



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:51 PM UTC

PDB ID : 4QNQ / pdb_00004qnq
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

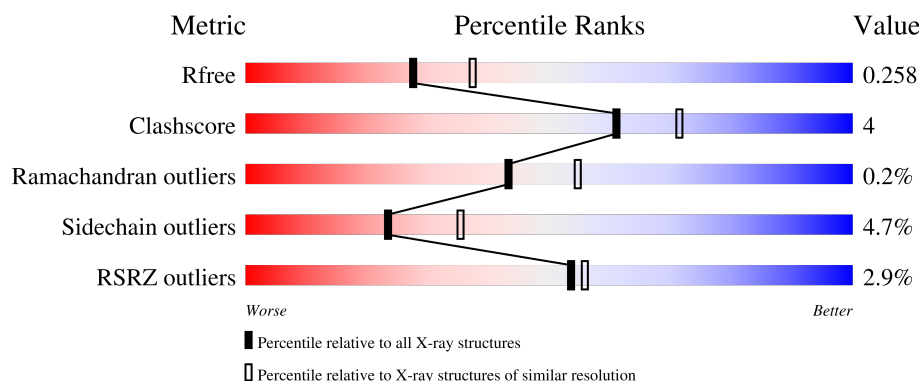
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	240	
1	B	240	
1	C	240	
1	D	240	
1	E	240	

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Mol	Chain	Length	Quality of chain
1	F	240	2% 56% 5% 38%
1	G	240	2% 51% 7% 42%
1	H	240	2% 52% 7% 41%
1	I	240	3% 55% 5% 39%
1	J	240	3% 54% 7% 38%
1	K	240	% 55% . 40%
1	L	240	3% 51% 7% 41%

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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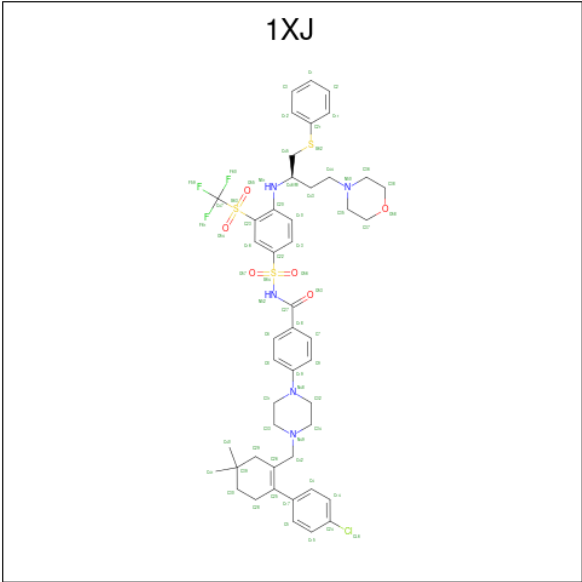
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	PRO	-	expression tag	UNP P53563
A	0	GLY	-	expression tag	UNP P53563
B	-6	GLY	-	expression tag	UNP P53563
B	-5	SER	-	expression tag	UNP P53563
B	-4	PRO	-	expression tag	UNP P53563
B	-3	GLU	-	expression tag	UNP P53563
B	-2	PHE	-	expression tag	UNP P53563
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 (CCD ID: 1XJ) (formula: C₄₇H₅₅ClF₃N₅O₆S₃).

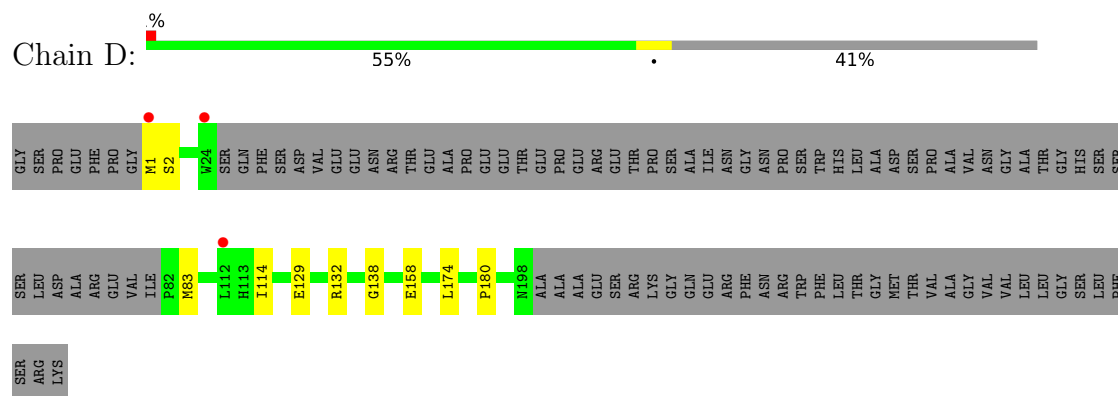


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	B	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	C	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	D	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	E	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	F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

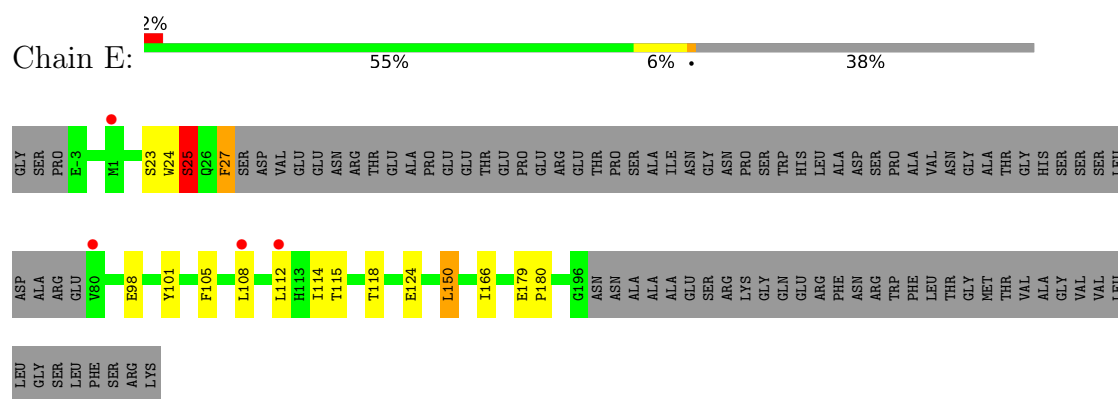
- Molecule 3 is water.

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

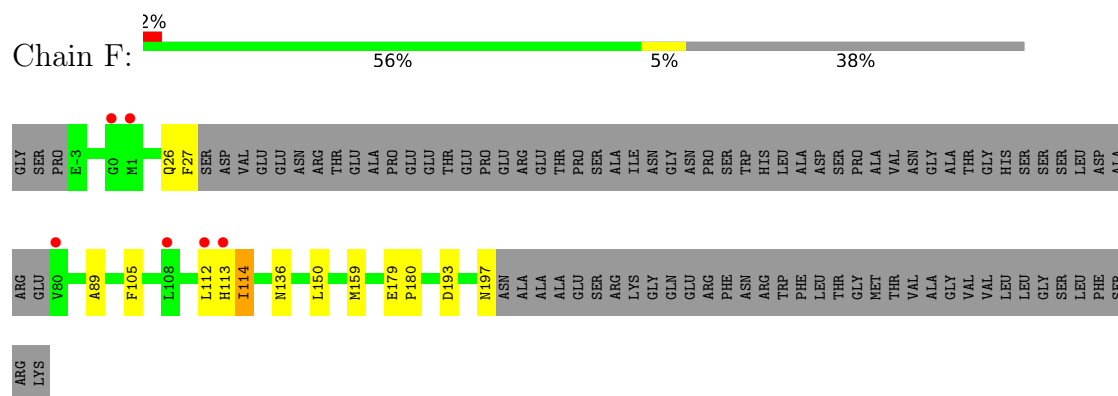
- Molecule 1: Bcl-2-like protein 1



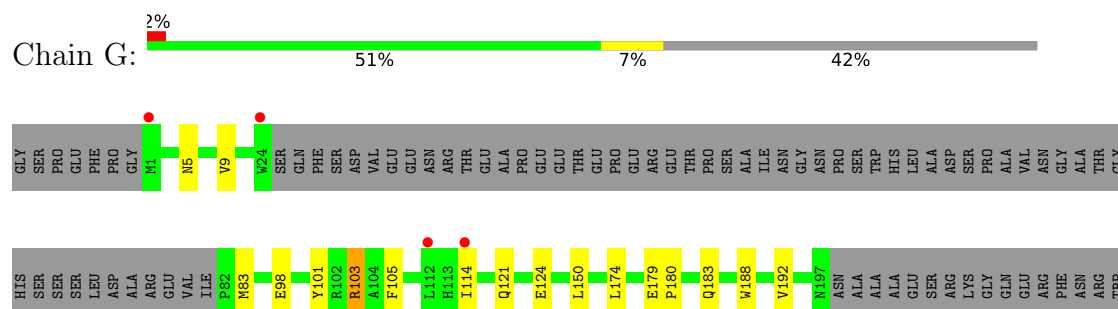
- Molecule 1: Bcl-2-like protein 1



- Molecule 1: Bcl-2-like protein 1



- Molecule 1: Bcl-2-like protein 1



PHE
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● Molecule 1: Bcl-2-like protein 1



GLY
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● Molecule 1: Bcl-2-like protein 1



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● Molecule 1: Bcl-2-like protein 1



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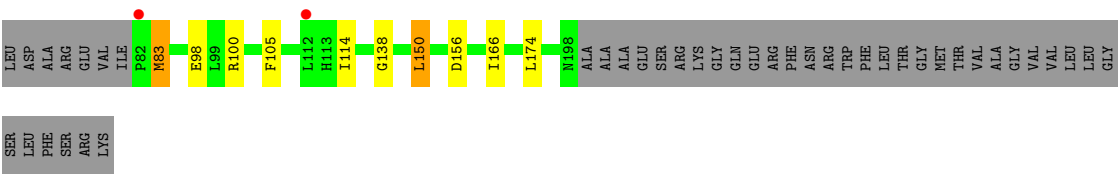
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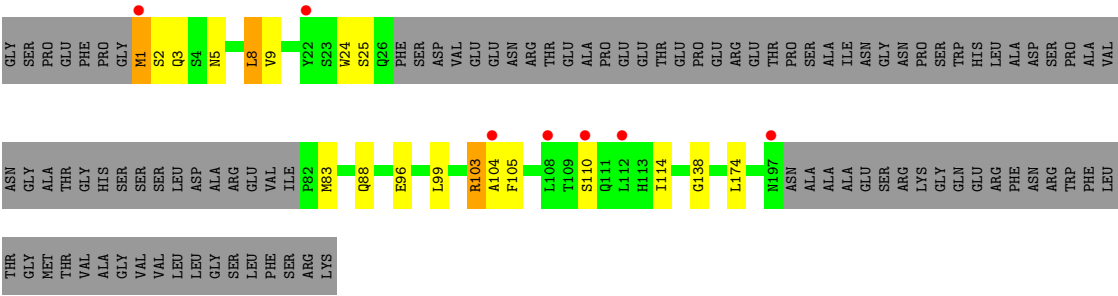
● Molecule 1: Bcl-2-like protein 1



GLY
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LEU
GLY
SER
SER
PHE
SER
ARG
LYS



● 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 85.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (85.00-2.30) 97.5 (85.00-2.30)	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 (4.84%)	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 , 46.7	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

5.1 Standard geometry

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	1.15	1/1198 (0.1%)	1.00	0/1621
1	B	1.06	0/1196	0.98	0/1618
1	C	0.99	0/1196	0.96	0/1618
1	D	1.20	0/1171	0.99	0/1584
1	E	1.04	0/1230	0.93	0/1665
1	F	1.12	1/1238 (0.1%)	0.97	0/1676
1	G	1.05	0/1163	0.95	0/1573
1	H	1.14	1/1178 (0.1%)	1.00	0/1593
1	I	1.01	0/1218	0.93	0/1649
1	J	1.09	1/1238 (0.1%)	0.96	1/1676 (0.1%)
1	K	0.97	0/1190	0.91	0/1610
1	L	0.92	0/1178	0.87	0/1593
All	All	1.06	4/14394 (0.0%)	0.96	1/19476 (0.0%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	14	SER	CA-C	-5.87	1.45	1.52
1	A	14	SER	CA-C	-5.22	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	142	ALA	N-CA	-5.10	1.40	1.46
1	F	89	ALA	C-O	5.02	1.30	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	26	GLN	N-CA-C	-5.13	104.53	111.55

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 [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	1169	0	1113	9	0
1	B	1167	0	1100	7	0
1	C	1167	0	1112	10	0
1	D	1143	0	1087	7	0
1	E	1199	0	1141	14	0
1	F	1207	0	1147	7	0
1	G	1135	0	1081	9	0
1	H	1150	0	1094	9	0
1	I	1188	0	1132	11	0
1	J	1207	0	1147	14	0
1	K	1161	0	1097	7	0
1	L	1150	0	1094	13	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	120	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.

All (120) 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:J:0:GLY:O	1:J:179:GLU:CD	2.37	0.68
1:C:81:ILE:HG23	1:L:99:LEU:HD22	1.79	0.65
1:J:105:PHE:CD1	2:J:301:1XJ:CL6	2.88	0.64
1:I:108:LEU:CD1	1:I:109:THR:HG23	2.28	0.63
2:C:301:1XJ:C25	2:C:301:1XJ:H44	2.30	0.62
1:I:108:LEU:HD13	1:I:109:THR:HG23	1.84	0.59
2:F:301:1XJ:C25	2:F:301:1XJ:H40	2.33	0.59
1:J:105:PHE:HD1	2:J:301:1XJ:CL6	2.24	0.57
1:E:115:THR:HG1	1:E:118:THR:HG1	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:PHE:CD1	2:F:301:1XJ:CL6	2.95	0.57
1:J:0:GLY:O	1:J:179:GLU:OE2	2.22	0.57
1:I:150:LEU:HB3	1:I:166:ILE:HD13	1.87	0.56
1:H:1:MET:HG3	1:H:2:SER:N	2.21	0.55
2:C:301:1XJ:O53	2:C:301:1XJ:C13	2.56	0.53
1:E:27:PHE:C	1:E:27:PHE:CD1	2.86	0.53
1:K:150:LEU:HB3	1:K:166:ILE:HD13	1.90	0.53
1:J:111:GLN:HB3	1:J:112:LEU:HD12	1.90	0.53
1:B:138:GLY:HA3	2:B:301:1XJ:H55	1.75	0.52
1:I:16:LYS:NZ	1:I:98:GLU:OE1	2.39	0.52
1:H:136:ASN:C	1:H:136:ASN:OD1	2.54	0.51
1:F:179:GLU:N	1:F:180:PRO:CD	2.74	0.51
1:C:1:MET:HE2	1:C:3:GLN:CB	2.41	0.51
1:L:1:MET:HG3	1:L:2:SER:N	2.25	0.51
2:C:301:1XJ:O53	2:C:301:1XJ:H7	2.11	0.50
2:A:301:1XJ:C4	2:A:301:1XJ:H45	2.42	0.50
1:I:105:PHE:O	1:I:108:LEU:CD1	2.40	0.50
1:K:138:GLY:HA3	2:K:301:1XJ:H55	1.76	0.50
1:L:96:GLU:OE2	2:L:301:1XJ:H32	2.11	0.50
1:C:3:GLN:HG3	1:L:88:GLN:HG2	1.92	0.49
1:L:1:MET:HE2	1:L:3:GLN:HB2	1.94	0.49
1:H:23:SER:C	1:H:25:SER:N	2.70	0.49
1:L:5:ASN:HA	1:L:8:LEU:HD22	1.93	0.49
1:F:114:ILE:O	1:F:159:MET:HE1	2.13	0.49
1:E:105:PHE:CD1	2:E:301:1XJ:CL6	3.03	0.49
1:K:105:PHE:CD2	2:K:301:1XJ:CL6	3.03	0.49
1:J:96:GLU:OE2	2:J:301:1XJ:H50	2.12	0.48
1:E:124:GLU:HG2	3:E:407:HOH:O	2.14	0.48
1:H:24:TRP:O	1:H:24:TRP:CD1	2.66	0.48
1:L:1:MET:HE2	1:L:3:GLN:CB	2.44	0.48
1:H:23:SER:C	1:H:25:SER:H	2.22	0.48
1:K:98:GLU:HG2	1:K:105:PHE:CE2	2.49	0.48
1:I:123:PHE:O	1:I:127:VAL:HG23	2.14	0.47
1:K:138:GLY:HA3	2:K:301:1XJ:N52	2.30	0.47
1:A:105:PHE:CD1	2:A:301:1XJ:CL6	3.04	0.47
1:B:101:TYR:CZ	2:B:301:1XJ:H5	2.50	0.47
1:B:8:LEU:CD2	1:B:83:MET:CE	2.93	0.46
1:J:150:LEU:HD23	1:J:150:LEU:HA	1.77	0.46
1:I:136:ASN:OD1	1:I:136:ASN:C	2.58	0.46
1:K:100:ARG:NH2	3:K:405:HOH:O	2.38	0.46
1:A:105:PHE:HD1	2:A:301:1XJ:CL6	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HG3	1:D:2:SER:N	2.29	0.46
1:L:138:GLY:HA3	2:L:301:1XJ:H55	1.81	0.46
1:G:5:ASN:O	1:G:9:VAL:HG23	2.15	0.46
1:E:23:SER:O	1:E:25:SER:N	2.45	0.45
1:G:103:ARG:H	1:G:103:ARG:CD	2.29	0.45
1:B:180:PRO:HG3	1:C:15:TYR:CE1	2.51	0.45
2:I:301:1XJ:H12	2:I:301:1XJ:C6	2.47	0.45
1:C:1:MET:HE2	1:C:3:GLN:HB2	1.98	0.45
2:I:301:1XJ:H51	2:I:301:1XJ:H49	1.60	0.45
1:J:179:GLU:N	1:J:180:PRO:CD	2.80	0.45
1:A:136:ASN:OD1	1:A:136:ASN:C	2.60	0.45
1:E:24:TRP:NE1	1:E:27:PHE:CD2	2.84	0.45
1:E:179:GLU:N	1:E:180:PRO:CD	2.80	0.45
1:A:15:TYR:CE1	1:D:180:PRO:HG3	2.52	0.44
1:G:105:PHE:CD1	2:G:301:1XJ:CL6	3.07	0.44
1:A:179:GLU:N	1:A:180:PRO:CD	2.81	0.44
1:E:101:TYR:CZ	2:E:301:1XJ:H5	2.52	0.44
1:L:24:TRP:O	1:L:24:TRP:CG	2.70	0.44
1:G:179:GLU:N	1:G:180:PRO:CD	2.81	0.44
1:I:105:PHE:CD1	2:I:301:1XJ:CL6	3.08	0.44
1:F:105:PHE:CE1	2:F:301:1XJ:CL6	3.08	0.44
1:J:112:LEU:HD12	1:J:112:LEU:N	2.32	0.44
1:G:98:GLU:HG2	1:G:105:PHE:CE1	2.53	0.43
1:B:83:MET:HE2	1:B:87:LYS:HE3	2.00	0.43
1:E:98:GLU:HG2	1:E:105:PHE:CE1	2.54	0.43
1:D:129:GLU:CD	1:D:132:ARG:HH12	2.19	0.43
1:J:150:LEU:HB3	1:J:166:ILE:HD13	2.00	0.43
1:E:124:GLU:OE2	3:E:407:HOH:O	2.21	0.43
1:C:194:LEU:HD21	1:G:121:GLN:HG3	2.01	0.43
1:E:27:PHE:C	1:E:27:PHE:HD1	2.26	0.43
1:G:183:GLN:HA	1:G:183:GLN:OE1	2.18	0.43
1:L:103:ARG:HG2	1:L:104:ALA:N	2.34	0.43
1:C:3:GLN:HG2	1:L:88:GLN:CB	2.48	0.42
1:F:179:GLU:HB3	1:F:180:PRO:HD3	2.01	0.42
1:C:1:MET:HG3	1:C:2:SER:N	2.35	0.42
1:H:90:LEU:HD12	1:H:90:LEU:HA	1.90	0.42
1:C:1:MET:HE2	1:C:3:GLN:HB3	2.01	0.42
1:E:23:SER:C	1:E:25:SER:H	2.27	0.42
1:E:150:LEU:HB3	1:E:166:ILE:HD13	2.02	0.42
1:H:16:LYS:NZ	1:H:98:GLU:OE2	2.51	0.42
2:C:301:1XJ:H14	2:C:301:1XJ:H24	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:THR:OG1	1:E:118:THR:OG1	2.26	0.42
1:K:83:MET:HA	1:K:83:MET:HE2	2.00	0.42
1:D:138:GLY:HA3	2:D:301:1XJ:H55	1.85	0.42
1:B:8:LEU:HD21	1:B:83:MET:CE	2.49	0.42
1:H:105:PHE:CD1	2:H:301:1XJ:CL6	3.10	0.42
1:J:26:GLN:HG2	1:J:160:GLN:HB3	2.02	0.42
1:A:117:GLY:HA2	1:F:136:ASN:HD22	1.85	0.42
1:D:138:GLY:HA3	2:D:301:1XJ:N52	2.34	0.42
1:G:101:TYR:CZ	2:G:301:1XJ:H5	2.54	0.42
1:I:108:LEU:HD13	1:I:109:THR:H	1.82	0.42
1:A:99:LEU:HD12	1:A:99:LEU:HA	1.86	0.42
2:J:301:1XJ:H14	2:J:301:1XJ:H24	1.89	0.41
1:J:86:VAL:HG22	1:J:192:VAL:HG21	2.01	0.41
1:L:5:ASN:O	1:L:9:VAL:HG23	2.20	0.41
1:L:105:PHE:CD1	2:L:301:1XJ:CL6	3.11	0.41
1:B:14:SER:HB2	1:H:26:GLN:HG2	2.02	0.41
2:F:301:1XJ:H5	2:F:301:1XJ:H25	1.77	0.41
1:J:195:TYR:O	2:J:301:1XJ:H34	2.21	0.41
1:A:111:GLN:HB3	1:A:112:LEU:HD13	2.03	0.41
1:G:188:TRP:O	1:G:192:VAL:HG23	2.21	0.41
2:A:301:1XJ:H15	2:A:301:1XJ:H51	1.80	0.40
1:F:193:ASP:O	1:F:197:ASN:HB2	2.21	0.40
1:A:15:TYR:CD1	1:D:180:PRO:HG3	2.56	0.40
1:C:136:ASN:OD1	1:C:136:ASN:C	2.65	0.40
1:J:96:GLU:OE2	2:J:301:1XJ:H32	2.22	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	18	23
1	I	143/240 (60%)	140 (98%)	3 (2%)	0	100	100
1	J	145/240 (60%)	139 (96%)	5 (3%)	1 (1%)	18	23
1	K	139/240 (58%)	137 (99%)	2 (1%)	0	100	100
1	L	138/240 (58%)	136 (99%)	1 (1%)	1 (1%)	18	23
All	All	1685/2880 (58%)	1652 (98%)	30 (2%)	3 (0%)	43	55

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%)	119 (96%)	5 (4%)	28	42
1	B	124/201 (62%)	119 (96%)	5 (4%)	28	42
1	C	124/201 (62%)	116 (94%)	8 (6%)	15	22
1	D	121/201 (60%)	117 (97%)	4 (3%)	33	50
1	E	127/201 (63%)	121 (95%)	6 (5%)	23	35
1	F	128/201 (64%)	122 (95%)	6 (5%)	23	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	120/201 (60%)	114 (95%)	6 (5%)	22	33
1	H	122/201 (61%)	115 (94%)	7 (6%)	18	27
1	I	126/201 (63%)	119 (94%)	7 (6%)	19	28
1	J	128/201 (64%)	124 (97%)	4 (3%)	35	52
1	K	123/201 (61%)	118 (96%)	5 (4%)	27	41
1	L	122/201 (61%)	115 (94%)	7 (6%)	18	27
All	All	1489/2412 (62%)	1419 (95%)	70 (5%)	23	35

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	112	LEU
1	A	121	GLN
1	A	156	ASP
1	A	174	LEU
1	B	102	ARG
1	B	112	LEU
1	B	114	ILE
1	B	156	ASP
1	B	174	LEU
1	C	81	ILE
1	C	83	MET
1	C	108	LEU
1	C	110	SER
1	C	114	ILE
1	C	121	GLN
1	C	156	ASP
1	C	174	LEU
1	D	83	MET
1	D	114	ILE
1	D	158	GLU
1	D	174	LEU
1	E	25	SER
1	E	27	PHE
1	E	108	LEU
1	E	112	LEU
1	E	114	ILE
1	E	150	LEU
1	F	26	GLN

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Mol	Chain	Res	Type
1	F	27	PHE
1	F	112	LEU
1	F	113	HIS
1	F	114	ILE
1	F	150	LEU
1	G	83	MET
1	G	103	ARG
1	G	114	ILE
1	G	124	GLU
1	G	150	LEU
1	G	174	LEU
1	H	1	MET
1	H	83	MET
1	H	112	LEU
1	H	114	ILE
1	H	124	GLU
1	H	156	ASP
1	H	174	LEU
1	I	6	ARG
1	I	25	SER
1	I	103	ARG
1	I	108	LEU
1	I	112	LEU
1	I	114	ILE
1	I	150	LEU
1	J	80	VAL
1	J	112	LEU
1	J	114	ILE
1	J	157	LYS
1	K	83	MET
1	K	114	ILE
1	K	150	LEU
1	K	156	ASP
1	K	174	LEU
1	L	1	MET
1	L	8	LEU
1	L	83	MET
1	L	103	ARG
1	L	110	SER
1	L	114	ILE
1	L	174	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	177	HIS
1	C	121	GLN
1	D	125	GLN
1	E	128	ASN
1	E	177	HIS
1	F	111	GLN
1	G	111	GLN
1	G	177	HIS
1	G	197	ASN
1	H	111	GLN
1	I	111	GLN
1	I	177	HIS
1	J	177	HIS
1	K	160	GLN
1	K	177	HIS
1	L	177	HIS

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 oligosaccharides 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	G	301	-	70,71,71	1.44	7 (10%)	91,104,104	3.03	32 (35%)
2	1XJ	E	301	-	70,71,71	1.36	8 (11%)	91,104,104	2.86	26 (28%)
2	1XJ	H	301	-	70,71,71	1.47	11 (15%)	91,104,104	2.80	28 (30%)
2	1XJ	C	301	-	70,71,71	1.42	9 (12%)	91,104,104	2.92	33 (36%)
2	1XJ	B	301	-	70,71,71	1.36	10 (14%)	91,104,104	2.73	29 (31%)
2	1XJ	K	301	-	70,71,71	1.33	10 (14%)	91,104,104	2.87	37 (40%)
2	1XJ	L	301	-	70,71,71	1.42	10 (14%)	91,104,104	2.64	35 (38%)
2	1XJ	A	301	-	70,71,71	1.90	15 (21%)	91,104,104	2.67	32 (35%)
2	1XJ	I	301	-	70,71,71	1.56	14 (20%)	91,104,104	2.97	32 (35%)
2	1XJ	D	301	-	70,71,71	1.68	11 (15%)	91,104,104	2.25	25 (27%)
2	1XJ	F	301	-	70,71,71	1.61	12 (17%)	91,104,104	2.95	36 (39%)
2	1XJ	J	301	-	70,71,71	1.50	11 (15%)	91,104,104	3.04	26 (28%)

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	G	301	-	-	6/56/89/89	0/7/7/7
2	1XJ	E	301	-	-	7/56/89/89	0/7/7/7
2	1XJ	H	301	-	-	6/56/89/89	0/7/7/7
2	1XJ	C	301	-	-	6/56/89/89	0/7/7/7
2	1XJ	B	301	-	-	5/56/89/89	0/7/7/7
2	1XJ	K	301	-	-	6/56/89/89	0/7/7/7
2	1XJ	L	301	-	-	5/56/89/89	0/7/7/7
2	1XJ	A	301	-	-	5/56/89/89	0/7/7/7
2	1XJ	I	301	-	-	7/56/89/89	0/7/7/7
2	1XJ	D	301	-	-	3/56/89/89	0/7/7/7
2	1XJ	F	301	-	-	9/56/89/89	0/7/7/7
2	1XJ	J	301	-	-	9/56/89/89	0/7/7/7

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	1XJ	O55-S63	6.34	1.50	1.44
2	F	301	1XJ	C26-C25	6.27	1.44	1.34
2	E	301	1XJ	C26-C25	6.23	1.44	1.34
2	H	301	1XJ	C26-C25	6.22	1.44	1.34
2	G	301	1XJ	C26-C25	6.21	1.44	1.34
2	J	301	1XJ	C26-C25	5.90	1.43	1.34
2	D	301	1XJ	C26-C25	5.87	1.43	1.34
2	C	301	1XJ	C26-C25	5.75	1.43	1.34
2	L	301	1XJ	C26-C25	5.68	1.43	1.34
2	A	301	1XJ	C26-C25	5.58	1.43	1.34
2	I	301	1XJ	C26-C25	5.55	1.43	1.34
2	B	301	1XJ	C26-C25	5.24	1.42	1.34
2	A	301	1XJ	O57-S64	5.21	1.49	1.43
2	D	301	1XJ	O55-S63	4.96	1.49	1.44
2	D	301	1XJ	O57-S64	4.66	1.48	1.43
2	J	301	1XJ	C45-S62	-4.65	1.71	1.81
2	H	301	1XJ	O57-S64	4.54	1.48	1.43
2	F	301	1XJ	C45-S62	-4.41	1.71	1.81
2	C	301	1XJ	O55-S63	4.21	1.48	1.44
2	A	301	1XJ	O54-S63	4.08	1.48	1.44
2	D	301	1XJ	S64-N52	-3.99	1.54	1.64
2	J	301	1XJ	O55-S63	3.88	1.48	1.44
2	A	301	1XJ	C32-N48	-3.86	1.40	1.46
2	K	301	1XJ	C26-C25	3.79	1.40	1.34
2	L	301	1XJ	C28-C25	-3.63	1.45	1.50
2	G	301	1XJ	O57-S64	3.44	1.47	1.43
2	A	301	1XJ	C28-C25	-3.43	1.45	1.50
2	I	301	1XJ	O57-S64	3.38	1.47	1.43
2	I	301	1XJ	C23-S63	-3.36	1.73	1.78
2	A	301	1XJ	C22-S64	-3.32	1.71	1.76
2	A	301	1XJ	C13-C10	3.18	1.43	1.38
2	F	301	1XJ	O55-S63	3.16	1.47	1.44
2	J	301	1XJ	C28-C25	-3.14	1.46	1.50
2	I	301	1XJ	C45-S62	-3.06	1.74	1.81
2	I	301	1XJ	C20-N51	3.06	1.44	1.37
2	I	301	1XJ	O55-S63	3.04	1.47	1.44
2	A	301	1XJ	C20-N51	3.03	1.44	1.37
2	J	301	1XJ	C31-N48	-3.02	1.41	1.46
2	G	301	1XJ	C32-N48	-3.00	1.41	1.46
2	B	301	1XJ	C28-C25	-3.00	1.46	1.50
2	H	301	1XJ	C27-N52	2.99	1.42	1.39
2	L	301	1XJ	O57-S64	2.98	1.47	1.43
2	K	301	1XJ	C28-C25	-2.93	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	1XJ	C32-N48	-2.91	1.41	1.46
2	J	301	1XJ	S64-N52	-2.88	1.57	1.64
2	E	301	1XJ	C28-C25	-2.87	1.46	1.50
2	D	301	1XJ	C28-C25	-2.86	1.46	1.50
2	K	301	1XJ	C20-N51	2.85	1.43	1.37
2	B	301	1XJ	C19-N48	2.84	1.46	1.38
2	A	301	1XJ	C23-S63	-2.84	1.74	1.78
2	G	301	1XJ	C28-C25	-2.80	1.46	1.50
2	A	301	1XJ	C10-C20	2.79	1.44	1.39
2	F	301	1XJ	O57-S64	2.74	1.46	1.43
2	F	301	1XJ	C10-C20	2.74	1.44	1.39
2	K	301	1XJ	C32-N48	-2.72	1.42	1.46
2	G	301	1XJ	C27-N52	2.66	1.42	1.39
2	I	301	1XJ	C31-N48	-2.65	1.42	1.46
2	D	301	1XJ	C32-N48	-2.64	1.42	1.46
2	D	301	1XJ	C31-N48	-2.62	1.42	1.46
2	D	301	1XJ	C27-N52	2.62	1.42	1.39
2	I	301	1XJ	C43-C46	-2.61	1.47	1.53
2	D	301	1XJ	C20-N51	2.60	1.43	1.37
2	C	301	1XJ	C23-S63	-2.58	1.74	1.78
2	B	301	1XJ	S64-N52	-2.54	1.58	1.64
2	L	301	1XJ	C19-N48	2.53	1.45	1.38
2	L	301	1XJ	C22-S64	-2.53	1.72	1.76
2	I	301	1XJ	C32-N48	-2.52	1.42	1.46
2	K	301	1XJ	C29-C26	-2.51	1.46	1.50
2	F	301	1XJ	C20-N51	2.50	1.43	1.37
2	H	301	1XJ	C16-C23	-2.48	1.35	1.39
2	C	301	1XJ	C20-N51	2.47	1.43	1.37
2	F	301	1XJ	C32-N48	-2.47	1.42	1.46
2	E	301	1XJ	C20-N51	2.46	1.43	1.37
2	C	301	1XJ	C19-N48	2.45	1.45	1.38
2	E	301	1XJ	C32-N48	-2.44	1.42	1.46
2	G	301	1XJ	O54-S63	-2.41	1.41	1.44
2	H	301	1XJ	C28-C25	-2.40	1.47	1.50
2	J	301	1XJ	C46-N51	-2.40	1.41	1.46
2	B	301	1XJ	C44-N50	-2.39	1.42	1.47
2	K	301	1XJ	O57-S64	2.39	1.46	1.43
2	A	301	1XJ	C43-C46	-2.38	1.47	1.53
2	B	301	1XJ	C32-N48	-2.38	1.42	1.46
2	L	301	1XJ	O55-S63	2.38	1.46	1.44
2	H	301	1XJ	C32-N48	-2.36	1.42	1.46
2	E	301	1XJ	C19-N48	2.35	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	1XJ	C19-N48	2.34	1.45	1.38
2	L	301	1XJ	C17-C25	-2.33	1.45	1.49
2	G	301	1XJ	C31-N48	-2.31	1.42	1.46
2	E	301	1XJ	C27-N52	2.30	1.41	1.39
2	C	301	1XJ	S64-N52	-2.30	1.58	1.64
2	L	301	1XJ	S64-N52	-2.29	1.58	1.64
2	F	301	1XJ	C28-C25	-2.28	1.47	1.50
2	B	301	1XJ	C7-C18	2.28	1.42	1.39
2	C	301	1XJ	C28-C25	-2.24	1.47	1.50
2	C	301	1XJ	C32-N48	-2.24	1.42	1.46
2	K	301	1XJ	S64-N52	-2.23	1.58	1.64
2	E	301	1XJ	C31-N48	-2.22	1.42	1.46
2	A	301	1XJ	C19-N48	2.22	1.44	1.38
2	K	301	1XJ	O55-S63	2.22	1.46	1.44
2	I	301	1XJ	C28-C25	-2.21	1.47	1.50
2	B	301	1XJ	C43-C46	-2.21	1.48	1.53
2	H	301	1XJ	C21-S62	-2.20	1.72	1.76
2	A	301	1XJ	C29-C26	-2.19	1.47	1.50
2	L	301	1XJ	C20-N51	2.18	1.42	1.37
2	F	301	1XJ	C9-C7	2.17	1.42	1.38
2	J	301	1XJ	C40-C39	-2.17	1.49	1.53
2	K	301	1XJ	C41-C39	-2.16	1.49	1.53
2	F	301	1XJ	C29-C26	-2.16	1.47	1.50
2	B	301	1XJ	C27-N52	2.16	1.41	1.39
2	H	301	1XJ	O56-S64	2.13	1.46	1.43
2	C	301	1XJ	O54-S63	2.13	1.46	1.44
2	H	301	1XJ	C40-C39	-2.09	1.49	1.53
2	I	301	1XJ	C19-N48	2.09	1.44	1.38
2	J	301	1XJ	C32-N48	-2.08	1.43	1.46
2	E	301	1XJ	C9-C7	2.08	1.42	1.38
2	H	301	1XJ	C19-N48	2.08	1.44	1.38
2	A	301	1XJ	C40-C39	-2.08	1.49	1.53
2	F	301	1XJ	S64-N52	-2.07	1.59	1.64
2	J	301	1XJ	C41-C39	-2.07	1.49	1.53
2	B	301	1XJ	C31-N48	-2.07	1.43	1.46
2	I	301	1XJ	C41-C39	-2.06	1.49	1.53
2	K	301	1XJ	C44-N50	-2.06	1.42	1.47
2	I	301	1XJ	O56-S64	2.05	1.45	1.43
2	I	301	1XJ	C13-C10	2.05	1.42	1.38
2	D	301	1XJ	C17-C25	-2.01	1.45	1.49
2	D	301	1XJ	C30-C39	2.01	1.57	1.53
2	H	301	1XJ	C8-C19	2.01	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	301	1XJ	C19-N48	2.00	1.44	1.38

All (371) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	1XJ	C42-N49-C34	16.92	137.46	111.14
2	J	301	1XJ	C42-N49-C34	16.20	136.33	111.14
2	K	301	1XJ	C42-N49-C34	15.65	135.49	111.14
2	H	301	1XJ	C42-N49-C34	15.12	134.66	111.14
2	J	301	1XJ	O57-S64-O56	-14.40	102.04	119.52
2	B	301	1XJ	C42-N49-C34	13.55	132.21	111.14
2	I	301	1XJ	C42-N49-C34	13.07	131.47	111.14
2	C	301	1XJ	C42-N49-C34	13.00	131.36	111.14
2	G	301	1XJ	C42-N49-C34	12.25	130.19	111.14
2	F	301	1XJ	C42-N49-C34	11.78	129.47	111.14
2	L	301	1XJ	C28-C25-C17	-11.45	94.95	116.20
2	D	301	1XJ	C42-N49-C34	10.96	128.19	111.14
2	C	301	1XJ	O55-S63-O54	-10.93	105.34	119.06
2	G	301	1XJ	C28-C25-C17	-10.77	96.20	116.20
2	G	301	1XJ	O55-S63-O54	-10.67	105.66	119.06
2	H	301	1XJ	C28-C25-C17	-10.40	96.89	116.20
2	I	301	1XJ	O57-S64-O56	-10.33	106.97	119.52
2	F	301	1XJ	C28-C25-C17	-10.31	97.06	116.20
2	C	301	1XJ	O57-S64-O56	-9.21	108.33	119.52
2	C	301	1XJ	C28-C25-C17	-9.15	99.22	116.20
2	A	301	1XJ	C42-N49-C34	8.98	125.11	111.14
2	F	301	1XJ	O55-S63-O54	-8.91	107.88	119.06
2	K	301	1XJ	C28-C25-C17	-8.87	99.73	116.20
2	E	301	1XJ	C28-C25-C17	-8.76	99.93	116.20
2	F	301	1XJ	O57-S64-O56	-8.33	109.40	119.52
2	I	301	1XJ	C28-C25-C17	-8.26	100.87	116.20
2	L	301	1XJ	C42-N49-C34	8.25	123.97	111.14
2	K	301	1XJ	O57-S64-O56	-8.20	109.57	119.52
2	B	301	1XJ	O55-S63-O54	-7.75	109.34	119.06
2	A	301	1XJ	C27-N52-S64	-7.60	113.42	123.38
2	A	301	1XJ	C4-C17-C25	-7.59	111.22	121.00
2	I	301	1XJ	O57-S64-C22	7.57	117.53	107.98
2	L	301	1XJ	O57-S64-O56	-7.43	110.50	119.52
2	B	301	1XJ	C28-C25-C17	-7.38	102.50	116.20
2	E	301	1XJ	O57-S64-O56	-7.27	110.69	119.52
2	H	301	1XJ	O55-S63-O54	-7.12	110.13	119.06
2	J	301	1XJ	C28-C25-C17	-7.01	103.19	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	1XJ	C28-C25-C17	-6.95	103.30	116.20
2	A	301	1XJ	C28-C25-C17	-6.78	103.61	116.20
2	E	301	1XJ	O55-S63-O54	-6.48	110.92	119.06
2	I	301	1XJ	C16-C23-C20	6.37	127.22	120.85
2	B	301	1XJ	O56-S64-C22	-6.23	100.12	107.98
2	F	301	1XJ	C43-C46-N51	6.22	120.70	110.49
2	I	301	1XJ	C16-C22-S64	-5.89	113.03	119.06
2	A	301	1XJ	O57-S64-O56	-5.81	112.46	119.52
2	B	301	1XJ	C8-C6-C18	-5.76	114.64	120.80
2	G	301	1XJ	O56-S64-C22	-5.69	100.80	107.98
2	C	301	1XJ	C22-C16-C23	-5.62	113.57	120.22
2	J	301	1XJ	C43-C44-N50	5.60	128.42	113.69
2	G	301	1XJ	C43-C44-N50	5.58	128.37	113.69
2	L	301	1XJ	O55-S63-O54	-5.54	112.11	119.06
2	J	301	1XJ	C42-N49-C33	-5.53	102.55	111.14
2	B	301	1XJ	O57-S64-O56	-5.52	112.82	119.52
2	A	301	1XJ	O53-C27-N52	-5.41	114.52	121.16
2	G	301	1XJ	C36-N50-C35	5.34	120.34	108.84
2	F	301	1XJ	C4-C17-C25	-5.26	114.22	121.00
2	L	301	1XJ	C22-C16-C23	-5.22	114.05	120.22
2	G	301	1XJ	C16-C22-S64	-5.21	113.73	119.06
2	K	301	1XJ	O56-S64-C22	5.19	114.53	107.98
2	A	301	1XJ	C5-C17-C25	5.11	127.60	121.00
2	E	301	1XJ	C42-N49-C33	-5.09	103.22	111.14
2	C	301	1XJ	C16-C23-C20	5.08	125.92	120.85
2	G	301	1XJ	O58-C37-C35	-5.02	100.95	111.77
2	C	301	1XJ	C27-N52-S64	-4.95	116.88	123.38
2	D	301	1XJ	C4-C17-C25	-4.94	114.64	121.00
2	D	301	1XJ	O55-S63-O54	-4.89	112.92	119.06
2	G	301	1XJ	C4-C17-C25	-4.84	114.76	121.00
2	I	301	1XJ	C45-S62-C21	4.83	114.98	103.79
2	H	301	1XJ	C22-C16-C23	-4.76	114.59	120.22
2	K	301	1XJ	O55-S63-O54	-4.65	113.22	119.06
2	I	301	1XJ	C43-C44-N50	4.56	125.69	113.69
2	H	301	1XJ	C36-N50-C35	4.55	118.64	108.84
2	H	301	1XJ	C8-C6-C18	-4.50	115.99	120.80
2	B	301	1XJ	C6-C8-C19	4.50	126.00	120.30
2	G	301	1XJ	C8-C6-C18	-4.50	115.99	120.80
2	D	301	1XJ	C8-C6-C18	-4.48	116.01	120.80
2	D	301	1XJ	C36-N50-C35	4.47	118.47	108.84
2	A	301	1XJ	C33-C31-N48	4.40	120.05	110.78
2	D	301	1XJ	C27-N52-S64	-4.40	117.61	123.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	1XJ	C7-C18-C6	4.35	124.10	118.57
2	I	301	1XJ	C22-C16-C23	-4.34	115.08	120.22
2	H	301	1XJ	C13-C22-C16	4.33	126.04	120.68
2	L	301	1XJ	O57-S64-C22	4.33	113.44	107.98
2	G	301	1XJ	C22-C16-C23	-4.31	115.13	120.22
2	I	301	1XJ	C13-C22-S64	4.28	124.46	119.76
2	I	301	1XJ	C30-C39-C29	-4.27	104.01	108.11
2	C	301	1XJ	C43-C44-N50	4.21	124.78	113.69
2	G	301	1XJ	C42-N49-C33	-4.19	104.62	111.14
2	F	301	1XJ	C31-C33-N49	4.17	119.05	110.65
2	A	301	1XJ	C18-C27-N52	4.16	121.03	116.08
2	L	301	1XJ	C36-N50-C35	4.13	117.75	108.84
2	F	301	1XJ	C43-C44-N50	4.10	124.48	113.69
2	E	301	1XJ	C4-C17-C25	-4.08	115.75	121.00
2	K	301	1XJ	C4-C17-C25	-4.07	115.75	121.00
2	B	301	1XJ	C36-N50-C35	4.07	117.60	108.84
2	K	301	1XJ	C14-C24-C15	4.05	126.26	121.24
2	L	301	1XJ	C5-C17-C4	4.03	123.69	118.57
2	L	301	1XJ	C8-C6-C18	-4.02	116.50	120.80
2	J	301	1XJ	O53-C27-C18	3.96	128.74	120.90
2	E	301	1XJ	O56-S64-C22	3.95	112.97	107.98
2	B	301	1XJ	O57-S64-N52	3.95	118.07	106.77
2	J	301	1XJ	C20-N51-C46	3.92	131.03	124.60
2	A	301	1XJ	C16-C23-S63	-3.92	110.67	116.43
2	G	301	1XJ	C32-N48-C31	3.89	120.31	111.57
2	A	301	1XJ	C32-N48-C31	3.85	120.22	111.57
2	F	301	1XJ	O54-S63-C47	3.83	116.53	104.70
2	L	301	1XJ	C16-C22-S64	-3.83	115.15	119.06
2	F	301	1XJ	C41-C39-C30	3.82	115.55	110.04
2	G	301	1XJ	C44-N50-C36	3.82	121.41	111.24
2	K	301	1XJ	C43-C44-N50	3.81	123.72	113.69
2	C	301	1XJ	C16-C22-S64	-3.78	115.20	119.06
2	F	301	1XJ	C13-C22-C16	3.77	125.34	120.68
2	A	301	1XJ	O55-S63-O54	-3.72	114.39	119.06
2	C	301	1XJ	O53-C27-N52	-3.70	116.61	121.16
2	B	301	1XJ	C22-C16-C23	-3.70	115.84	120.22
2	A	301	1XJ	O54-S63-C23	3.70	116.36	107.90
2	B	301	1XJ	O54-S63-C23	3.70	116.36	107.90
2	D	301	1XJ	C7-C18-C6	3.67	123.23	118.57
2	J	301	1XJ	C8-C6-C18	-3.65	116.90	120.80
2	E	301	1XJ	C22-C16-C23	-3.64	115.92	120.22
2	L	301	1XJ	O54-S63-C23	3.62	116.18	107.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	1XJ	C16-C23-C20	3.62	124.46	120.85
2	J	301	1XJ	O57-S64-N52	3.59	117.06	106.77
2	E	301	1XJ	C18-C27-N52	3.57	120.34	116.08
2	E	301	1XJ	C20-N51-C46	3.57	130.45	124.60
2	I	301	1XJ	C42-N49-C33	-3.56	105.60	111.14
2	B	301	1XJ	C4-C17-C25	-3.56	116.41	121.00
2	E	301	1XJ	C16-C23-C20	3.56	124.40	120.85
2	L	301	1XJ	C32-C34-N49	3.55	117.82	110.65
2	J	301	1XJ	C32-N48-C31	3.55	119.56	111.57
2	H	301	1XJ	C7-C18-C6	3.52	123.04	118.57
2	D	301	1XJ	C22-C16-C23	-3.51	116.07	120.22
2	A	301	1XJ	C14-C24-CL6	-3.51	114.19	119.36
2	A	301	1XJ	C16-C23-C20	3.50	124.35	120.85
2	G	301	1XJ	C23-C20-N51	-3.50	118.81	122.18
2	H	301	1XJ	C16-C22-S64	-3.49	115.50	119.06
2	K	301	1XJ	C40-C39-C30	-3.48	105.02	110.04
2	J	301	1XJ	C18-C27-N52	-3.48	111.94	116.08
2	F	301	1XJ	C45-S62-C21	-3.48	95.75	103.79
2	K	301	1XJ	C8-C6-C18	-3.47	117.09	120.80
2	F	301	1XJ	C15-C5-C17	-3.46	117.10	120.80
2	I	301	1XJ	O58-C38-C36	3.46	119.22	111.77
2	D	301	1XJ	C38-O58-C37	3.46	121.06	109.88
2	F	301	1XJ	C8-C19-N48	-3.45	116.60	121.39
2	K	301	1XJ	C41-C39-C30	3.45	115.01	110.04
2	A	301	1XJ	C22-C16-C23	-3.44	116.15	120.22
2	H	301	1XJ	C4-C17-C25	-3.44	116.56	121.00
2	D	301	1XJ	C16-C23-C20	3.44	124.28	120.85
2	H	301	1XJ	C43-C44-N50	3.42	122.68	113.69
2	A	301	1XJ	O57-S64-C22	-3.41	103.67	107.98
2	L	301	1XJ	C32-N48-C31	3.41	119.23	111.57
2	H	301	1XJ	C32-N48-C31	3.40	119.21	111.57
2	A	301	1XJ	C43-C46-N51	-3.39	104.93	110.49
2	E	301	1XJ	C16-C23-S63	-3.38	111.46	116.43
2	K	301	1XJ	C22-C16-C23	-3.37	116.23	120.22
2	H	301	1XJ	C30-C28-C25	-3.35	105.45	111.92
2	F	301	1XJ	C40-C39-C30	-3.35	105.22	110.04
2	I	301	1XJ	C23-C20-N51	-3.34	118.96	122.18
2	J	301	1XJ	C27-N52-S64	-3.34	119.00	123.38
2	L	301	1XJ	C30-C39-C29	-3.33	104.91	108.11
2	H	301	1XJ	C27-N52-S64	-3.33	119.02	123.38
2	B	301	1XJ	C43-C44-N50	3.29	122.36	113.69
2	B	301	1XJ	C42-N49-C33	-3.28	106.04	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	1XJ	C22-S64-N52	3.28	111.29	106.06
2	G	301	1XJ	C5-C17-C4	3.27	122.73	118.57
2	B	301	1XJ	C7-C18-C6	3.27	122.72	118.57
2	F	301	1XJ	C44-N50-C35	3.27	119.95	111.24
2	A	301	1XJ	C8-C6-C18	-3.27	117.31	120.80
2	F	301	1XJ	C32-N48-C31	3.26	118.91	111.57
2	K	301	1XJ	C5-C17-C4	3.25	122.70	118.57
2	B	301	1XJ	C16-C22-S64	-3.25	115.74	119.06
2	A	301	1XJ	C40-C39-C29	-3.24	104.74	109.85
2	E	301	1XJ	C44-N50-C35	3.23	119.85	111.24
2	J	301	1XJ	C10-C13-C22	3.23	122.58	119.44
2	H	301	1XJ	C20-N51-C46	3.23	129.89	124.60
2	C	301	1XJ	C13-C22-C16	3.23	124.67	120.68
2	I	301	1XJ	C32-N48-C31	3.22	118.81	111.57
2	C	301	1XJ	C4-C17-C25	-3.20	116.87	121.00
2	A	301	1XJ	C7-C18-C6	3.19	122.62	118.57
2	K	301	1XJ	O53-C27-N52	-3.14	117.31	121.16
2	E	301	1XJ	C32-N48-C19	3.14	126.66	118.11
2	K	301	1XJ	C27-N52-S64	-3.13	119.27	123.38
2	E	301	1XJ	C43-C44-N50	3.13	121.93	113.69
2	I	301	1XJ	C4-C17-C25	-3.12	116.98	121.00
2	I	301	1XJ	C32-C34-N49	3.11	116.92	110.65
2	J	301	1XJ	C22-C16-C23	-3.11	116.55	120.22
2	F	301	1XJ	O53-C27-N52	-3.09	117.37	121.16
2	J	301	1XJ	O57-S64-C22	3.06	111.83	107.98
2	K	301	1XJ	C20-N51-C46	3.05	129.60	124.60
2	J	301	1XJ	C30-C28-C25	-3.02	106.10	111.92
2	D	301	1XJ	C32-N48-C31	3.01	118.34	111.57
2	B	301	1XJ	C41-C39-C30	3.00	114.37	110.04
2	E	301	1XJ	O53-C27-N52	-2.99	117.49	121.16
2	L	301	1XJ	C13-C22-C16	2.98	124.36	120.68
2	F	301	1XJ	C9-C19-N48	2.98	125.52	121.39
2	K	301	1XJ	C41-C39-C29	-2.98	105.16	109.85
2	F	301	1XJ	C10-C13-C22	-2.95	116.57	119.44
2	I	301	1XJ	C41-C39-C30	2.92	114.25	110.04
2	H	301	1XJ	C44-N50-C36	2.92	119.02	111.24
2	I	301	1XJ	C8-C19-N48	-2.92	117.34	121.39
2	J	301	1XJ	O56-S64-N52	2.90	115.08	106.77
2	D	301	1XJ	C16-C22-S64	-2.89	116.11	119.06
2	F	301	1XJ	C10-C20-N51	-2.88	117.77	122.31
2	G	301	1XJ	C18-C27-N52	2.88	119.51	116.08
2	L	301	1XJ	C14-C24-C15	2.88	124.81	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	1XJ	O57-S64-O56	-2.87	116.03	119.52
2	A	301	1XJ	C13-C22-C16	2.84	124.19	120.68
2	K	301	1XJ	C5-C15-C24	-2.84	116.39	119.24
2	L	301	1XJ	C6-C8-C19	2.83	123.88	120.30
2	L	301	1XJ	O53-C27-N52	-2.83	117.69	121.16
2	C	301	1XJ	C42-N49-C33	-2.81	106.78	111.14
2	L	301	1XJ	C15-C5-C17	-2.79	117.82	120.80
2	G	301	1XJ	C14-C24-C15	2.79	124.69	121.24
2	E	301	1XJ	C6-C8-C19	2.76	123.79	120.30
2	A	301	1XJ	O57-S64-N52	2.75	114.64	106.77
2	B	301	1XJ	C4-C14-C24	-2.74	116.48	119.24
2	B	301	1XJ	O57-S64-C22	-2.73	104.54	107.98
2	G	301	1XJ	O57-S64-N52	2.72	114.56	106.77
2	I	301	1XJ	C8-C6-C18	-2.70	117.92	120.80
2	F	301	1XJ	C38-C36-N50	2.69	114.21	110.12
2	C	301	1XJ	C6-C8-C19	2.69	123.70	120.30
2	H	301	1XJ	C10-C20-N51	-2.68	118.09	122.31
2	L	301	1XJ	O56-S64-C22	-2.67	104.61	107.98
2	K	301	1XJ	C40-C39-C29	2.66	114.05	109.85
2	F	301	1XJ	C8-C6-C18	-2.66	117.96	120.80
2	I	301	1XJ	C44-N50-C36	2.66	118.32	111.24
2	F	301	1XJ	O58-C37-C35	2.65	117.49	111.77
2	G	301	1XJ	C16-C23-C20	2.65	123.50	120.85
2	L	301	1XJ	C43-C44-N50	2.65	120.66	113.69
2	K	301	1XJ	O57-S64-C22	2.65	111.32	107.98
2	G	301	1XJ	C13-C22-S64	2.65	122.67	119.76
2	E	301	1XJ	C30-C39-C29	2.64	110.65	108.11
2	C	301	1XJ	C8-C6-C18	-2.64	117.98	120.80
2	F	301	1XJ	C5-C17-C25	2.64	124.40	121.00
2	B	301	1XJ	C13-C22-C16	2.63	123.94	120.68
2	L	301	1XJ	C33-C31-N48	2.62	116.31	110.78
2	L	301	1XJ	O57-S64-N52	2.62	114.27	106.77
2	K	301	1XJ	O57-S64-N52	2.61	114.24	106.77
2	I	301	1XJ	C37-C35-N50	2.61	114.08	110.12
2	I	301	1XJ	C7-C18-C6	2.59	121.86	118.57
2	H	301	1XJ	C32-C34-N49	2.58	115.85	110.65
2	J	301	1XJ	C38-C36-N50	2.58	114.04	110.12
2	K	301	1XJ	C18-C27-N52	2.57	119.14	116.08
2	K	301	1XJ	O54-S63-C47	2.57	112.64	104.70
2	F	301	1XJ	C4-C14-C24	-2.57	116.66	119.24
2	J	301	1XJ	C16-C23-C20	2.56	123.40	120.85
2	K	301	1XJ	C10-C20-N51	-2.55	118.29	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	301	1XJ	C4-C14-C24	-2.55	116.68	119.24
2	H	301	1XJ	O55-S63-C47	2.55	112.57	104.70
2	H	301	1XJ	F59-C47-S63	2.55	117.18	110.25
2	F	301	1XJ	C22-C16-C23	-2.55	117.21	120.22
2	G	301	1XJ	C9-C7-C18	-2.55	118.08	120.80
2	G	301	1XJ	C30-C28-C25	-2.54	107.02	111.92
2	H	301	1XJ	C10-C20-C23	2.53	121.35	117.81
2	C	301	1XJ	C32-N48-C31	2.52	117.25	111.57
2	F	301	1XJ	C6-C8-C19	2.51	123.48	120.30
2	I	301	1XJ	C5-C17-C4	2.50	121.75	118.57
2	D	301	1XJ	C42-N49-C33	-2.49	107.27	111.14
2	L	301	1XJ	C5-C17-C25	-2.49	117.79	121.00
2	J	301	1XJ	O55-S63-O54	-2.49	115.94	119.06
2	K	301	1XJ	C6-C8-C19	2.48	123.44	120.30
2	D	301	1XJ	C43-C44-N50	2.48	120.20	113.69
2	H	301	1XJ	C6-C8-C19	2.47	123.42	120.30
2	I	301	1XJ	O55-S63-O54	-2.46	115.98	119.06
2	K	301	1XJ	C44-N50-C36	2.45	117.78	111.24
2	D	301	1XJ	O56-S64-C22	-2.45	104.89	107.98
2	G	301	1XJ	C44-N50-C35	2.44	117.74	111.24
2	L	301	1XJ	O53-C27-C18	2.44	125.73	120.90
2	C	301	1XJ	O56-S64-N52	2.43	113.71	106.77
2	D	301	1XJ	C8-C19-N48	-2.42	118.02	121.39
2	H	301	1XJ	C12-C21-C11	2.42	122.78	118.85
2	C	301	1XJ	F61-C47-S63	-2.41	103.67	110.25
2	L	301	1XJ	C4-C14-C24	-2.41	116.81	119.24
2	C	301	1XJ	C28-C25-C26	-2.41	118.60	121.92
2	C	301	1XJ	F59-C47-S63	2.40	116.77	110.25
2	B	301	1XJ	C16-C23-C20	2.38	123.23	120.85
2	J	301	1XJ	O54-S63-C47	2.38	112.05	104.70
2	I	301	1XJ	C38-C36-N50	2.38	113.73	110.12
2	L	301	1XJ	O55-S63-C23	2.37	113.33	107.90
2	G	301	1XJ	O54-S63-C47	2.37	112.03	104.70
2	G	301	1XJ	C20-N51-C46	2.37	128.49	124.60
2	E	301	1XJ	O54-S63-C47	2.37	112.01	104.70
2	G	301	1XJ	C13-C22-C16	2.36	123.60	120.68
2	K	301	1XJ	C7-C18-C6	2.36	121.57	118.57
2	C	301	1XJ	C14-C24-C15	2.36	124.16	121.24
2	D	301	1XJ	C16-C23-S63	-2.36	112.97	116.43
2	C	301	1XJ	O54-S63-C47	2.35	111.95	104.70
2	E	301	1XJ	C5-C17-C4	2.34	121.54	118.57
2	F	301	1XJ	C30-C39-C29	-2.34	105.87	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	1XJ	C33-C31-N48	2.34	115.70	110.78
2	C	301	1XJ	C44-N50-C36	2.34	117.46	111.24
2	I	301	1XJ	C43-C46-N51	2.33	114.32	110.49
2	E	301	1XJ	C16-C22-S64	-2.33	116.68	119.06
2	F	301	1XJ	O58-C38-C36	2.33	116.79	111.77
2	I	301	1XJ	O55-S63-C47	2.33	111.90	104.70
2	J	301	1XJ	C6-C8-C19	2.33	123.25	120.30
2	F	301	1XJ	C38-O58-C37	2.33	117.40	109.88
2	D	301	1XJ	C1-C3-C12	-2.33	117.37	120.24
2	K	301	1XJ	C14-C24-CL6	-2.33	115.93	119.36
2	B	301	1XJ	O56-S64-N52	2.32	113.41	106.77
2	C	301	1XJ	C32-C34-N49	2.32	115.33	110.65
2	L	301	1XJ	C10-C20-N51	-2.32	118.66	122.31
2	B	301	1XJ	C5-C17-C4	2.31	121.51	118.57
2	B	301	1XJ	C15-C5-C17	-2.31	118.33	120.80
2	L	301	1XJ	C16-C23-S63	-2.31	113.04	116.43
2	D	301	1XJ	C41-C39-C30	2.30	113.36	110.04
2	H	301	1XJ	C16-C23-C20	2.30	123.15	120.85
2	B	301	1XJ	C20-N51-C46	2.29	128.35	124.60
2	D	301	1XJ	C3-C1-C2	2.29	123.00	119.87
2	C	301	1XJ	O55-S63-C47	2.29	111.77	104.70
2	G	301	1XJ	C4-C14-C24	-2.28	116.95	119.24
2	A	301	1XJ	C15-C24-CL6	2.28	122.72	119.36
2	A	301	1XJ	C38-O58-C37	2.28	117.24	109.88
2	L	301	1XJ	O58-C37-C35	-2.27	106.87	111.77
2	A	301	1XJ	C34-C32-N48	-2.27	106.00	110.78
2	J	301	1XJ	C41-C39-C29	-2.26	106.28	109.85
2	L	301	1XJ	C44-N50-C35	2.26	117.27	111.24
2	D	301	1XJ	C32-C34-N49	2.26	115.21	110.65
2	D	301	1XJ	C43-C46-N51	-2.26	106.78	110.49
2	J	301	1XJ	C7-C18-C6	2.26	121.44	118.57
2	D	301	1XJ	O55-S63-C47	2.25	111.66	104.70
2	I	301	1XJ	O57-S64-N52	2.24	113.18	106.77
2	E	301	1XJ	C32-N48-C31	2.24	116.61	111.57
2	L	301	1XJ	C34-C32-N48	2.23	115.47	110.78
2	A	301	1XJ	C9-C19-N48	-2.22	118.31	121.39
2	A	301	1XJ	C40-C39-C30	2.22	113.24	110.04
2	G	301	1XJ	C32-C34-N49	2.20	115.09	110.65
2	C	301	1XJ	C41-C39-C30	-2.20	106.88	110.04
2	K	301	1XJ	C38-O58-C37	2.20	116.98	109.88
2	F	301	1XJ	O53-C27-C18	2.19	125.25	120.90
2	I	301	1XJ	C38-O58-C37	2.19	116.96	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	301	1XJ	C34-N49-C33	2.19	113.56	108.84
2	K	301	1XJ	C13-C22-C16	2.18	123.37	120.68
2	I	301	1XJ	C9-C19-N48	2.18	124.41	121.39
2	E	301	1XJ	C41-C39-C29	-2.17	106.42	109.85
2	B	301	1XJ	C23-C20-N51	-2.17	120.09	122.18
2	H	301	1XJ	C43-C46-N51	-2.15	106.96	110.49
2	C	301	1XJ	C5-C17-C4	2.15	121.30	118.57
2	E	301	1XJ	C8-C6-C18	-2.15	118.50	120.80
2	C	301	1XJ	C38-O58-C37	2.14	116.81	109.88
2	B	301	1XJ	C37-C35-N50	-2.14	106.87	110.12
2	K	301	1XJ	C32-N48-C19	2.14	123.94	118.11
2	L	301	1XJ	C14-C24-CL6	-2.13	116.21	119.36
2	K	301	1XJ	C33-C31-N48	2.13	115.28	110.78
2	L	301	1XJ	C4-C17-C25	-2.13	118.26	121.00
2	A	301	1XJ	C23-C20-N51	2.13	124.23	122.18
2	F	301	1XJ	C22-S64-N52	2.13	109.45	106.06
2	F	301	1XJ	O57-S64-N52	2.12	112.84	106.77
2	E	301	1XJ	C13-C22-C16	2.12	123.30	120.68
2	C	301	1XJ	C23-C20-N51	-2.11	120.14	122.18
2	B	301	1XJ	C8-C19-N48	-2.10	118.47	121.39
2	K	301	1XJ	C36-N50-C35	2.10	113.37	108.84
2	C	301	1XJ	C40-C39-C29	-2.10	106.54	109.85
2	K	301	1XJ	C32-N48-C31	2.09	116.26	111.57
2	H	301	1XJ	O55-S63-C23	2.08	112.65	107.90
2	A	301	1XJ	C10-C20-N51	-2.07	119.05	122.31
2	J	301	1XJ	C4-C17-C25	-2.06	118.34	121.00
2	H	301	1XJ	C10-C13-C22	-2.06	117.44	119.44
2	G	301	1XJ	C15-C5-C17	-2.06	118.60	120.80
2	C	301	1XJ	C44-N50-C35	2.06	116.72	111.24
2	D	301	1XJ	C5-C17-C25	2.05	123.65	121.00
2	B	301	1XJ	C9-C19-N48	2.05	124.23	121.39
2	C	301	1XJ	C18-C27-N52	2.04	118.51	116.08
2	E	301	1XJ	C30-C28-C25	-2.03	108.00	111.92
2	F	301	1XJ	C5-C17-C4	2.03	121.14	118.57
2	H	301	1XJ	C16-C23-S63	-2.02	113.46	116.43
2	I	301	1XJ	C34-N49-C33	2.02	113.20	108.84
2	K	301	1XJ	F61-C47-S63	2.02	115.74	110.25
2	A	301	1XJ	C7-C18-C27	-2.01	114.08	120.60
2	K	301	1XJ	C31-C33-N49	2.01	114.71	110.65
2	C	301	1XJ	O58-C37-C35	-2.01	107.44	111.77

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	1XJ	C26-C42-N49-C33
2	A	301	1XJ	C26-C42-N49-C34
2	B	301	1XJ	C45-C46-N51-C20
2	C	301	1XJ	C26-C42-N49-C33
2	E	301	1XJ	C26-C42-N49-C33
2	F	301	1XJ	C23-C20-N51-C46
2	F	301	1XJ	C26-C42-N49-C33
2	F	301	1XJ	S62-C45-C46-N51
2	G	301	1XJ	C45-C46-N51-C20
2	H	301	1XJ	C26-C42-N49-C33
2	I	301	1XJ	C26-C42-N49-C33
2	I	301	1XJ	C46-C43-C44-N50
2	J	301	1XJ	C44-C43-C46-C45
2	J	301	1XJ	S62-C45-C46-C43
2	J	301	1XJ	S62-C45-C46-N51
2	K	301	1XJ	C26-C42-N49-C33
2	K	301	1XJ	C26-C42-N49-C34
2	L	301	1XJ	C26-C42-N49-C33
2	G	301	1XJ	C43-C44-N50-C36
2	I	301	1XJ	C43-C44-N50-C36
2	J	301	1XJ	C43-C44-N50-C35
2	E	301	1XJ	C43-C44-N50-C35
2	L	301	1XJ	C44-C43-C46-N51
2	J	301	1XJ	C43-C44-N50-C36
2	C	301	1XJ	C43-C44-N50-C36
2	H	301	1XJ	C26-C42-N49-C34
2	F	301	1XJ	C10-C20-N51-C46
2	F	301	1XJ	C43-C44-N50-C35
2	G	301	1XJ	C44-C43-C46-N51
2	F	301	1XJ	S62-C45-C46-C43
2	J	301	1XJ	C44-C43-C46-N51
2	D	301	1XJ	C46-C43-C44-N50
2	F	301	1XJ	C46-C43-C44-N50
2	J	301	1XJ	C26-C42-N49-C33
2	C	301	1XJ	C20-C23-S63-O55
2	F	301	1XJ	C11-C21-S62-C45
2	G	301	1XJ	C26-C42-N49-C33
2	E	301	1XJ	C44-C43-C46-N51
2	J	301	1XJ	C11-C21-S62-C45
2	I	301	1XJ	C44-C43-C46-C45
2	I	301	1XJ	C11-C21-S62-C45
2	A	301	1XJ	C23-C20-N51-C46

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Mol	Chain	Res	Type	Atoms
2	A	301	1XJ	C44-C43-C46-N51
2	I	301	1XJ	S62-C45-C46-C43
2	B	301	1XJ	C12-C21-S62-C45
2	G	301	1XJ	C12-C21-S62-C45
2	L	301	1XJ	C43-C44-N50-C35
2	H	301	1XJ	C44-C43-C46-N51
2	E	301	1XJ	C12-C21-S62-C45
2	C	301	1XJ	C44-C43-C46-C45
2	D	301	1XJ	C12-C21-S62-C45
2	C	301	1XJ	C12-C21-S62-C45
2	B	301	1XJ	C44-C43-C46-N51
2	E	301	1XJ	C11-C21-S62-C45
2	B	301	1XJ	C11-C21-S62-C45
2	C	301	1XJ	C11-C21-S62-C45
2	D	301	1XJ	C11-C21-S62-C45
2	K	301	1XJ	C11-C21-S62-C45
2	H	301	1XJ	C11-C21-S62-C45
2	H	301	1XJ	C12-C21-S62-C45
2	I	301	1XJ	C12-C21-S62-C45
2	K	301	1XJ	C12-C21-S62-C45
2	G	301	1XJ	C11-C21-S62-C45
2	L	301	1XJ	C12-C21-S62-C45
2	F	301	1XJ	C12-C21-S62-C45
2	J	301	1XJ	C12-C21-S62-C45
2	L	301	1XJ	C11-C21-S62-C45
2	B	301	1XJ	C46-C43-C44-N50
2	E	301	1XJ	C46-C43-C44-N50
2	K	301	1XJ	C46-C43-C44-N50
2	A	301	1XJ	C12-C21-S62-C45
2	K	301	1XJ	C43-C44-N50-C36
2	E	301	1XJ	C5-C17-C25-C28
2	H	301	1XJ	C43-C44-N50-C35

There are no ring outliers.

12 monomers are involved in 37 short contacts:

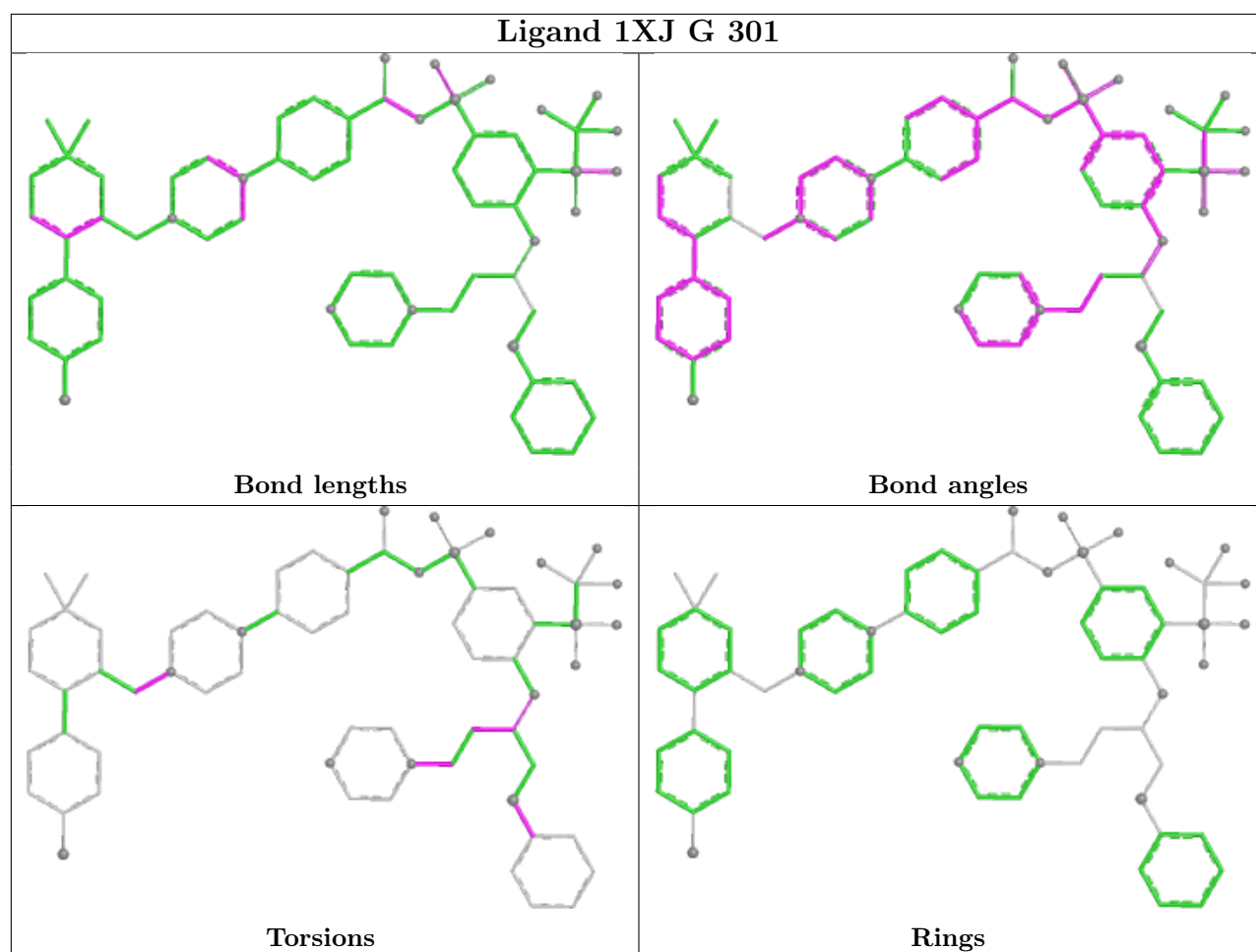
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	1XJ	3	0
2	E	301	1XJ	2	0
2	H	301	1XJ	1	0
2	C	301	1XJ	4	0
2	B	301	1XJ	2	0

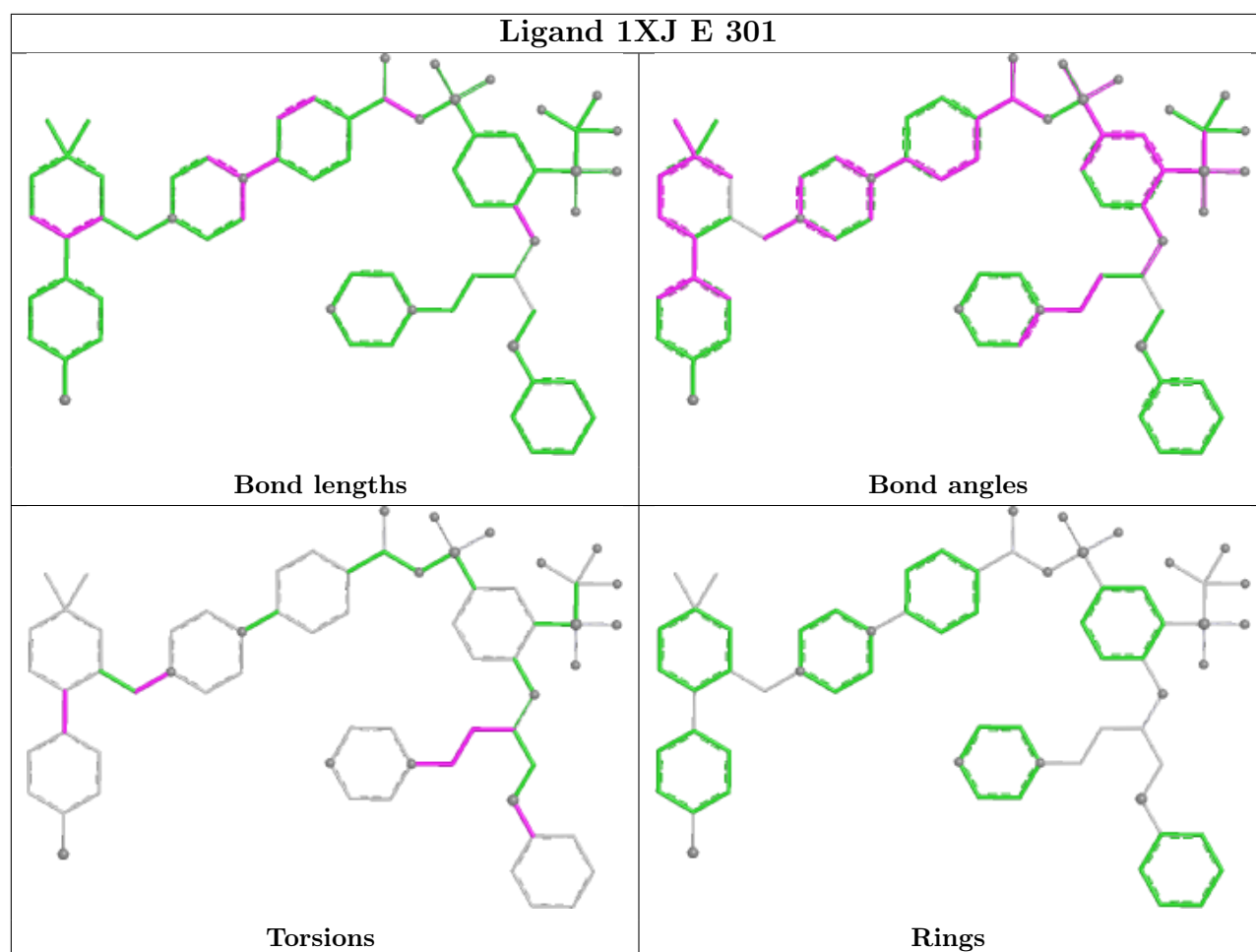
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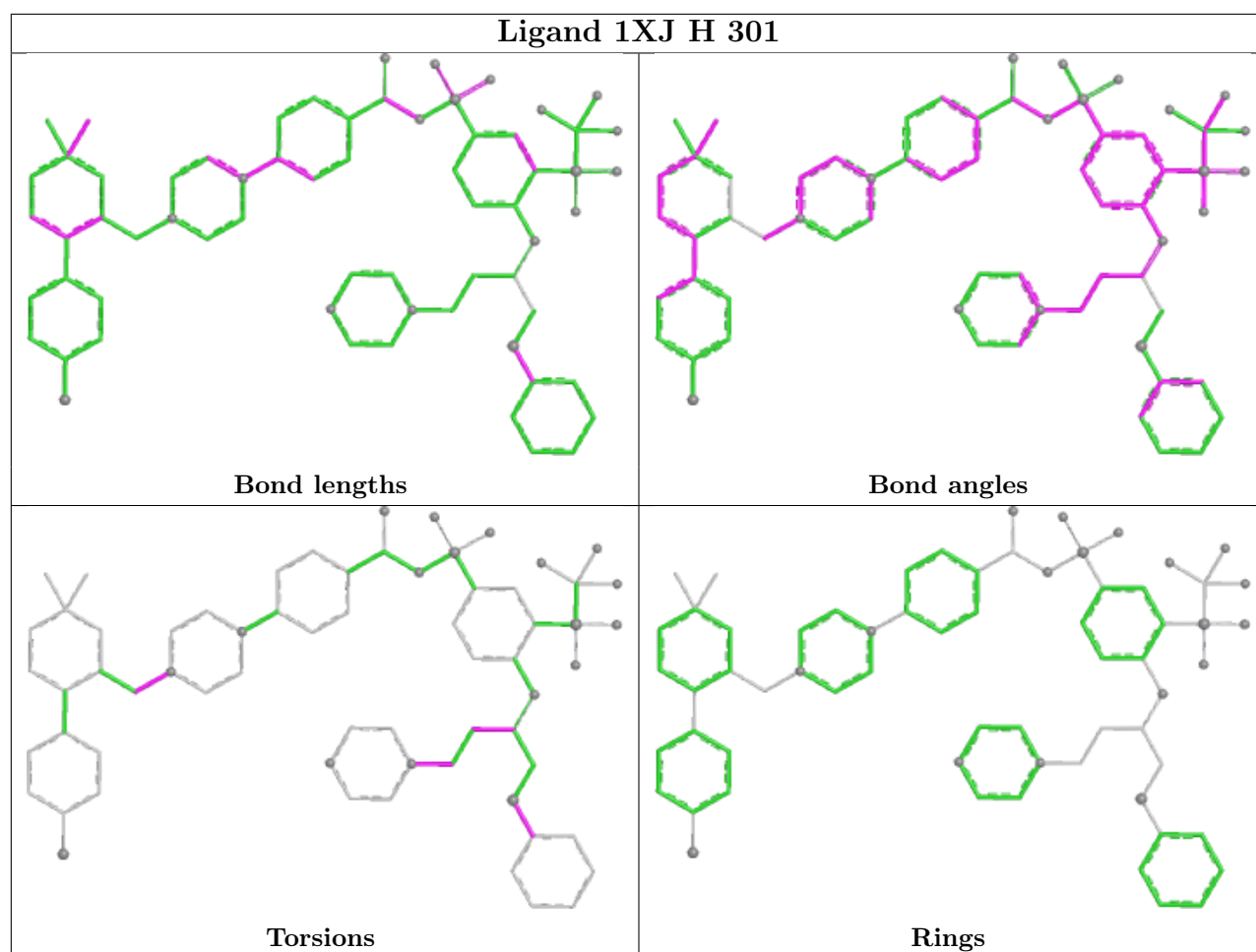
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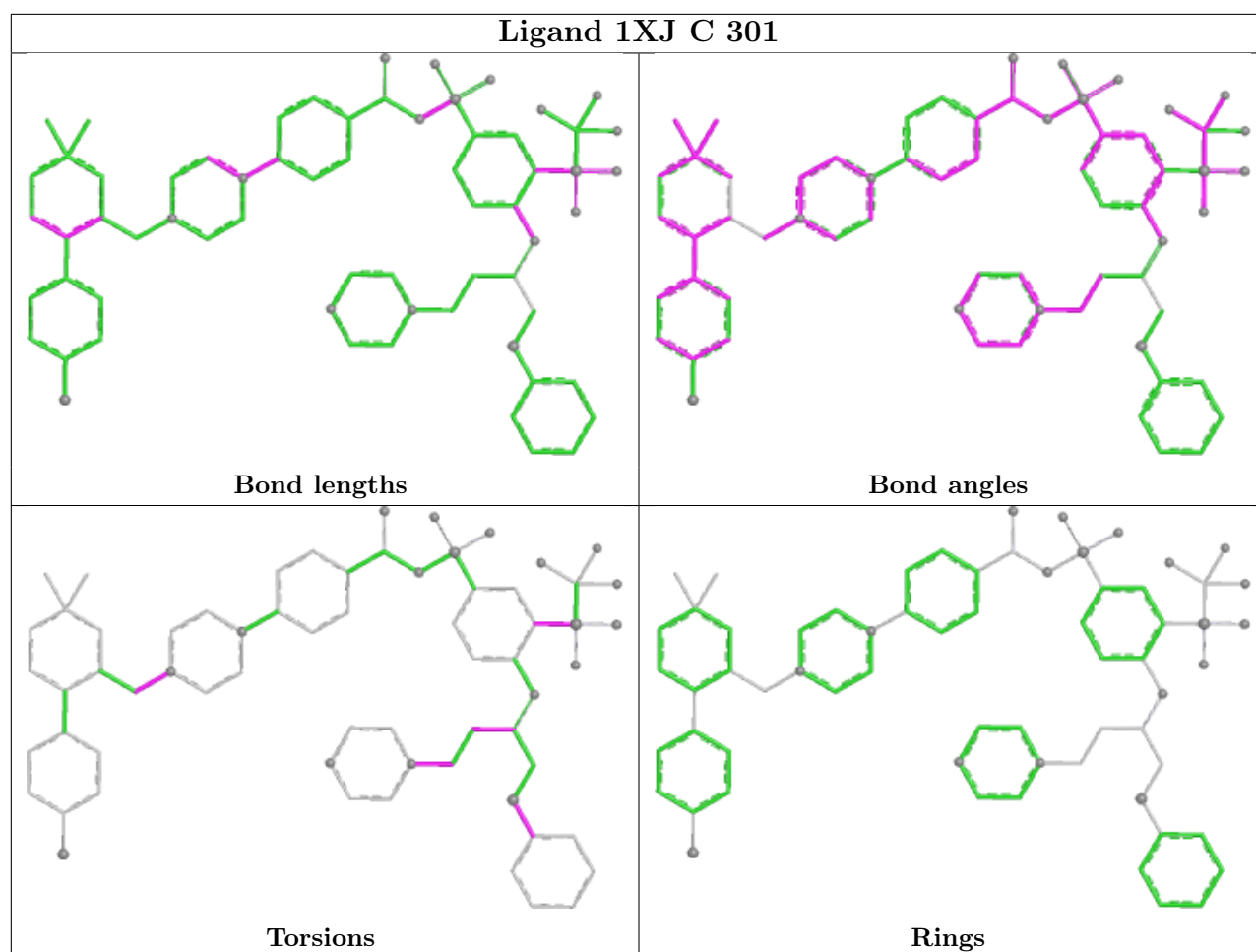
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	301	1XJ	3	0
2	L	301	1XJ	3	0
2	A	301	1XJ	4	0
2	I	301	1XJ	3	0
2	D	301	1XJ	2	0
2	F	301	1XJ	4	0
2	J	301	1XJ	6	0

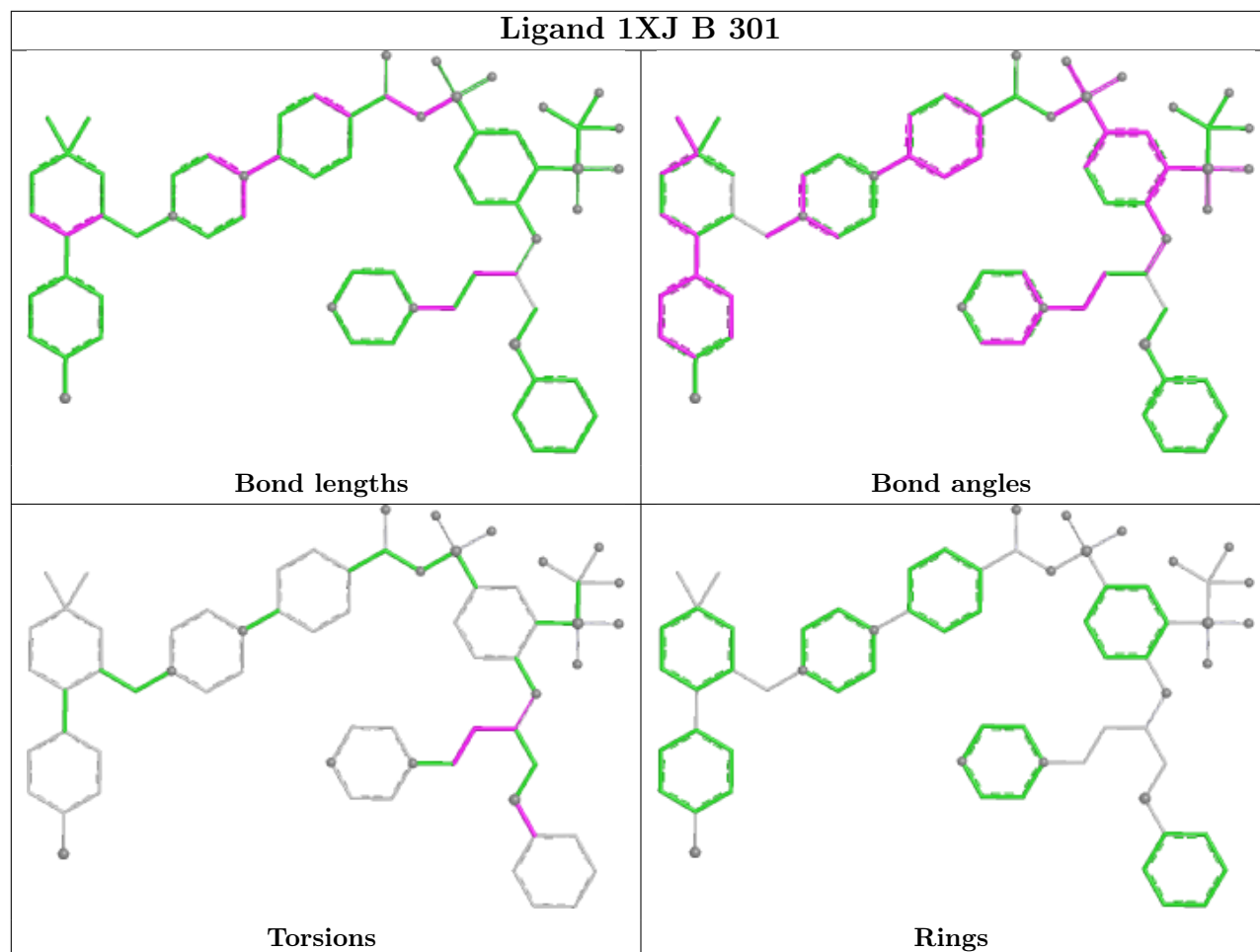
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



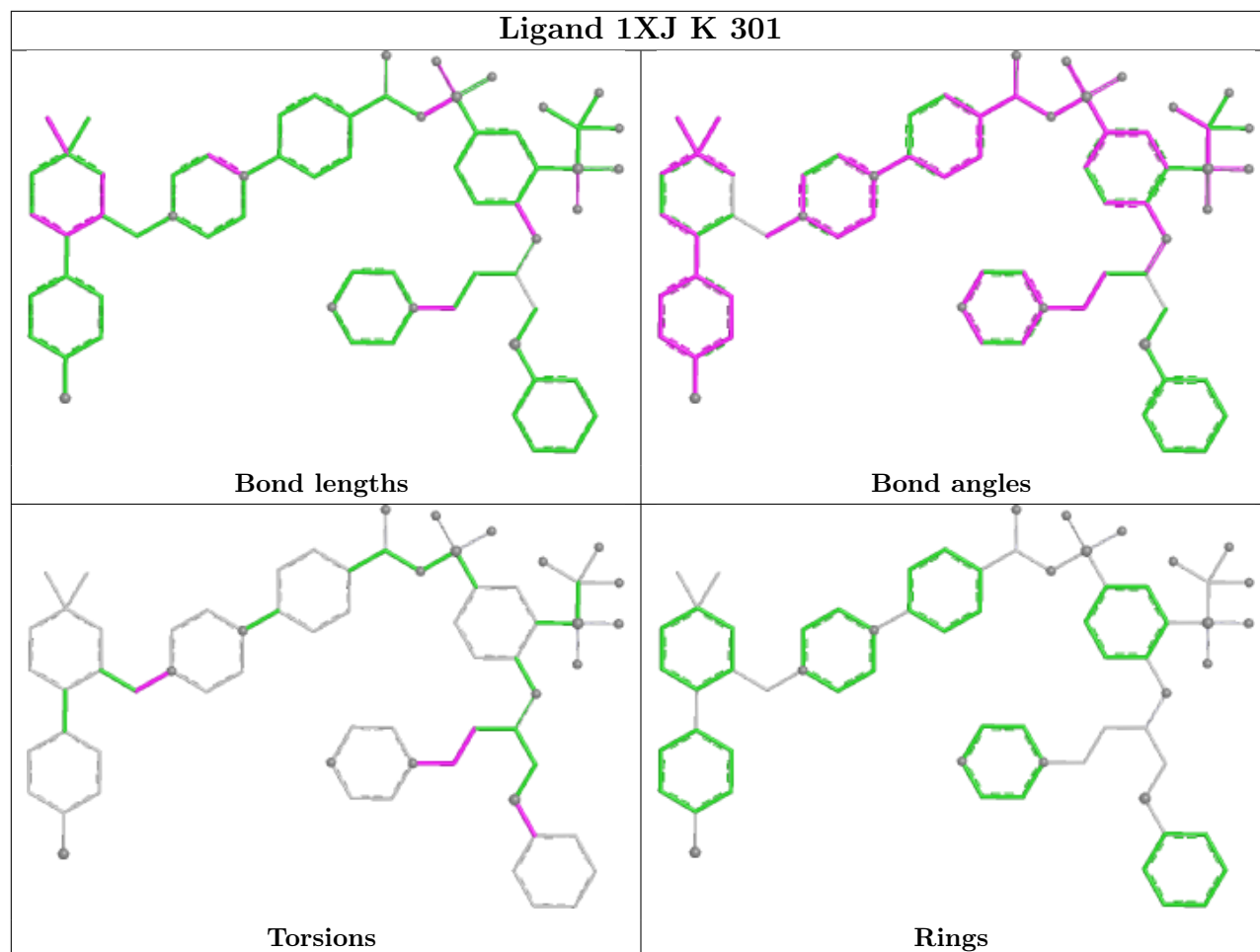


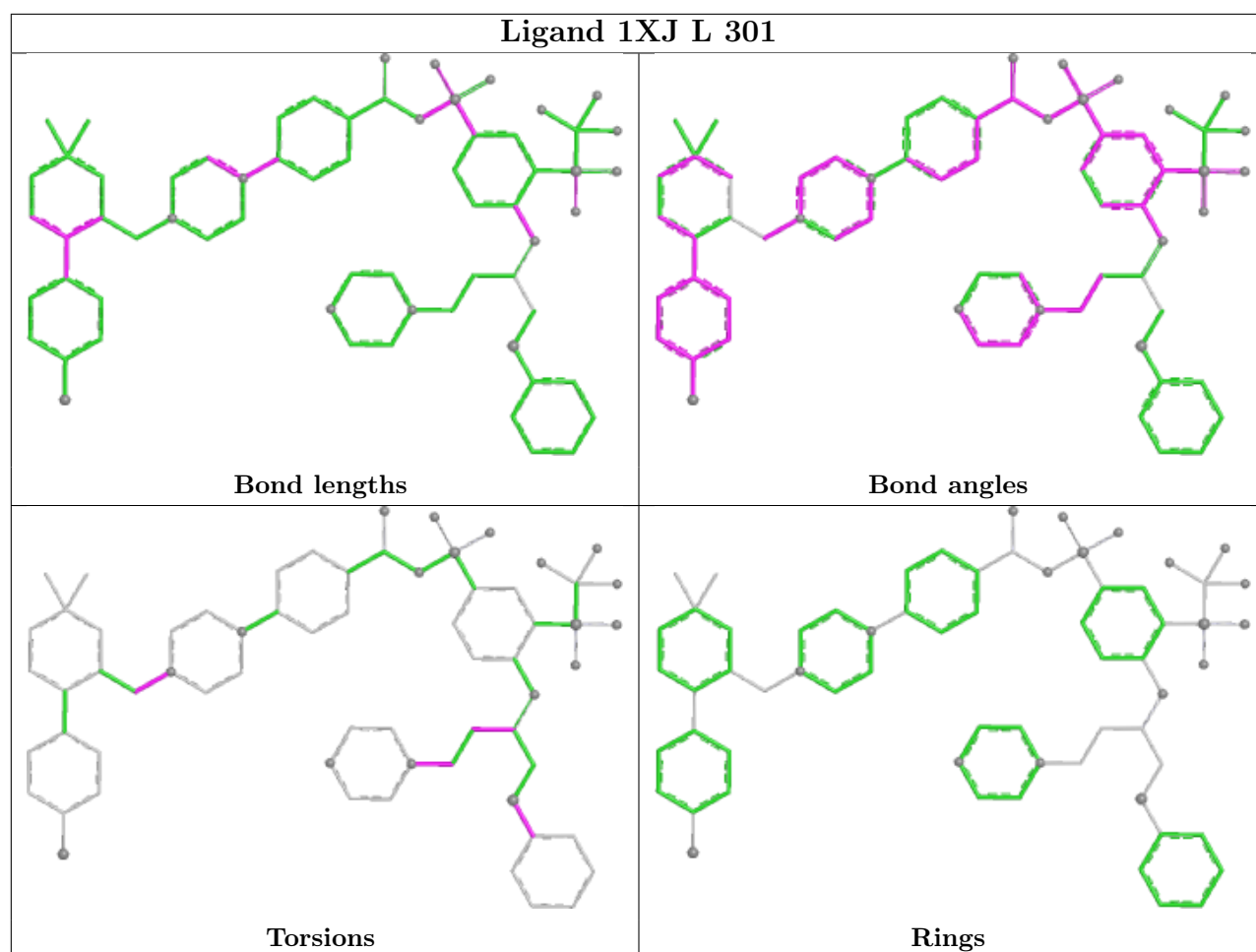


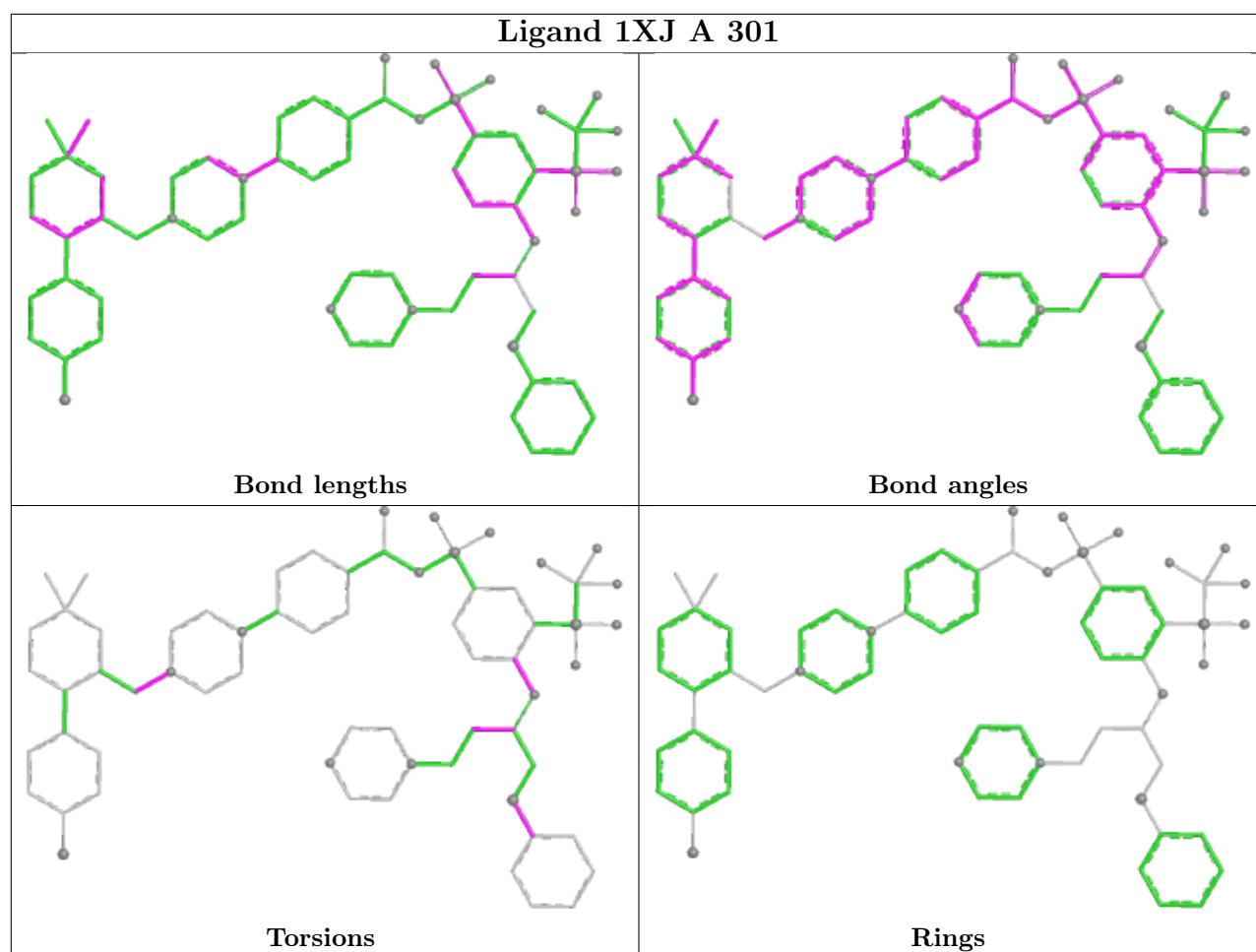


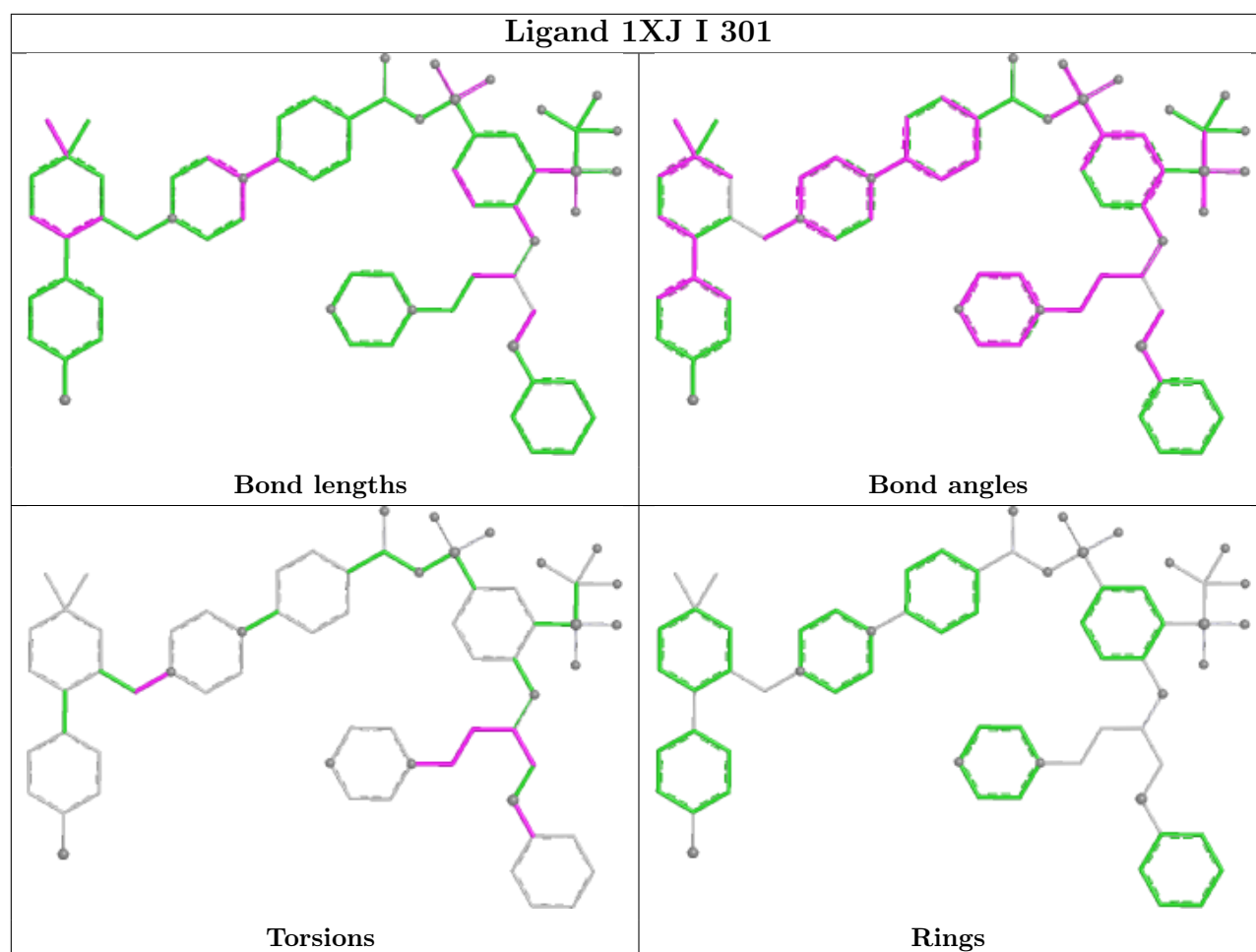


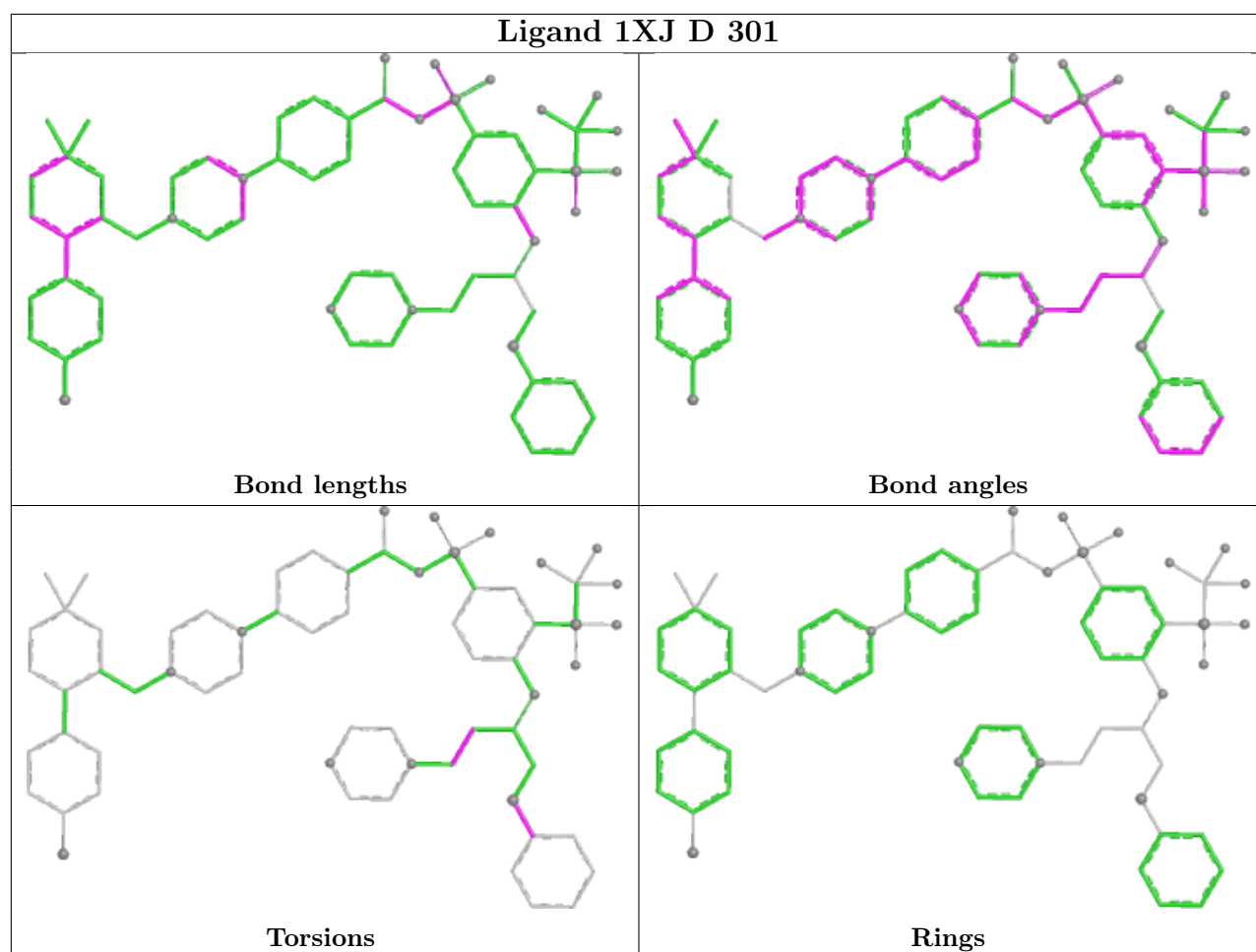
Ligand 1XJ K 301

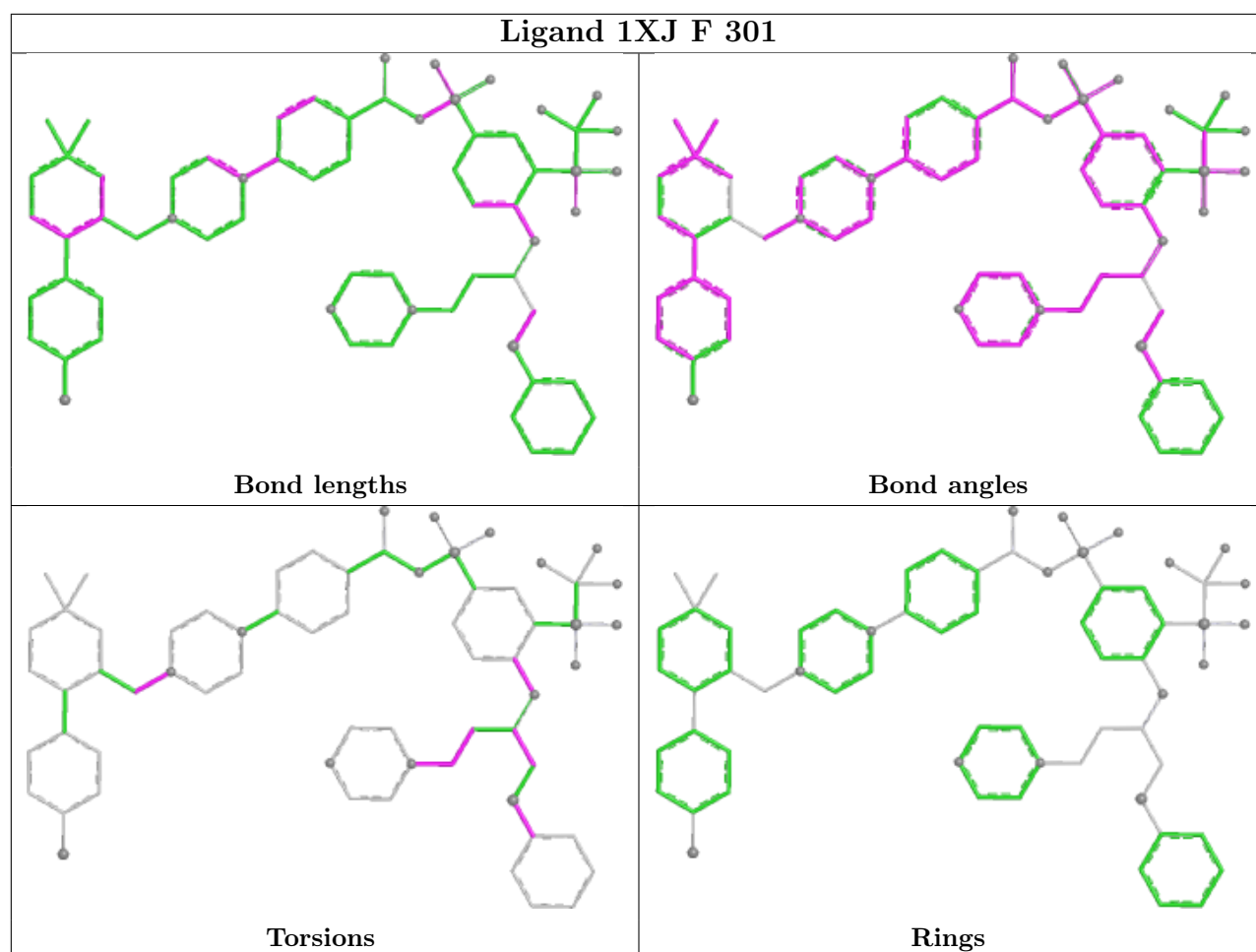


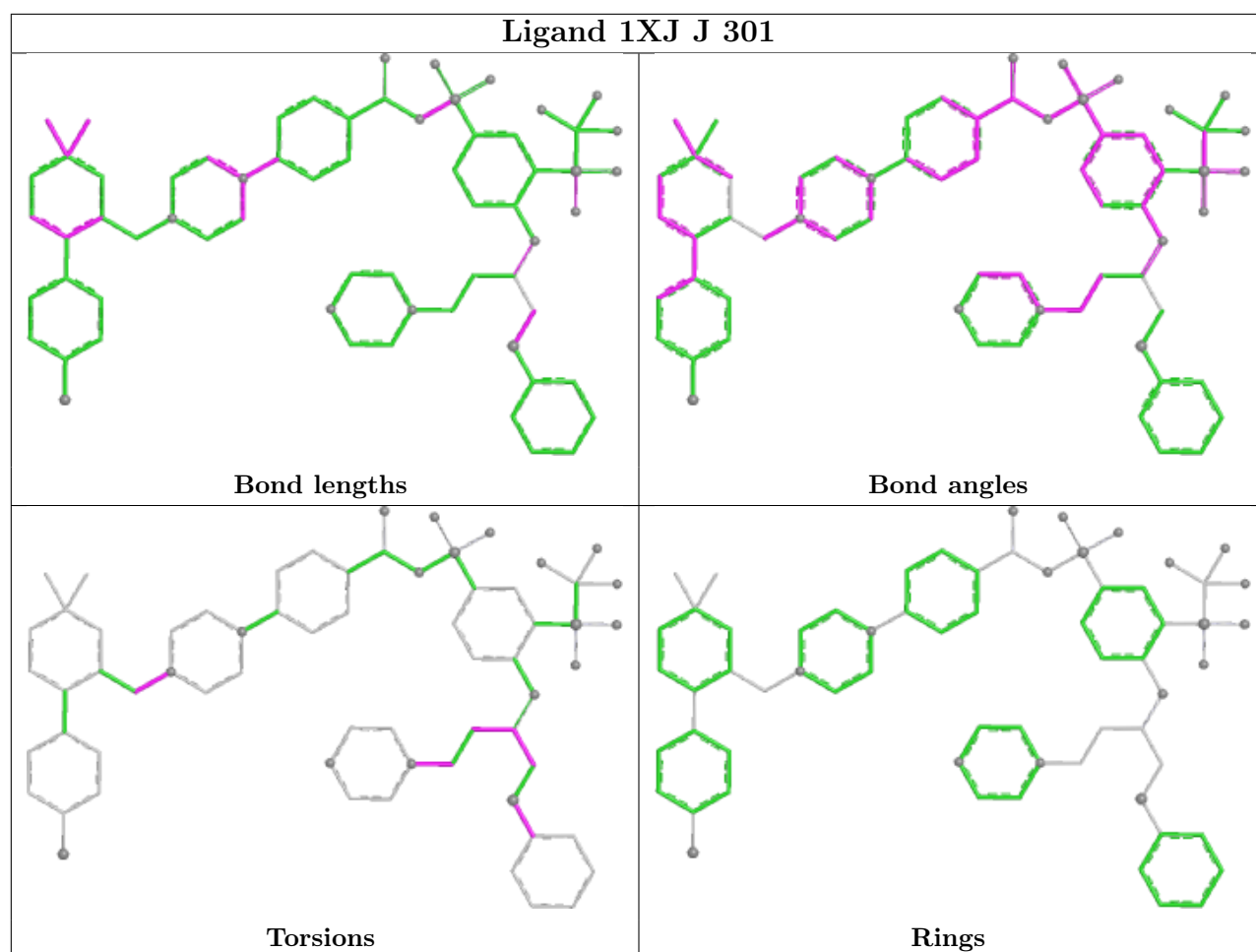












5.7 Other polymers [i](#)

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%)	-0.04	1 (0%) 84 85	26, 40, 75, 98	0
1	B	144/240 (60%)	-0.06	1 (0%) 84 85	29, 44, 86, 108	0
1	C	144/240 (60%)	0.17	3 (2%) 63 65	33, 51, 95, 111	0
1	D	141/240 (58%)	-0.08	3 (2%) 63 65	23, 39, 83, 105	0
1	E	148/240 (61%)	0.11	4 (2%) 56 58	31, 49, 98, 122	0
1	F	149/240 (62%)	0.03	6 (4%) 42 44	27, 44, 98, 117	0
1	G	140/240 (58%)	0.21	4 (2%) 53 56	34, 53, 93, 114	0
1	H	142/240 (59%)	-0.07	4 (2%) 55 57	25, 42, 81, 113	0
1	I	147/240 (61%)	0.16	7 (4%) 35 37	32, 51, 101, 142	0
1	J	149/240 (62%)	0.02	8 (5%) 31 33	22, 43, 98, 123	0
1	K	143/240 (59%)	0.11	3 (2%) 63 65	29, 51, 94, 121	0
1	L	142/240 (59%)	0.28	7 (4%) 35 36	34, 56, 108, 134	0
All	All	1733/2880 (60%)	0.07	51 (2%) 53 56	22, 48, 97, 142	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	112	LEU	4.3
1	C	112	LEU	4.0
1	B	112	LEU	3.7
1	G	112	LEU	3.6
1	H	112	LEU	3.6
1	I	112	LEU	3.3
1	C	108	LEU	3.3
1	F	0	GLY	3.3
1	H	24	TRP	3.3
1	G	24	TRP	3.2
1	K	112	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	80	VAL	3.0
1	J	27	PHE	2.9
1	J	108	LEU	2.8
1	I	109	THR	2.8
1	C	81	ILE	2.7
1	A	112	LEU	2.7
1	F	112	LEU	2.7
1	F	80	VAL	2.7
1	D	112	LEU	2.6
1	I	108	LEU	2.6
1	F	1	MET	2.5
1	G	1	MET	2.5
1	I	80	VAL	2.5
1	H	26	GLN	2.5
1	E	112	LEU	2.5
1	D	24	TRP	2.5
1	F	108	LEU	2.5
1	L	104	ALA	2.5
1	F	113	HIS	2.4
1	K	82	PRO	2.4
1	H	1	MET	2.4
1	I	1	MET	2.4
1	J	109	THR	2.4
1	I	196	GLY	2.3
1	E	80	VAL	2.3
1	G	114	ILE	2.3
1	J	25	SER	2.3
1	E	1	MET	2.3
1	E	108	LEU	2.2
1	L	110	SER	2.2
1	L	1	MET	2.2
1	J	104	ALA	2.2
1	L	22	TYR	2.1
1	J	105	PHE	2.1
1	I	110	SER	2.1
1	D	1	MET	2.1
1	K	27	PHE	2.1
1	L	197	ASN	2.0
1	J	112	LEU	2.0
1	L	108	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

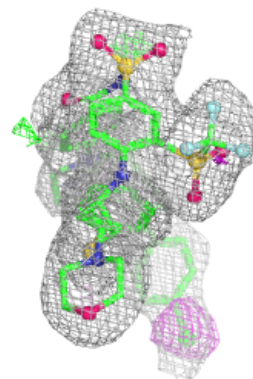
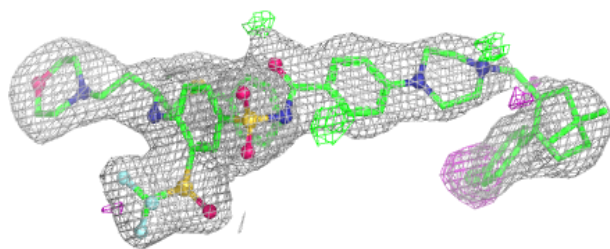
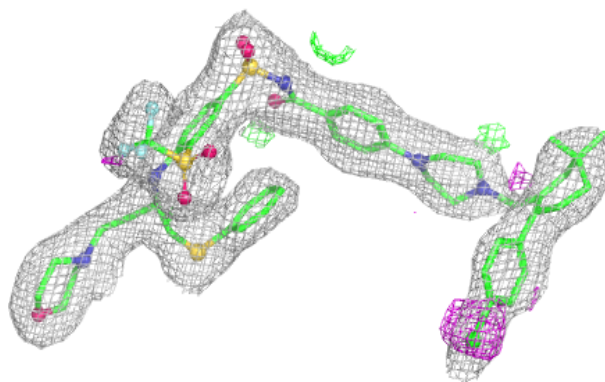
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	1XJ	F	301	65/65	0.95	0.08	30,42,63,64	0
2	1XJ	I	301	65/65	0.95	0.09	36,49,68,80	0
2	1XJ	J	301	65/65	0.95	0.09	33,46,70,80	0
2	1XJ	C	301	65/65	0.96	0.08	32,47,62,66	0
2	1XJ	K	301	65/65	0.96	0.07	31,39,61,67	0
2	1XJ	L	301	65/65	0.96	0.08	34,44,76,81	0
2	1XJ	H	301	65/65	0.97	0.07	26,32,72,80	0
2	1XJ	A	301	65/65	0.97	0.07	24,31,61,63	0
2	1XJ	E	301	65/65	0.97	0.08	36,48,77,79	0
2	1XJ	B	301	65/65	0.97	0.07	28,37,67,72	0
2	1XJ	G	301	65/65	0.97	0.07	33,42,72,77	0
2	1XJ	D	301	65/65	0.98	0.07	25,32,69,74	0

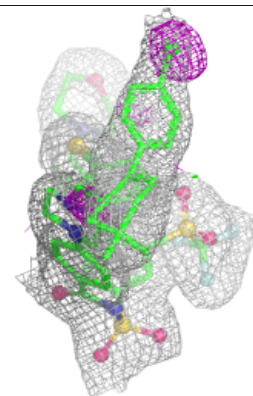
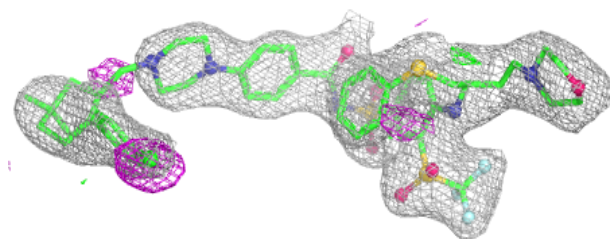
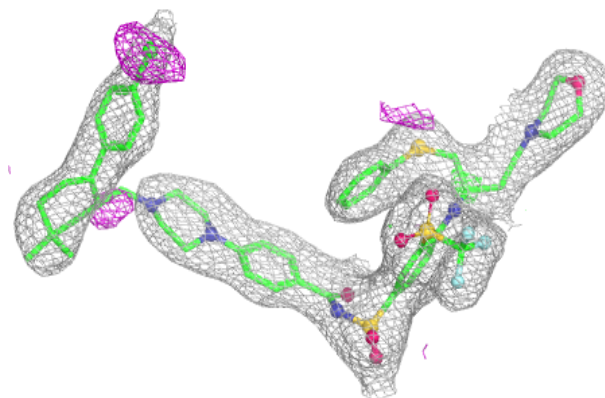
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1XJ 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)

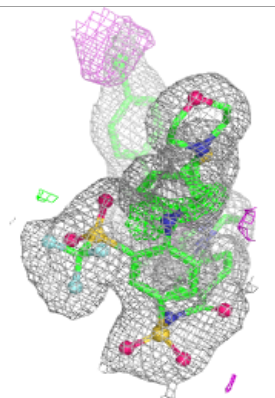
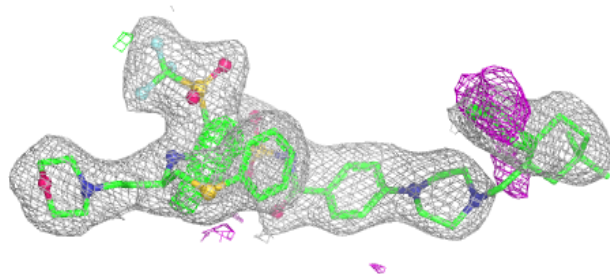
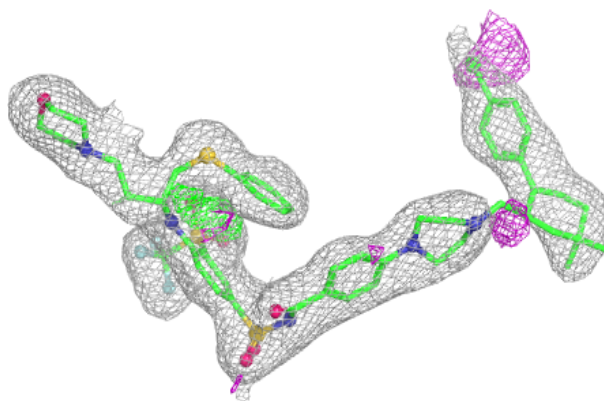
**Electron density around 1XJ I 301:**

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

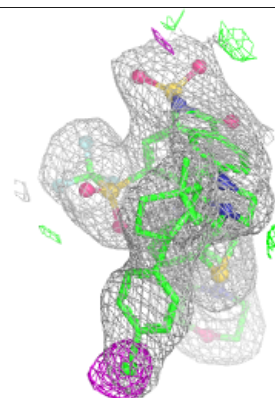
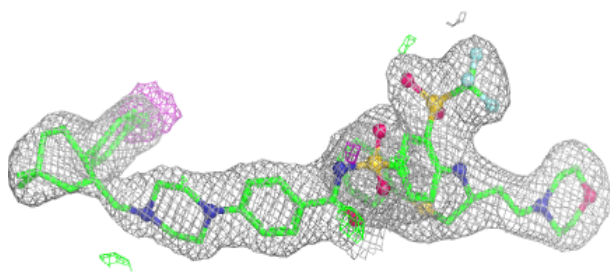
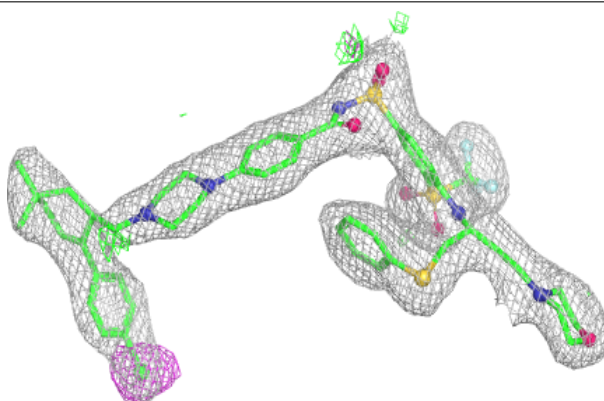


Electron density around 1XJ J 301:

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

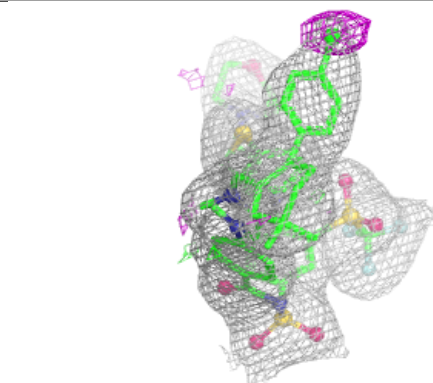
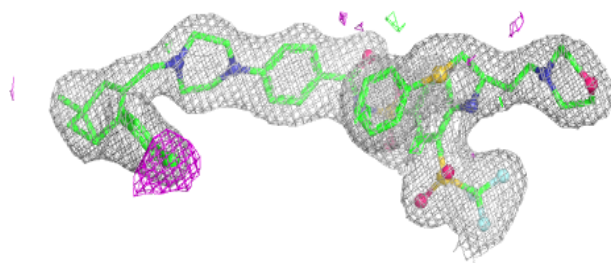
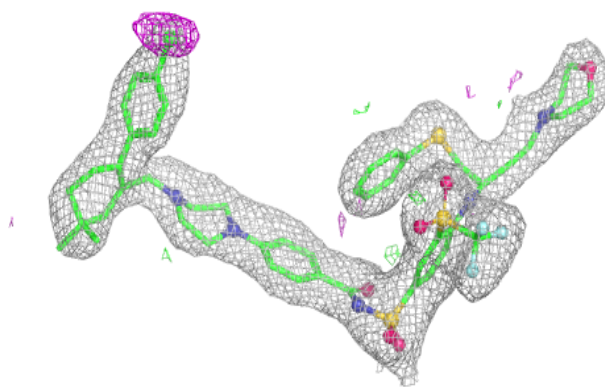
**Electron density around 1XJ C 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

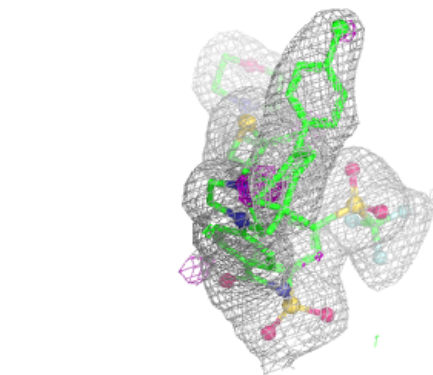
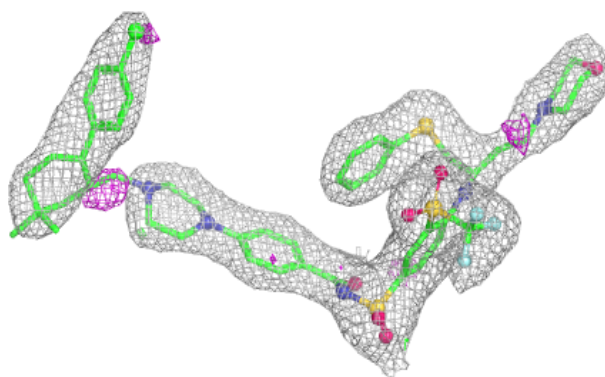


Electron density around 1XJ K 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

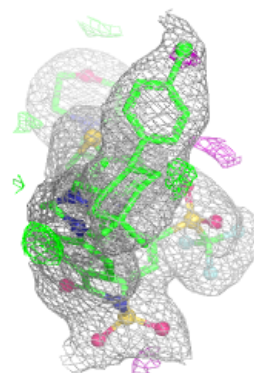
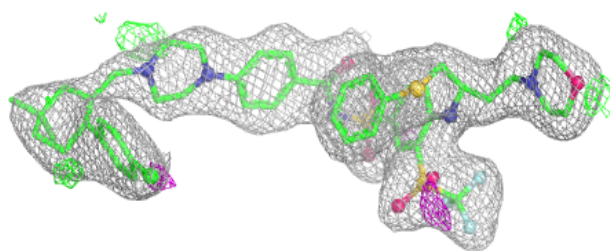
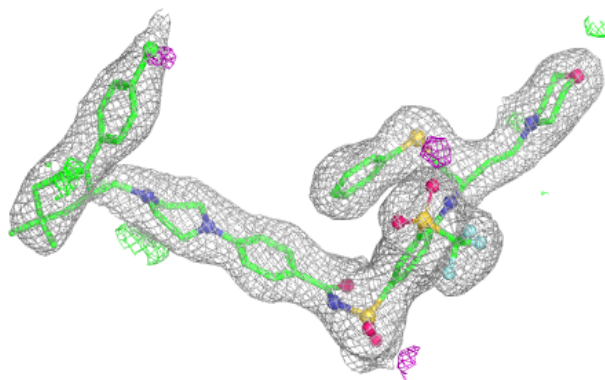
**Electron density around 1XJ L 301:**

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and green (positive)

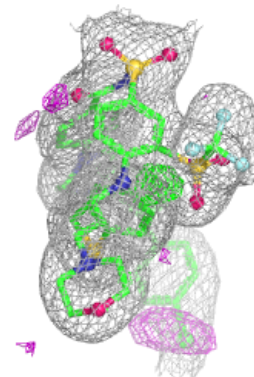
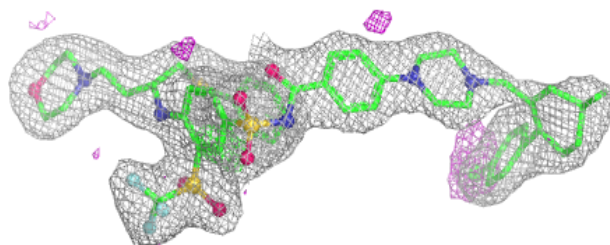
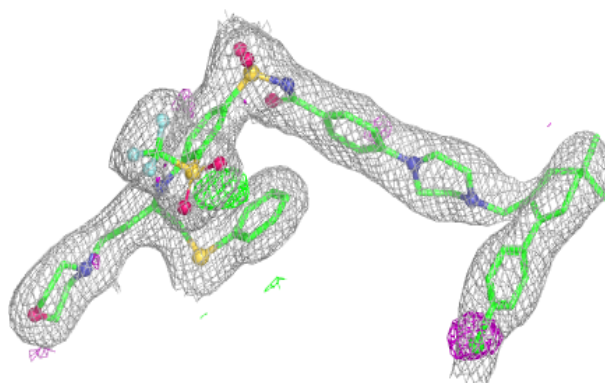


Electron density around 1XJ H 301:

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and green (positive)

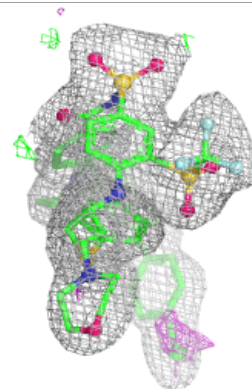
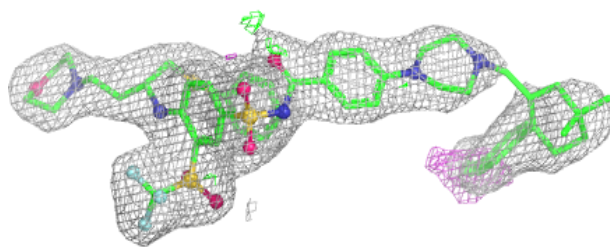
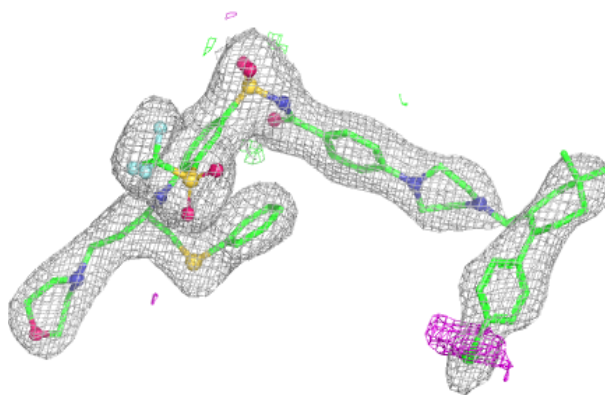
**Electron density around 1XJ A 301:**

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

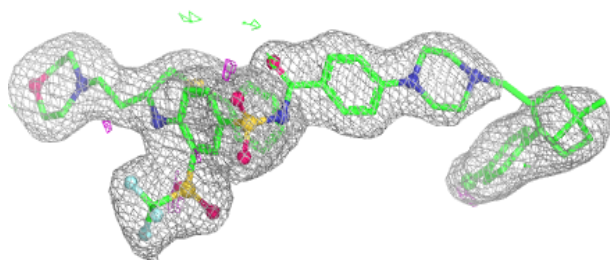
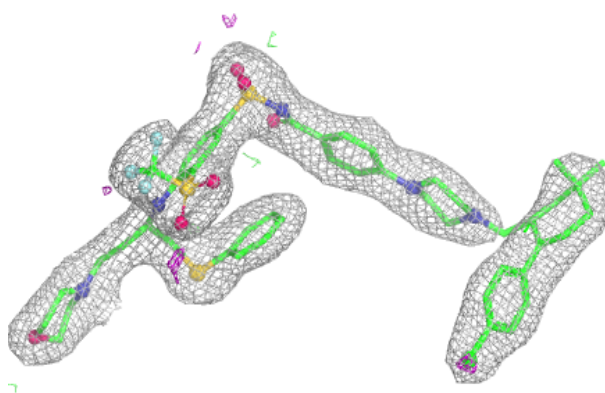


Electron density around 1XJ E 301:

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

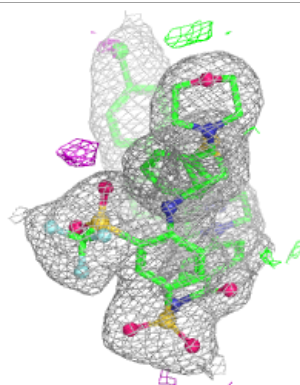
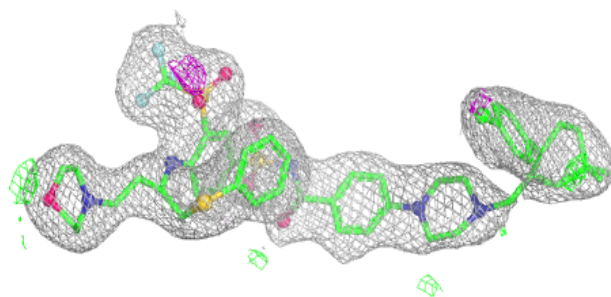
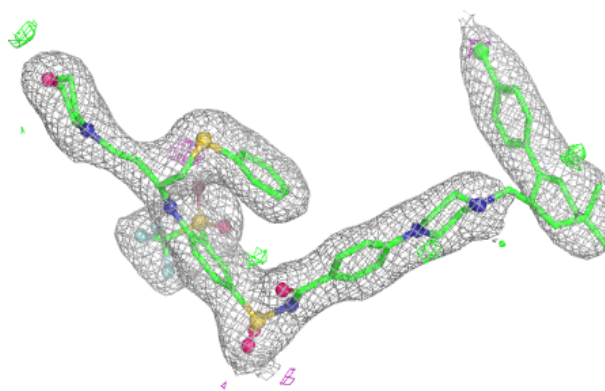
**Electron density around 1XJ B 301:**

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

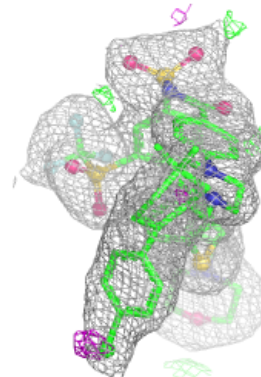
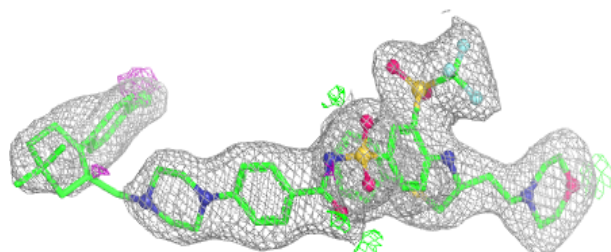
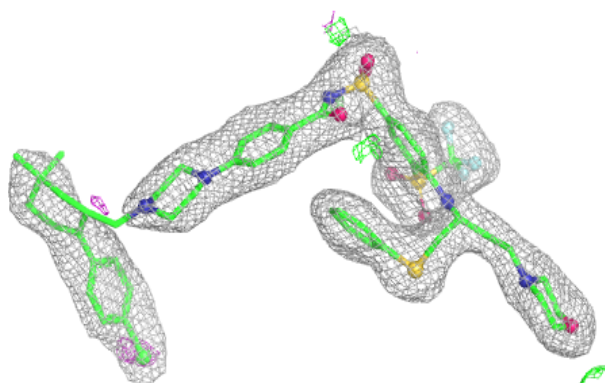


Electron density around 1XJ G 301:

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

**Electron density around 1XJ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.