



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:58 AM UTC

PDB ID : 8KE7 / pdb_00008ke7
Title : Crystal structure of DNA binding and cleavage core of human topoisomerase 2-beta in a DNA binding-competent conformation
Authors : Chan, N.L.; Liu, K.T.; Chen, S.F.
Deposited on : 2023-08-11
Resolution : 2.80 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

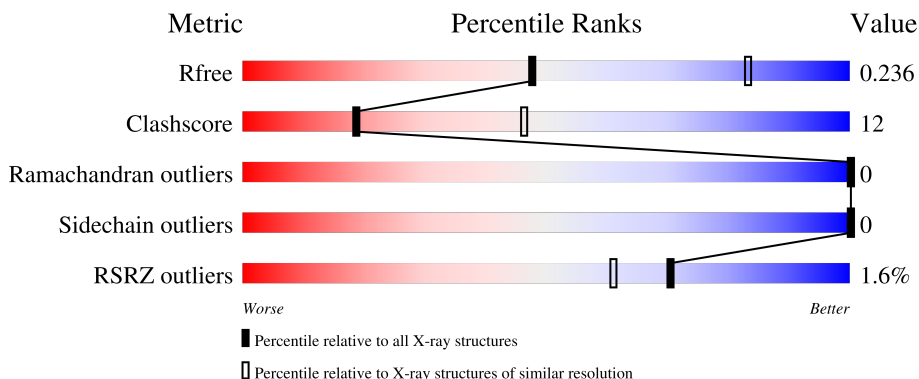
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

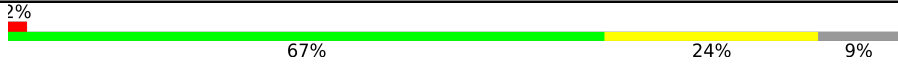
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	803	
1	B	803	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11767 atoms, of which 101 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 DNA topoisomerase 2-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	2	0
			5714	3654	970	1065	25			
1	B	728	Total	C	H	N	O	S	0	3
			5846	3688	74	976	1082	26		0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	MET	-	expression tag	UNP Q02880
A	420	ALA	-	expression tag	UNP Q02880
A	421	SER	-	expression tag	UNP Q02880
A	422	TRP	-	expression tag	UNP Q02880
A	423	SER	-	expression tag	UNP Q02880
A	424	HIS	-	expression tag	UNP Q02880
A	425	PRO	-	expression tag	UNP Q02880
A	426	GLN	-	expression tag	UNP Q02880
A	427	PHE	-	expression tag	UNP Q02880
A	428	GLU	-	expression tag	UNP Q02880
A	429	LYS	-	expression tag	UNP Q02880
A	430	GLY	-	expression tag	UNP Q02880
A	431	ALA	-	expression tag	UNP Q02880
A	432	ASP	-	expression tag	UNP Q02880
A	433	ASP	-	expression tag	UNP Q02880
A	434	ASP	-	expression tag	UNP Q02880
A	435	ASP	-	expression tag	UNP Q02880
A	436	LYS	-	expression tag	UNP Q02880
A	437	VAL	-	expression tag	UNP Q02880
A	438	PRO	-	expression tag	UNP Q02880
A	439	ASP	-	expression tag	UNP Q02880
A	440	PRO	-	expression tag	UNP Q02880
A	441	THR	-	expression tag	UNP Q02880
A	442	SER	-	expression tag	UNP Q02880
A	443	VAL	-	expression tag	UNP Q02880

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Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASP	-	expression tag	UNP Q02880
A	1202	GLY	-	expression tag	UNP Q02880
A	1203	ALA	-	expression tag	UNP Q02880
A	1204	PRO	-	expression tag	UNP Q02880
A	1205	GLY	-	expression tag	UNP Q02880
A	1206	PHE	-	expression tag	UNP Q02880
A	1207	SER	-	expression tag	UNP Q02880
A	1208	SER	-	expression tag	UNP Q02880
A	1209	ILE	-	expression tag	UNP Q02880
A	1210	SER	-	expression tag	UNP Q02880
A	1211	ALA	-	expression tag	UNP Q02880
A	1212	HIS	-	expression tag	UNP Q02880
A	1213	HIS	-	expression tag	UNP Q02880
A	1214	HIS	-	expression tag	UNP Q02880
A	1215	HIS	-	expression tag	UNP Q02880
A	1216	HIS	-	expression tag	UNP Q02880
A	1217	HIS	-	expression tag	UNP Q02880
A	1218	HIS	-	expression tag	UNP Q02880
A	1219	HIS	-	expression tag	UNP Q02880
A	1220	HIS	-	expression tag	UNP Q02880
A	1221	HIS	-	expression tag	UNP Q02880
B	419	MET	-	expression tag	UNP Q02880
B	420	ALA	-	expression tag	UNP Q02880
B	421	SER	-	expression tag	UNP Q02880
B	422	TRP	-	expression tag	UNP Q02880
B	423	SER	-	expression tag	UNP Q02880
B	424	HIS	-	expression tag	UNP Q02880
B	425	PRO	-	expression tag	UNP Q02880
B	426	GLN	-	expression tag	UNP Q02880
B	427	PHE	-	expression tag	UNP Q02880
B	428	GLU	-	expression tag	UNP Q02880
B	429	LYS	-	expression tag	UNP Q02880
B	430	GLY	-	expression tag	UNP Q02880
B	431	ALA	-	expression tag	UNP Q02880
B	432	ASP	-	expression tag	UNP Q02880
B	433	ASP	-	expression tag	UNP Q02880
B	434	ASP	-	expression tag	UNP Q02880
B	435	ASP	-	expression tag	UNP Q02880
B	436	LYS	-	expression tag	UNP Q02880
B	437	VAL	-	expression tag	UNP Q02880
B	438	PRO	-	expression tag	UNP Q02880
B	439	ASP	-	expression tag	UNP Q02880

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Chain	Residue	Modelled	Actual	Comment	Reference
B	440	PRO	-	expression tag	UNP Q02880
B	441	THR	-	expression tag	UNP Q02880
B	442	SER	-	expression tag	UNP Q02880
B	443	VAL	-	expression tag	UNP Q02880
B	444	ASP	-	expression tag	UNP Q02880
B	1202	GLY	-	expression tag	UNP Q02880
B	1203	ALA	-	expression tag	UNP Q02880
B	1204	PRO	-	expression tag	UNP Q02880
B	1205	GLY	-	expression tag	UNP Q02880
B	1206	PHE	-	expression tag	UNP Q02880
B	1207	SER	-	expression tag	UNP Q02880
B	1208	SER	-	expression tag	UNP Q02880
B	1209	ILE	-	expression tag	UNP Q02880
B	1210	SER	-	expression tag	UNP Q02880
B	1211	ALA	-	expression tag	UNP Q02880
B	1212	HIS	-	expression tag	UNP Q02880
B	1213	HIS	-	expression tag	UNP Q02880
B	1214	HIS	-	expression tag	UNP Q02880
B	1215	HIS	-	expression tag	UNP Q02880
B	1216	HIS	-	expression tag	UNP Q02880
B	1217	HIS	-	expression tag	UNP Q02880
B	1218	HIS	-	expression tag	UNP Q02880
B	1219	HIS	-	expression tag	UNP Q02880
B	1220	HIS	-	expression tag	UNP Q02880
B	1221	HIS	-	expression tag	UNP Q02880

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	B	1	Total	C	H	O	0	0
			7	2	3	2		
2	B	1	Total	C	H	O	0	0
			7	2	3	2		
2	B	1	Total	C	H	O	0	0
			7	2	3	2		

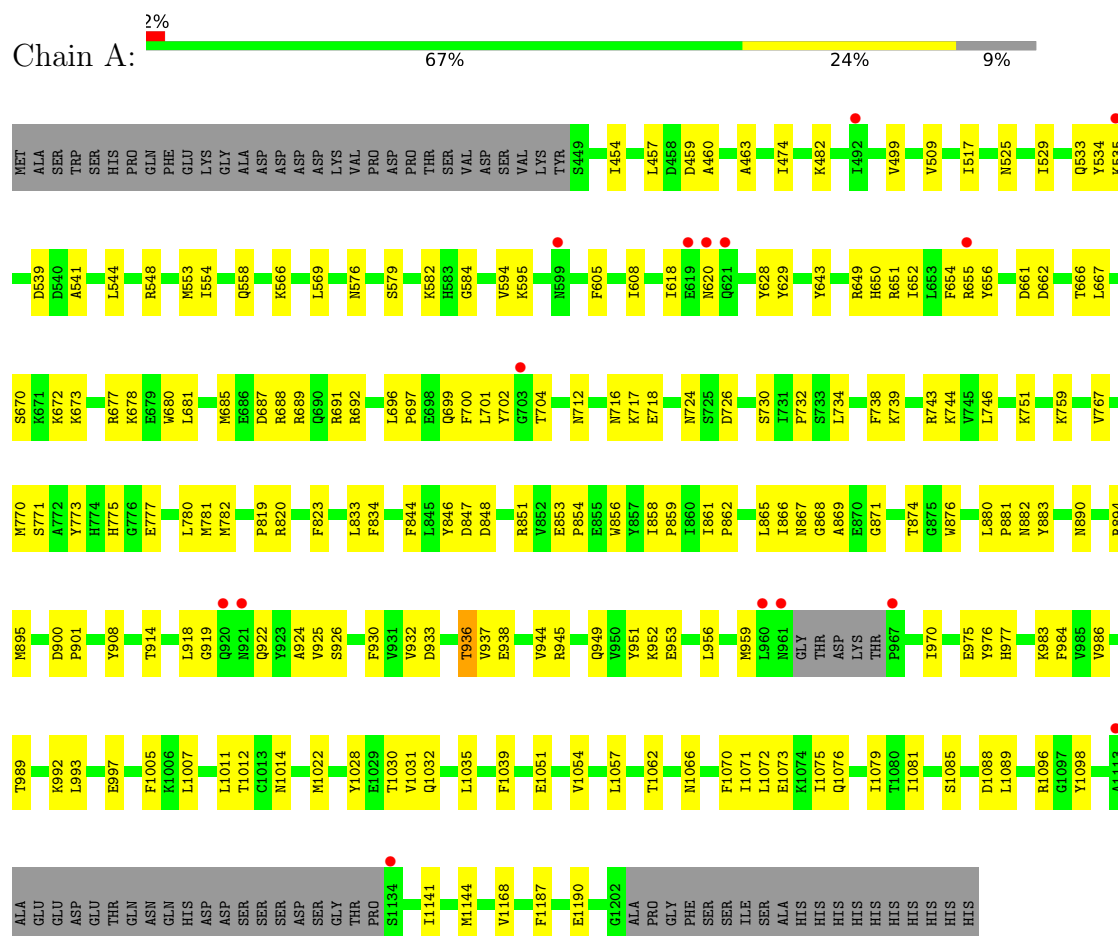
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total	O	0	0
			59	59		
3	B	85	Total	O	0	0
			85	85		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA topoisomerase 2-beta



SER	T1080	V944	Q805	I652
SER	I1081	R945	H811	L653
ILE	E1082	Q949	P819	F654
SER	N1083	M959	H831	K671
ALA	R1084	L960	A836	I674
HIS	M1082	N961	GLY	K678
HIS	R1096	THR	D839	M685
HIS	S1100	ASP	L842	E686
HIS	D1101	LYS	K645	R689
HIS	P1102	THR	F844	Q690
HIS	V1103	PRO	D847	L693
HIS	W1106	A968	D848	L696
	A1113	L969	P854	P697
ALA	GLU	I970	W856	F700
GLU	ASP	K983	I858	L701
ASP	GLU	M988	T861	Y702
GLU	THR	E991	R862	G703
GLN	THR	Q995	W864	T704
ASN	GLN	F1005	I866	ALA
GLN	ASP	K1006	A869	T706
HIS	HIS	L1007	G875	K707
ASP	ASP	T1012	Y883	H708
ASP	ASP	C1013	T886	Y711
SER	SER	M1014	L896	M712
SER	SER	V1017	T914	D713
ASP	ASP	H1021	N921	K717
GLY	GLY	M1022	E928	E718
THR	THR	G1023	I929	I731
PRO	PRO	C1024	F930	P732
S1134	S1134	L1025	V931	S733
I1141	I1141	K1026	V932	L734
M1144	M1144	V1031	K1080	V735
S1145	S1145	F1038	V1054	L746
L1146	L1146	L1041	G1055	K751
T1150	T1150	R1042	M1056	R752
V1154	V1154	K1080	V1064	S766
S1177	S1177	V1054	G1055	M770
L1184	L1184	V1188	M1056	Y773
V1188	V1188	A1203	K1083	H774
A1203	A1203	PRO	E941	H775
PRO	GLY	L942	I940	M781
PHE	PHE	P943	P943	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.72Å 113.71Å 209.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 2.80 19.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.83-2.80) 97.8 (19.83-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.194 , 0.238 0.195 , 0.236	Depositor DCC
R_{free} test set	2000 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11767	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	0.17	0/5828	0.46	3/7879 (0.0%)
1	B	0.23	2/5886 (0.0%)	0.48	2/7948 (0.0%)
All	All	0.20	2/11714 (0.0%)	0.47	5/15827 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	608	ILE	CA-CB	-6.19	1.51	1.54
1	B	522	GLU	CD-OE2	5.60	1.35	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	847	ASP	CA-C-N	5.83	132.68	121.54
1	A	847	ASP	C-N-CA	5.83	132.68	121.54
1	A	936	THR	OG1-CB-CG2	5.21	119.71	109.30
1	B	847	ASP	CA-C-N	5.04	131.17	121.54
1	B	847	ASP	C-N-CA	5.04	131.17	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5714	0	5519	156	0
1	B	5772	74	5651	117	0
2	A	20	15	15	0	0
2	B	16	12	12	0	0
3	A	59	0	0	3	0
3	B	85	0	0	4	0
All	All	11666	101	11197	270	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 12.

All (270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:ILE:HD13	1:B:569:LEU:HD22	1.32	1.05
1:B:685:MET:HE1	1:B:1025:LEU:HD12	1.45	0.97
1:A:976:TYR:HB2	1:A:983:LYS:HG2	1.52	0.90
1:B:466:LYS:O	1:B:467:HIS:HB2	1.70	0.90
1:B:1012:THR:HG22	1:B:1014:ASN:H	1.35	0.89
1:A:751:LYS:HB3	1:A:770:MET:HE1	1.52	0.89
1:A:1012:THR:HG22	1:A:1014:ASN:H	1.39	0.88
1:A:895:MET:HE1	1:A:1035:LEU:HG	1.54	0.88
1:B:944:VAL:HG12	1:B:945:ARG:HG2	1.61	0.80
1:B:1022:MET:HA	1:B:1022:MET:HE2	1.63	0.80
1:A:1030:THR:HG22	1:A:1032:GLN:H	1.47	0.79
1:B:811:HIS:CE1	1:B:949:GLN:HG3	2.18	0.79
1:A:651:ARG:O	1:A:652:ILE:HD13	1.85	0.77
1:B:589:PHE:O	1:B:590:ILE:HD13	1.86	0.76
1:B:988:MET:HE3	1:B:1005:PHE:HZ	1.50	0.76
1:A:554:ILE:HD12	1:A:569:LEU:HD22	1.70	0.73
1:B:674:ILE:H	1:B:674:ILE:HD12	1.56	0.71
1:A:539:ASP:OD1	1:A:579:SER:OG	2.08	0.71
1:B:473:LEU:HD23	1:B:530:VAL:HG22	1.73	0.71
1:A:558:GLN:NE2	1:A:702:TYR:O	2.24	0.70
1:B:700:PHE:CE1	1:B:718:GLU:HG3	2.27	0.70
1:B:482:LYS:HD3	3:B:1483:HOH:O	1.90	0.69
1:A:751:LYS:HD3	1:A:770:MET:CE	2.22	0.69
1:A:1081:ILE:HG22	1:A:1089:LEU:HD11	1.74	0.69
1:A:1051:GLU:O	1:A:1054:VAL:HG12	1.92	0.69
1:B:594:VAL:HG13	1:B:605:PHE:HB2	1.74	0.69
1:A:688:ARG:O	1:A:692:ARG:HG3	1.93	0.68
1:B:1024:CYS:SG	1:B:1026:LYS:HE3	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:PRO:HG3	1:A:1035:LEU:HD13	1.76	0.68
1:A:594:VAL:HG13	1:A:605:PHE:HB2	1.77	0.67
1:A:744:LYS:HG2	1:A:771:SER:HB2	1.76	0.67
1:A:781[B]:MET:HE2	1:A:819:PRO:HG2	1.76	0.67
1:A:582:LYS:HG2	1:A:656:TYR:CD2	2.30	0.67
1:A:751:LYS:CB	1:A:770:MET:HE1	2.24	0.67
1:A:751:LYS:HD3	1:A:770:MET:HE3	1.77	0.66
1:A:726:ASP:HB3	1:A:874:THR:OG1	1.95	0.66
1:A:482:LYS:HG3	1:A:499:VAL:CG1	2.25	0.65
1:A:700:PHE:CE2	1:A:718:GLU:HG3	2.32	0.65
1:B:558:GLN:OE1	1:B:590:ILE:HG23	1.96	0.65
1:B:555:MET:HE3	1:B:589:PHE:CD2	2.32	0.65
1:B:593:ILE:HD12	1:B:702:TYR:O	1.97	0.64
1:A:1071:ILE:O	1:A:1075:ILE:HG12	1.97	0.64
1:B:988:MET:HE3	1:B:1005:PHE:CZ	2.32	0.64
1:B:678:LYS:HE2	1:B:875:GLY:O	1.97	0.64
1:A:970:ILE:HG21	1:A:986:VAL:HG21	1.80	0.64
1:B:1184:LEU:O	1:B:1188:VAL:HG23	1.98	0.64
1:A:867:ASN:C	1:A:882:ASN:ND2	2.57	0.63
1:A:699:GLN:HG2	1:A:717:LYS:HE3	1.80	0.63
1:A:773:TYR:CE1	1:A:775:HIS:HB2	2.34	0.63
1:A:628:TYR:CE1	1:A:848:ASP:O	2.52	0.63
1:B:513:SER:O	1:B:517:ILE:HG13	1.99	0.62
1:A:670:SER:HB3	1:A:673:LYS:HG3	1.81	0.62
1:A:1073:GLU:CD	1:A:1096:ARG:HH12	2.07	0.62
1:A:454:ILE:HD11	1:A:525:ASN:OD1	2.01	0.61
1:A:554:ILE:HD13	1:A:566:LYS:HA	1.81	0.61
1:A:654:PHE:C	1:A:655:ARG:HE	2.08	0.61
1:A:732:PRO:HG2	1:A:869:ALA:HB1	1.82	0.61
1:B:530:VAL:HB	1:B:532:LEU:HD23	1.81	0.61
1:A:652:ILE:HG13	1:A:704:THR:HG22	1.82	0.60
1:B:574:HIS:HB2	1:B:581:LEU:HD11	1.82	0.60
1:B:1141:ILE:HA	1:B:1144:MET:HE2	1.83	0.60
1:A:689:ARG:NH2	1:A:1022:MET:HB2	2.17	0.60
1:A:868:GLY:N	1:A:882:ASN:HD22	2.00	0.60
1:A:882:ASN:OD1	1:A:908:TYR:CE2	2.55	0.59
1:A:1070:PHE:HE2	1:B:1146:LEU:HD13	1.67	0.59
1:B:671:LYS:O	1:B:674:ILE:HD11	2.02	0.59
1:A:482:LYS:HG3	1:A:499:VAL:HG11	1.85	0.59
1:A:652:ILE:HG13	1:A:704:THR:CG2	2.33	0.59
1:A:687:ASP:O	1:A:691:ARG:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:PRO:HG2	1:B:869:ALA:HB1	1.85	0.59
1:B:628:TYR:CE2	1:B:848:ASP:O	2.56	0.59
1:B:862:PRO:HD2	1:B:888:ILE:HG21	1.85	0.59
1:B:991:GLU:O	1:B:995:GLN:HG3	2.03	0.59
1:A:759:LYS:HE2	1:A:820:ARG:O	2.03	0.58
1:A:883:TYR:CZ	1:A:1031:VAL:HG21	2.38	0.58
1:A:895:MET:CE	1:A:1035:LEU:HG	2.30	0.58
1:A:1141:ILE:O	1:A:1144:MET:HG3	2.03	0.58
1:B:555:MET:HE3	1:B:589:PHE:CE2	2.39	0.57
1:B:921:ASN:HB3	1:B:1013:CYS:HB2	1.85	0.57
1:B:1092[A]:MET:HE3	1:B:1096:ARG:HD2	1.87	0.57
1:B:1025:LEU:O	1:B:1026:LYS:HD3	2.04	0.56
1:A:951:TYR:OH	1:A:1007:LEU:HD21	2.05	0.56
1:B:706:THR:HB	1:B:708:HIS:O	2.05	0.56
1:A:918:LEU:HD13	1:A:924:ALA:HB2	1.87	0.56
1:A:594:VAL:CG1	1:A:605:PHE:HB2	2.35	0.56
1:A:696:LEU:HB3	1:A:697:PRO:CD	2.35	0.56
1:A:858:ILE:HG23	1:A:858:ILE:O	2.06	0.56
1:A:952:LYS:HD2	1:A:975:GLU:OE2	2.04	0.56
1:B:896:LEU:HD22	1:B:1177:SER:HB3	1.87	0.56
1:A:1062:THR:HG21	3:A:1455:HOH:O	2.05	0.56
1:A:654:PHE:N	1:A:655:ARG:HH21	2.04	0.55
1:A:890[A]:ASN:O	1:A:894:ARG:HG3	2.06	0.55
1:A:541:ALA:O	1:A:544:LEU:HG	2.05	0.55
1:A:1073:GLU:OE1	1:A:1098:TYR:OH	2.21	0.55
1:A:482:LYS:HG3	1:A:499:VAL:HG12	1.89	0.55
1:A:975:GLU:HG2	1:A:977:HIS:HE2	1.72	0.55
1:B:649:ARG:HG3	1:B:649:ARG:O	2.06	0.55
1:A:730:SER:O	1:A:739:LYS:HE2	2.07	0.54
1:B:1017:VAL:HG12	1:B:1025:LEU:HD22	1.88	0.54
1:A:861:ILE:HB	1:A:862:PRO:HD2	1.89	0.54
1:B:1050:LYS:O	1:B:1054:VAL:HG23	2.08	0.54
1:B:537:SER:OG	1:B:539:ASP:OD1	2.14	0.54
1:B:858:ILE:HG23	1:B:858:ILE:O	2.07	0.54
1:A:662:ASP:O	1:A:666:THR:HG23	2.08	0.54
1:B:862:PRO:HG3	1:B:1038:PHE:CD2	2.42	0.54
1:B:773:TYR:CE1	1:B:775:HIS:HB2	2.43	0.54
1:A:833:LEU:HD21	1:A:1187:PHE:CE1	2.43	0.53
1:A:751:LYS:CD	1:A:770:MET:HE3	2.38	0.53
1:A:654:PHE:O	1:A:655:ARG:NH2	2.42	0.53
1:A:865:LEU:HD11	1:A:1031:VAL:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:932:VAL:CG2	1:B:936:THR:HB	2.38	0.53
1:A:608:ILE:HB	1:A:701:LEU:HD13	1.91	0.53
1:A:880:LEU:HD23	1:A:881:PRO:O	2.09	0.53
1:B:526:ILE:O	1:B:530:VAL:HG23	2.09	0.53
1:B:751:LYS:HD2	1:B:770:MET:SD	2.48	0.53
1:A:866:ILE:O	1:A:882:ASN:HB3	2.09	0.52
1:B:752:ARG:NH1	1:B:766:SER:OG	2.42	0.52
1:A:944:VAL:O	1:A:945:ARG:HB2	2.10	0.52
1:B:556:THR:OG1	1:B:566:LYS:HE3	2.09	0.52
1:A:667:LEU:O	1:A:677:ARG:NH2	2.43	0.52
1:B:811:HIS:HE1	1:B:949:GLN:HG3	1.70	0.52
1:A:977:HIS:O	1:B:494:ARG:NH2	2.43	0.52
1:A:865:LEU:CD1	1:A:1031:VAL:HG13	2.39	0.52
1:A:649:ARG:O	1:A:649:ARG:HG2	2.08	0.52
1:A:834:PHE:CE1	1:A:859:PRO:HB3	2.45	0.52
1:A:777:GLU:O	1:A:781[A]:MET:HG2	2.09	0.51
1:A:584:GLY:HA3	1:A:655:ARG:HH12	1.76	0.51
1:A:781[B]:MET:HG2	1:A:782:MET:HE2	1.93	0.51
1:A:975:GLU:HG2	1:A:977:HIS:NE2	2.25	0.51
1:B:589:PHE:C	1:B:590:ILE:HD13	2.34	0.51
1:B:831:ARG:NH1	1:B:836:ALA:HA	2.25	0.51
1:B:1063:LYS:HD2	1:B:1103:VAL:CG2	2.41	0.51
1:A:914:THR:HG1	1:A:926:SER:HG	1.59	0.51
1:A:895:MET:HE1	1:A:1035:LEU:CG	2.32	0.51
1:A:956:LEU:O	1:A:959:MET:HB2	2.10	0.51
1:B:1056:MET:HE2	1:B:1106:TRP:CE3	2.46	0.50
1:B:781[B]:MET:HG3	1:B:819:PRO:HG3	1.93	0.50
1:B:864:VAL:HG12	3:B:1426:HOH:O	2.11	0.50
1:A:678:LYS:HG3	1:A:876:TRP:CH2	2.46	0.50
1:B:883:TYR:CZ	1:B:1031:VAL:HG11	2.47	0.50
1:B:614:TRP:O	1:B:620:ASN:HB2	2.12	0.49
1:B:696:LEU:HB3	1:B:697:PRO:HD2	1.95	0.49
1:B:858:ILE:O	1:B:1042:ARG:NH1	2.45	0.49
1:A:959:MET:HE1	1:A:1005:PHE:HA	1.93	0.49
1:A:643:TYR:HA	1:A:650:HIS:CE1	2.48	0.49
1:A:930:PHE:O	1:A:937:VAL:HG23	2.12	0.48
1:A:767:VAL:HB	1:A:780:LEU:HD21	1.95	0.48
1:A:993:LEU:HD23	1:A:997:GLU:HB2	1.95	0.48
1:B:1017:VAL:CG1	1:B:1025:LEU:HD22	2.43	0.48
1:A:933:ASP:OD1	1:A:933:ASP:C	2.56	0.48
1:A:993:LEU:HD23	1:A:993:LEU:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:ARG:NH1	1:B:693:LEU:HD11	2.29	0.48
1:B:527:ILE:HG23	1:B:532:LEU:HB2	1.96	0.48
1:B:735:VAL:HG11	1:B:856:TRP:CE3	2.48	0.48
1:B:861:ILE:HD12	1:B:866:ILE:HD11	1.96	0.47
1:A:584:GLY:CA	1:A:655:ARG:NH1	2.77	0.47
1:B:574:HIS:O	1:B:578:PRO:HD3	2.14	0.47
1:A:685:MET:HE2	1:A:724:ASN:OD1	2.15	0.47
1:A:759:LYS:HG3	1:A:823:PHE:CE2	2.48	0.47
1:A:666:THR:O	1:A:670:SER:HB2	2.14	0.47
1:A:534:TYR:HE1	1:A:576:ASN:ND2	2.13	0.47
1:A:901:PRO:HG2	1:A:1032:GLN:CD	2.40	0.47
1:B:473:LEU:HG	1:B:475:LEU:CD1	2.45	0.47
1:B:746:LEU:HD12	1:B:746:LEU:HA	1.74	0.47
1:B:1074:LYS:HZ1	1:B:1082:GLU:CD	2.23	0.47
1:A:595:LYS:HD2	1:A:629:TYR:CZ	2.50	0.47
1:A:649:ARG:HG3	3:A:1458:HOH:O	2.15	0.46
1:A:661:ASP:OD1	1:A:712:ASN:HB2	2.15	0.46
1:A:696:LEU:HB3	1:A:697:PRO:HD2	1.97	0.46
1:A:867:ASN:C	1:A:882:ASN:HD22	2.22	0.46
1:A:744:LYS:HE2	1:A:853:GLU:OE2	2.14	0.46
1:B:1084:ARG:HH12	1:B:1092[B]:MET:CE	2.29	0.46
1:A:894:ARG:NH2	1:A:900:ASP:O	2.47	0.46
1:A:533:GLN:HG2	1:A:535:LYS:HG2	1.97	0.46
1:A:751:LYS:CD	1:A:770:MET:CE	2.93	0.46
1:A:959:MET:HE1	1:A:1005:PHE:CD2	2.50	0.46
1:A:1057:LEU:HB3	1:A:1168:VAL:HG22	1.98	0.46
1:B:608:ILE:HB	1:B:609:PRO:HD3	1.98	0.46
1:A:938:GLU:HA	1:A:984:PHE:O	2.16	0.46
1:A:584:GLY:HA3	1:A:655:ARG:NH1	2.31	0.46
1:A:680:TRP:HE1	1:A:716:ASN:HD22	1.64	0.46
1:A:1079:ILE:HD11	1:A:1096:ARG:HD3	1.96	0.46
1:B:654:PHE:HB3	1:B:711:TYR:CZ	2.52	0.45
1:B:686:GLU:O	1:B:690:GLN:HG2	2.16	0.45
1:A:846:TYR:CZ	1:A:851:ARG:HG3	2.51	0.45
1:B:941:GLU:HA	1:B:941:GLU:OE2	2.16	0.45
1:A:919:GLY:O	1:A:922:GLN:HB2	2.17	0.45
1:A:952:LYS:HE2	1:B:455:PRO:O	2.17	0.45
1:A:993:LEU:HD23	1:A:993:LEU:O	2.17	0.45
1:B:550:GLY:O	1:B:551:LYS:HG3	2.17	0.45
1:B:594:VAL:CG1	1:B:605:PHE:HB2	2.43	0.45
1:B:959:MET:HE2	1:B:970:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:PHE:HA	1:A:854:PRO:HA	1.99	0.45
1:B:1080:THR:HG23	1:B:1084:ARG:HD2	1.99	0.45
1:B:534:TYR:HE2	1:B:576:ASN:ND2	2.15	0.45
1:B:559:ASP:OD2	1:B:559:ASP:C	2.60	0.45
1:A:584:GLY:CA	1:A:655:ARG:HH12	2.30	0.44
1:A:734:LEU:HD13	1:A:1028:TYR:CZ	2.52	0.44
1:A:925:VAL:HG21	1:A:1011:LEU:HG	1.99	0.44
1:A:738:PHE:CZ	1:A:746:LEU:HD22	2.53	0.44
1:B:1084:ARG:NH1	1:B:1092[B]:MET:SD	2.90	0.44
1:A:554:ILE:CD1	1:A:566:LYS:HA	2.46	0.44
1:A:1072:LEU:O	1:A:1076:GLN:HG2	2.17	0.44
1:A:1039:PHE:CD2	1:A:1039:PHE:C	2.96	0.44
1:B:474:ILE:HG12	1:B:553:MET:HE2	1.98	0.44
1:B:652:ILE:HD12	1:B:706:THR:O	2.18	0.44
1:A:861:ILE:HD12	1:A:866:ILE:HD11	2.00	0.44
1:B:457:LEU:HD22	1:B:529:ILE:HG12	2.00	0.43
1:B:930:PHE:O	1:B:937:VAL:HA	2.18	0.43
1:B:482:LYS:HG3	1:B:499:VAL:HG12	2.00	0.43
1:B:713:ASP:O	1:B:717:LYS:HB2	2.16	0.43
1:A:744:LYS:NZ	1:A:771:SER:O	2.51	0.43
1:A:1085:SER:HB3	1:A:1088:ASP:HB2	1.99	0.43
1:B:544:LEU:HD21	1:B:580:LEU:CD2	2.48	0.43
1:B:523:ILE:O	1:B:527:ILE:HG13	2.18	0.43
1:A:901:PRO:HB2	1:A:1032:GLN:HE22	1.83	0.43
1:B:988:MET:CE	1:B:1005:PHE:CZ	3.00	0.43
1:A:970:ILE:HG21	1:A:986:VAL:CG2	2.47	0.43
1:B:506:ILE:O	1:B:568:LEU:HD13	2.19	0.43
1:B:580:LEU:HD23	1:B:580:LEU:HA	1.84	0.43
1:A:474:ILE:HA	1:A:553:MET:O	2.18	0.43
1:A:618:ILE:C	1:A:620:ASN:H	2.26	0.43
1:A:651:ARG:C	1:A:652:ILE:HD13	2.44	0.43
1:A:667:LEU:HA	1:A:673:LYS:HD2	1.99	0.43
1:B:465:GLY:O	1:B:468:SER:OG	2.31	0.43
1:A:457:LEU:HD21	1:A:459:ASP:HB2	2.01	0.42
1:A:509:VAL:HG12	1:A:517:ILE:HG12	2.01	0.42
1:A:949:GLN:O	1:A:953:GLU:HG3	2.19	0.42
1:B:734:LEU:HD23	1:B:734:LEU:C	2.44	0.42
1:A:548:ARG:HG2	1:A:548:ARG:HH11	1.84	0.42
1:A:681:LEU:HD22	1:A:724:ASN:HB2	2.01	0.42
1:B:473:LEU:CD2	1:B:530:VAL:HG22	2.46	0.42
1:B:928:GLU:HB2	1:B:941:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:THR:OG1	1:A:992:LYS:HG2	2.19	0.42
1:B:932:VAL:HG23	1:B:936:THR:HB	2.01	0.42
1:A:730:SER:O	1:A:871:GLY:HA3	2.19	0.42
1:A:959:MET:HE1	1:A:1005:PHE:HD2	1.82	0.42
1:A:672:LYS:O	1:A:673:LYS:HG2	2.20	0.42
1:B:1150:THR:O	1:B:1154:VAL:HG23	2.20	0.42
1:A:525:ASN:O	1:A:529:ILE:HG13	2.20	0.42
1:B:700:PHE:HE1	1:B:702:TYR:CE1	2.37	0.42
1:A:654:PHE:O	1:A:655:ARG:CZ	2.67	0.42
1:A:925:VAL:CG2	1:A:1011:LEU:HG	2.49	0.42
1:B:671:LYS:O	1:B:674:ILE:CD1	2.68	0.42
1:B:836:ALA:O	1:B:839:ASP:HB2	2.19	0.42
1:B:844:PHE:HA	1:B:854:PRO:HA	2.02	0.41
1:B:1100:SER:O	1:B:1101:ASP:C	2.63	0.41
1:B:805:GLN:NE2	3:B:1413:HOH:O	2.52	0.41
1:B:943:PRO:HG3	1:B:1007:LEU:O	2.20	0.41
1:B:1022:MET:HA	1:B:1022:MET:CE	2.44	0.41
1:A:945:ARG:HD3	1:A:945:ARG:HA	1.85	0.41
1:A:701:LEU:O	1:A:702:TYR:HB2	2.21	0.41
1:A:781[B]:MET:HG3	1:A:819:PRO:HG3	2.03	0.41
1:A:932:VAL:CG1	1:A:936:THR:HG22	2.50	0.41
1:A:1190:GLU:HA	1:A:1190:GLU:OE1	2.20	0.41
1:A:743:ARG:NE	1:A:856:TRP:HA	2.36	0.41
1:B:1063:LYS:HD2	1:B:1103:VAL:HG23	2.01	0.41
1:A:959:MET:SD	1:A:1005:PHE:CE2	3.13	0.41
1:B:731:ILE:HA	1:B:732:PRO:HD3	1.90	0.41
1:B:839:ASP:HA	1:B:842:LEU:HD12	2.02	0.41
1:B:939:ILE:O	1:B:983:LYS:HA	2.21	0.41
1:B:1021:HIS:HB3	1:B:1041:LEU:HD22	2.02	0.41
1:A:460:ALA:HB3	1:A:463:ALA:HB2	2.03	0.41
1:B:1063:LYS:HD2	1:B:1103:VAL:HG21	2.03	0.41
1:B:554:ILE:O	1:B:554:ILE:CG2	2.69	0.41
1:A:584:GLY:HA2	1:A:655:ARG:NH1	2.36	0.40
1:B:530:VAL:HB	1:B:532:LEU:CD2	2.48	0.40
1:A:1066:ASN:ND2	3:A:1403:HOH:O	2.54	0.40
1:B:914:THR:HA	3:B:1435:HOH:O	2.21	0.40
1:A:654:PHE:C	1:A:655:ARG:NE	2.75	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	725/803 (90%)	706 (97%)	19 (3%)	0	100	100
1	B	723/803 (90%)	707 (98%)	16 (2%)	0	100	100
All	All	1448/1606 (90%)	1413 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	577/704 (82%)	577 (100%)	0	100	100
1	B	604/704 (86%)	604 (100%)	0	100	100
All	All	1181/1408 (84%)	1181 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	650	HIS
1	A	712	ASN
1	A	716	ASN
1	A	786	ASN
1	A	882	ASN
1	A	907	ASN

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Mol	Chain	Res	Type
1	A	1021	HIS
1	A	1032	GLN
1	A	1197	GLN
1	B	524	ASN
1	B	558	GLN
1	B	583	HIS
1	B	801	GLN
1	B	811	HIS
1	B	890	ASN
1	B	935	ASN
1	B	1065	ASN
1	B	1160	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	ACT	A	1304	-	3,3,3	1.01	0	3,3,3	0.81	0
2	ACT	A	1301	-	3,3,3	0.97	0	3,3,3	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	B	1301	-	3,3,3	0.99	0	3,3,3	0.78	0
2	ACT	B	1304	-	3,3,3	0.98	0	3,3,3	0.87	0
2	ACT	B	1303	-	3,3,3	0.98	0	3,3,3	0.89	0
2	ACT	A	1303	-	3,3,3	0.98	0	3,3,3	0.86	0
2	ACT	A	1305	-	3,3,3	0.98	0	3,3,3	0.85	0
2	ACT	A	1302	-	3,3,3	0.98	0	3,3,3	0.91	0
2	ACT	B	1302	-	3,3,3	0.99	0	3,3,3	0.81	0

There are no bond length outliers.

There are no bond angle outliers.

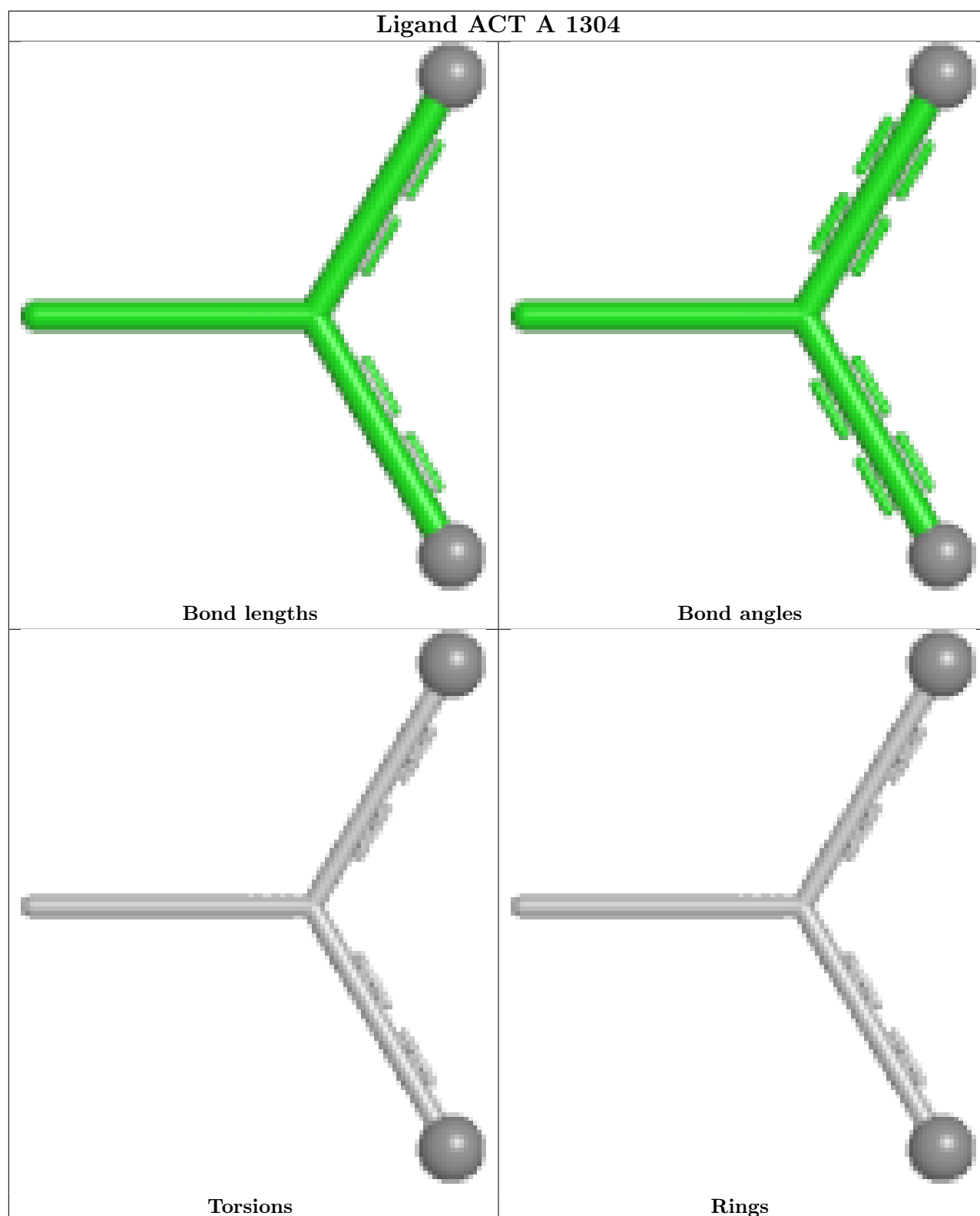
There are no chirality outliers.

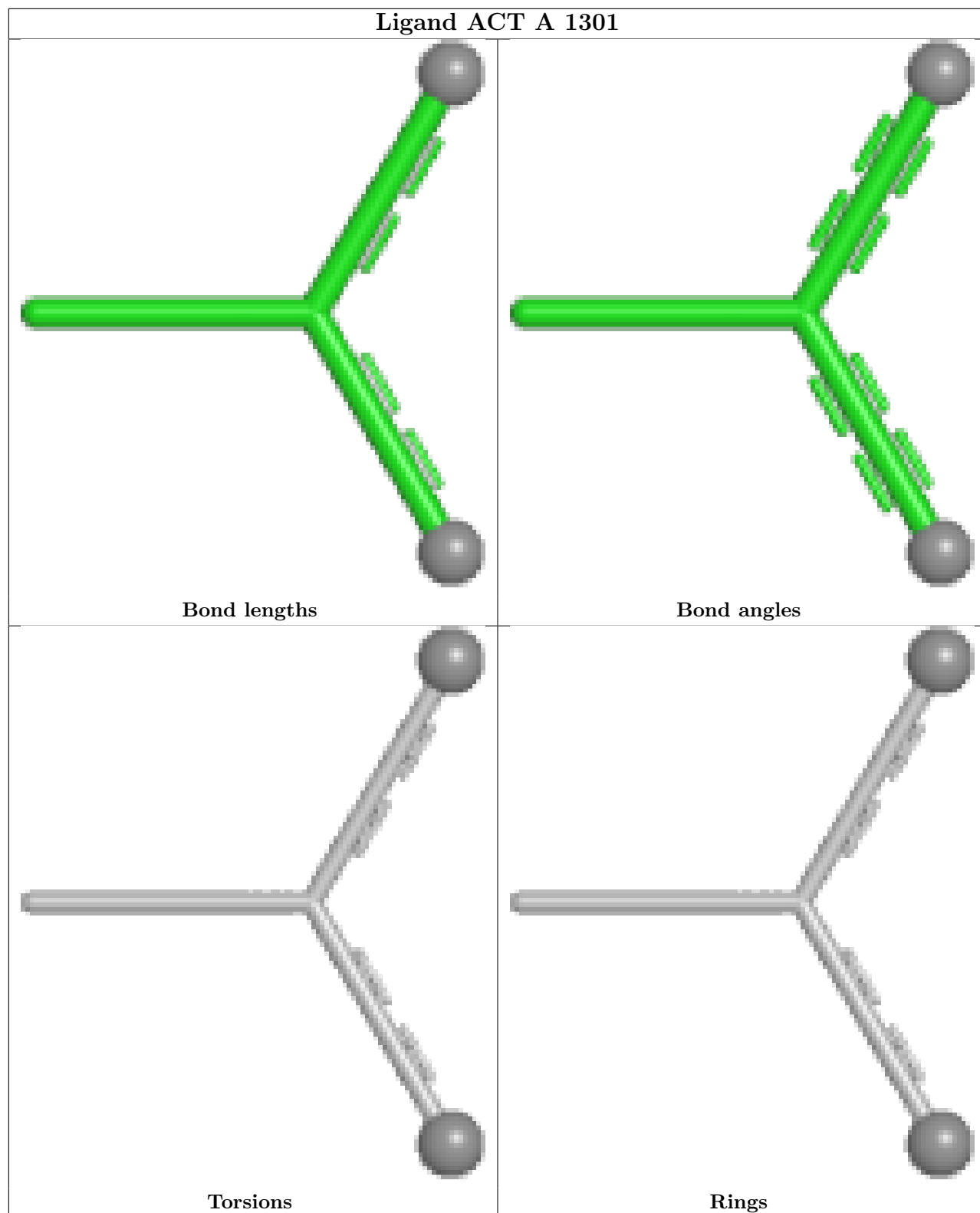
There are no torsion outliers.

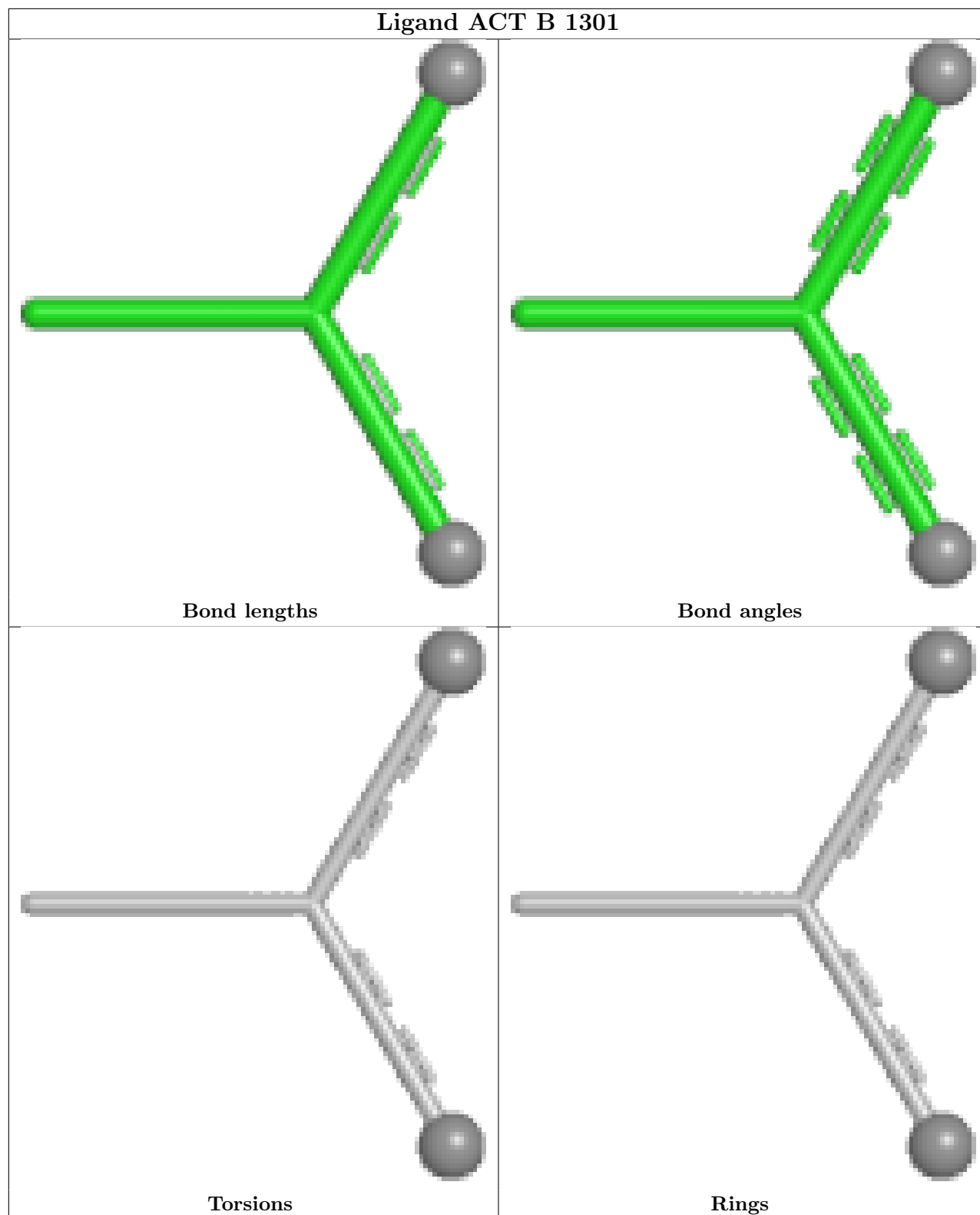
There are no ring outliers.

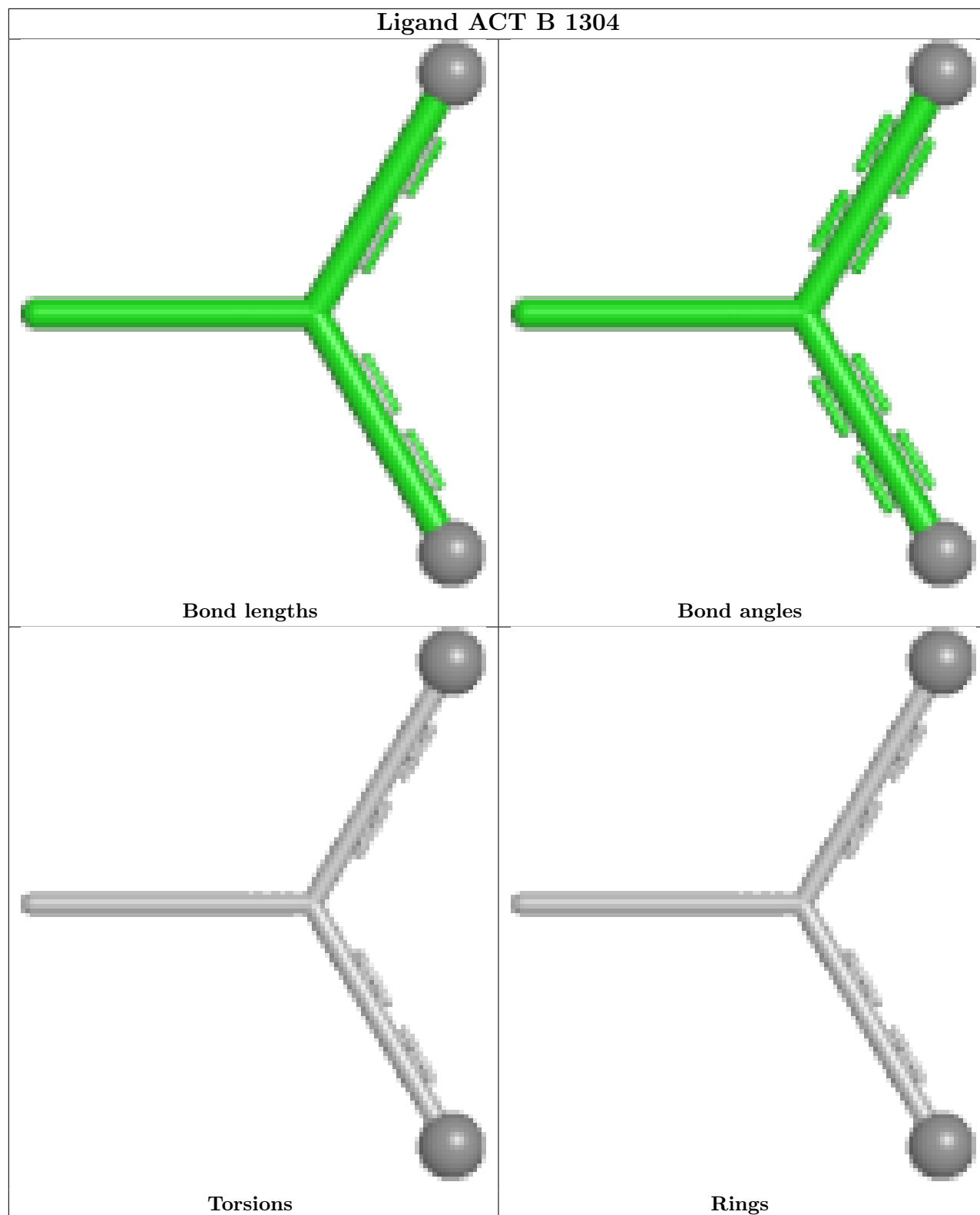
No monomer is involved in short contacts.

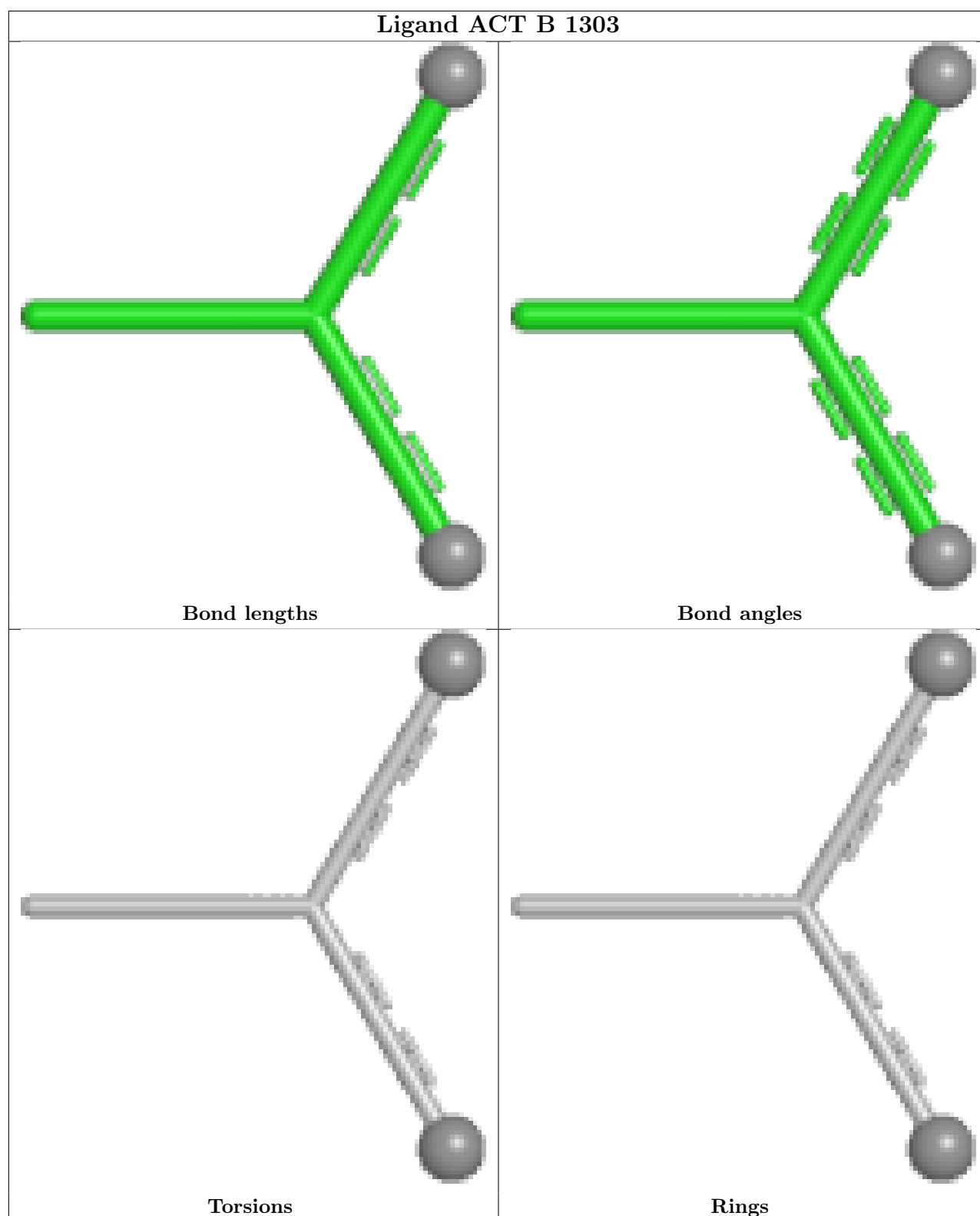
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

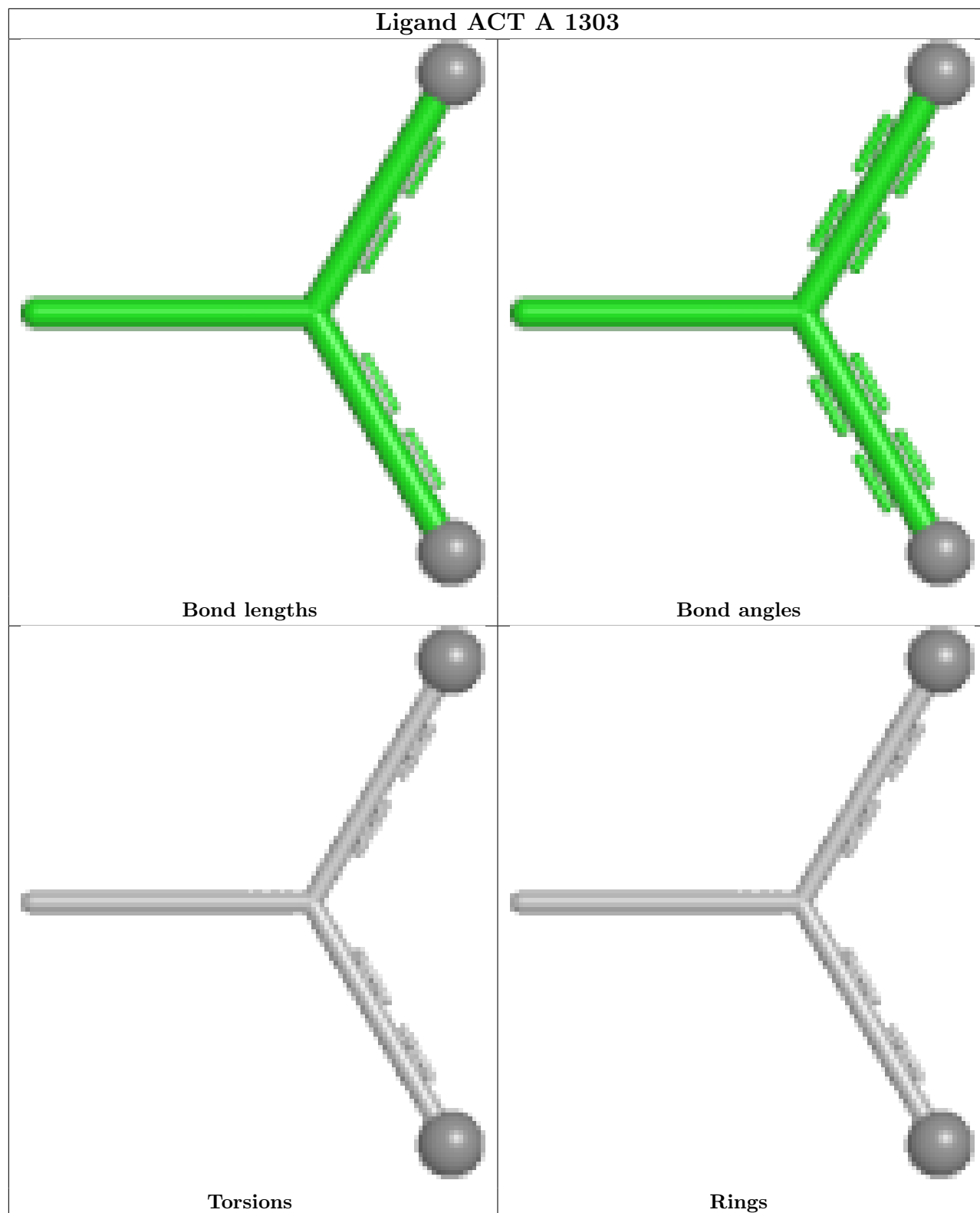


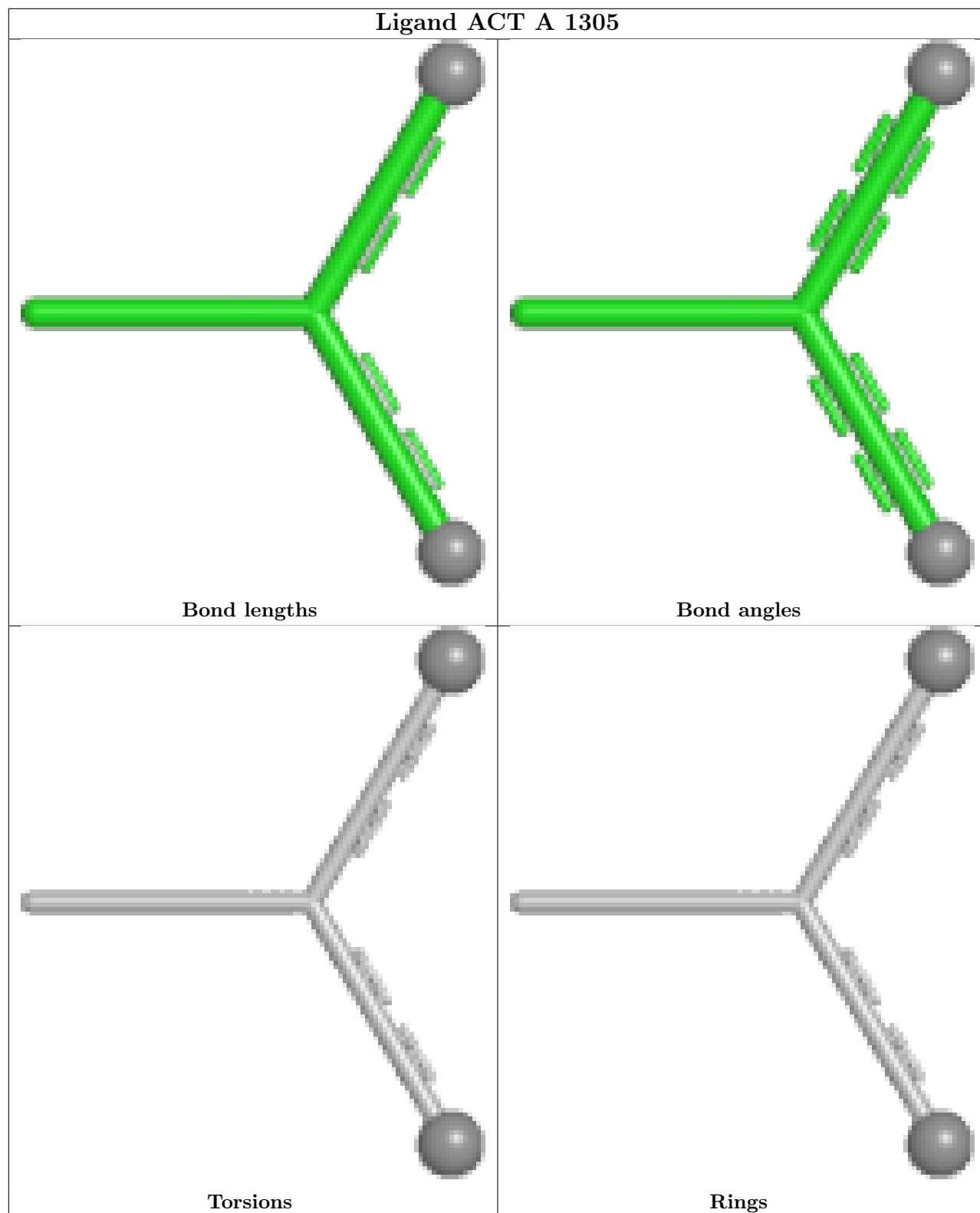


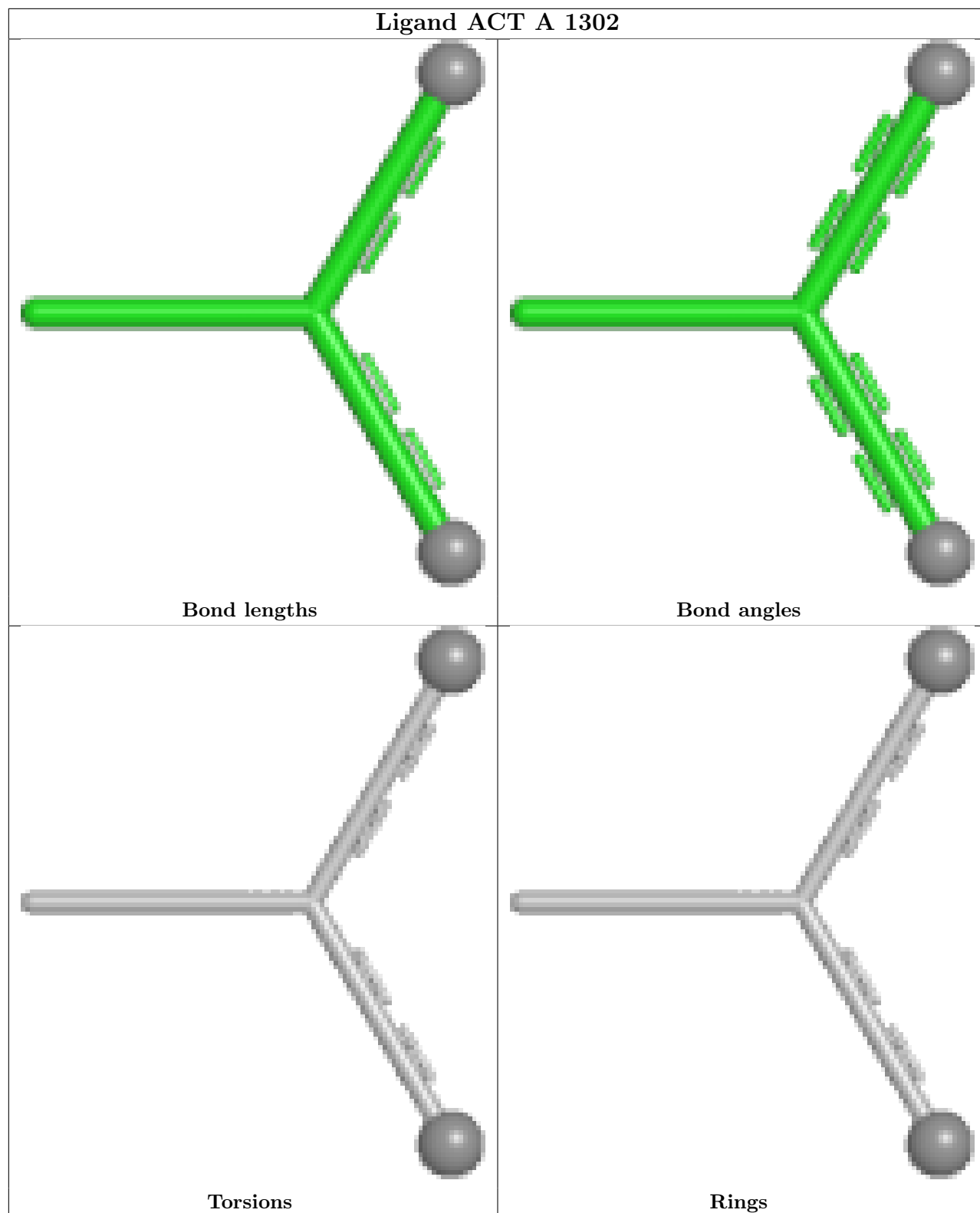


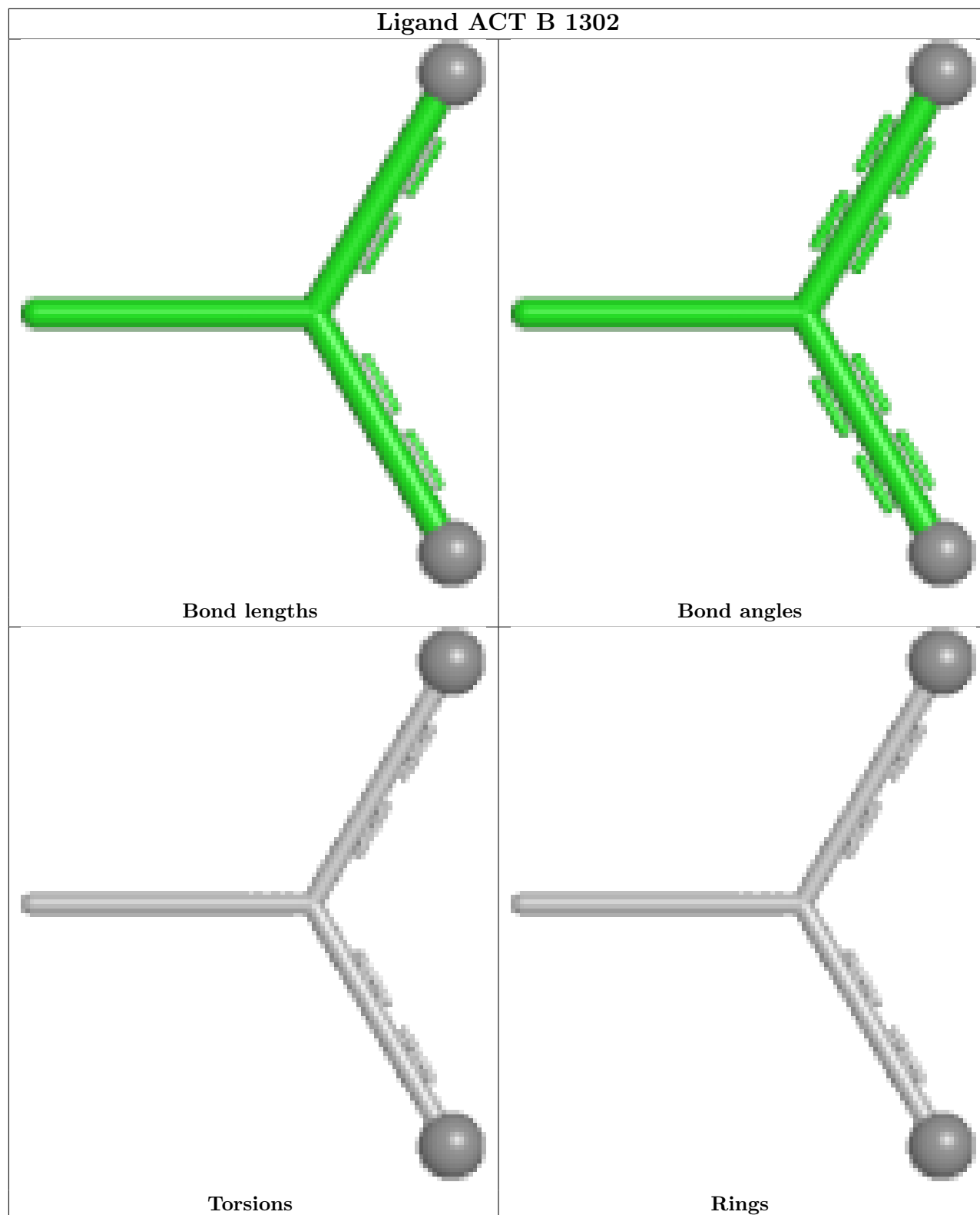












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	729/803 (90%)	-0.24	15 (2%) 63 54	25, 58, 100, 123	2 (0%)
1	B	728/803 (90%)	-0.33	8 (1%) 78 70	23, 56, 97, 123	3 (0%)
All	All	1457/1606 (90%)	-0.29	23 (1%) 70 61	23, 58, 98, 123	5 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	961	ASN	4.1
1	A	921	ASN	3.3
1	A	619	GLU	3.1
1	A	703	GLY	2.9
1	A	620	ASN	2.9
1	A	960	LEU	2.8
1	A	1113	ALA	2.8
1	B	704	THR	2.7
1	A	655	ARG	2.6
1	B	1113	ALA	2.5
1	B	703	GLY	2.5
1	B	706	THR	2.5
1	A	621	GLN	2.3
1	A	920	GLN	2.3
1	B	921	ASN	2.2
1	A	1134	SER	2.2
1	A	967	PRO	2.2
1	A	535	LYS	2.2
1	A	492	ILE	2.1
1	A	599	ASN	2.1
1	B	1203	ALA	2.1
1	B	467	HIS	2.0
1	B	540	ASP	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](#)

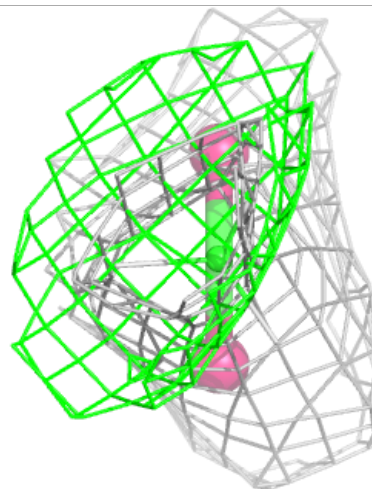
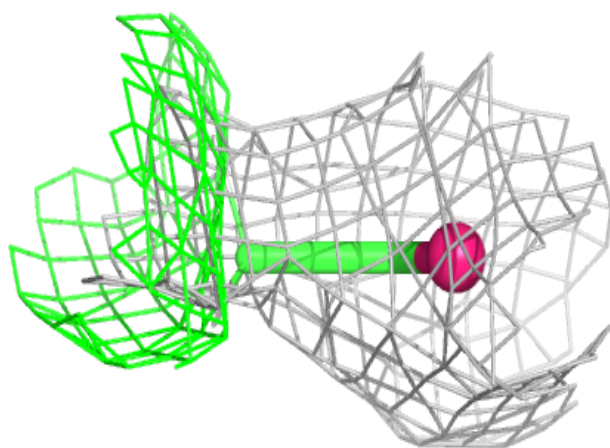
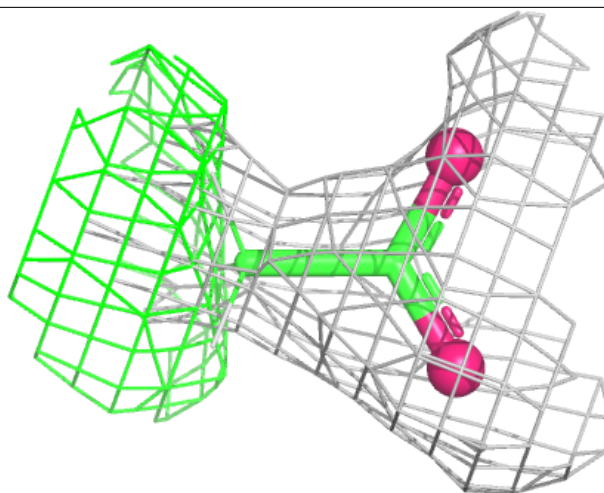
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	B	1301	4/4	0.47	0.21	83,100,104,104	0
2	ACT	A	1302	4/4	0.67	0.15	60,68,72,75	0
2	ACT	A	1301	4/4	0.69	0.32	71,76,85,85	0
2	ACT	B	1303	4/4	0.76	0.14	65,68,81,81	0
2	ACT	A	1304	4/4	0.83	0.14	64,69,83,83	0
2	ACT	A	1305	4/4	0.85	0.15	68,80,96,96	0
2	ACT	A	1303	4/4	0.88	0.08	49,57,59,60	0
2	ACT	B	1302	4/4	0.90	0.09	50,54,64,64	0
2	ACT	B	1304	4/4	0.92	0.10	51,59,62,62	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.

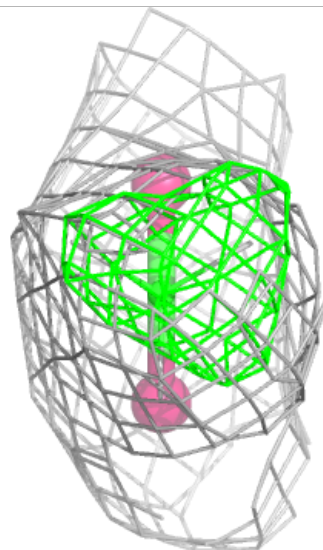
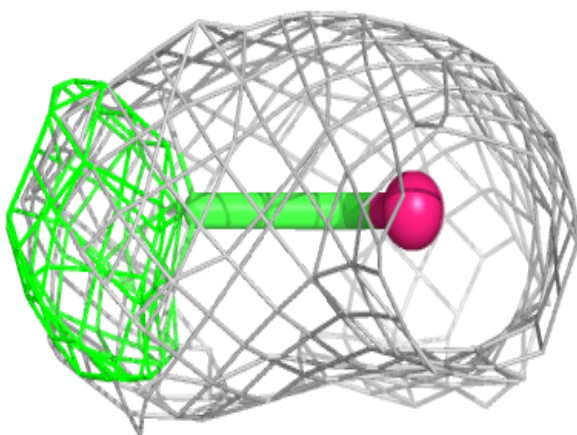
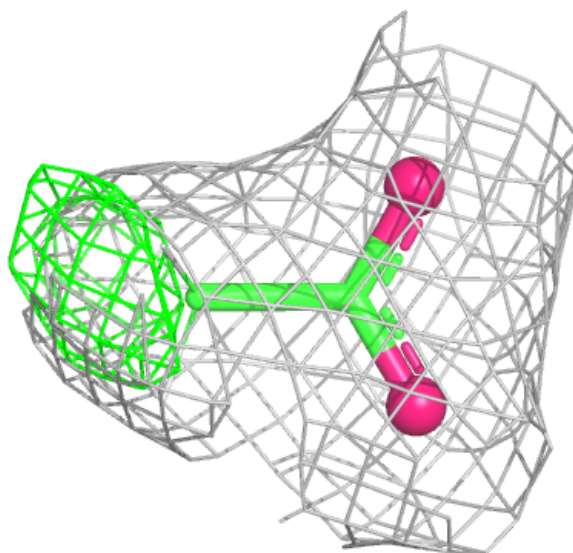
Electron density around ACT B 1301:

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



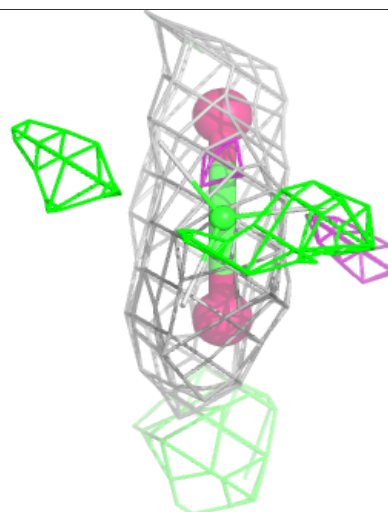
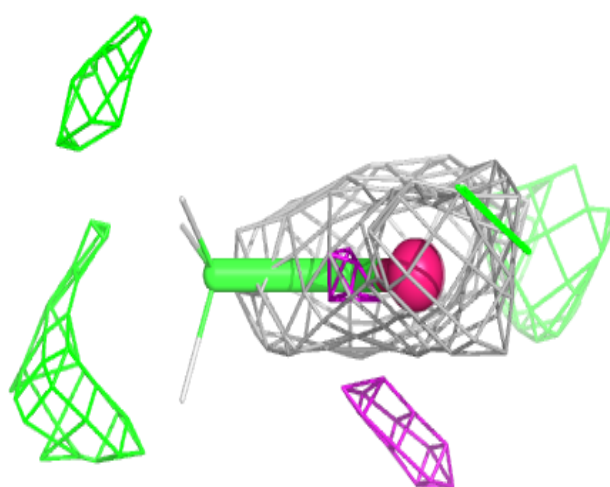
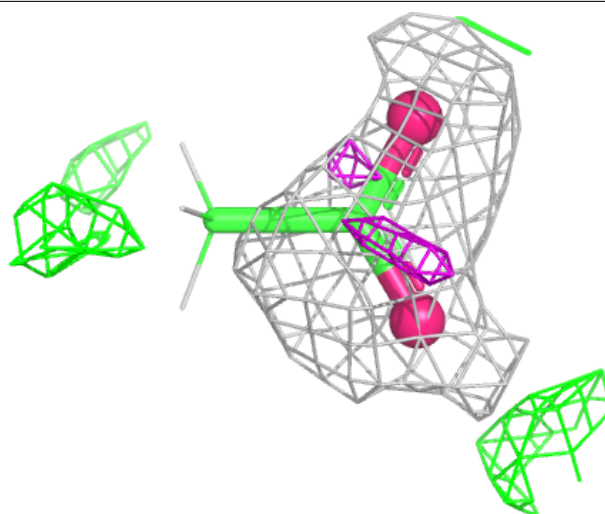
Electron density around ACT A 1302:

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



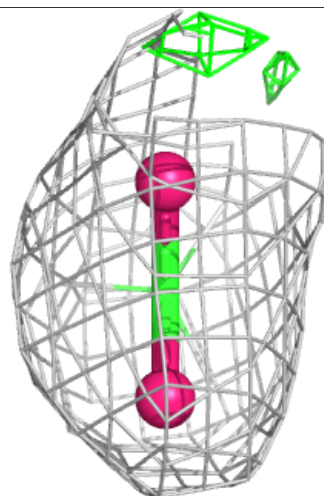
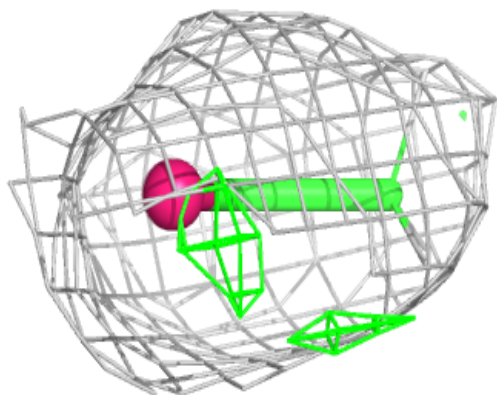
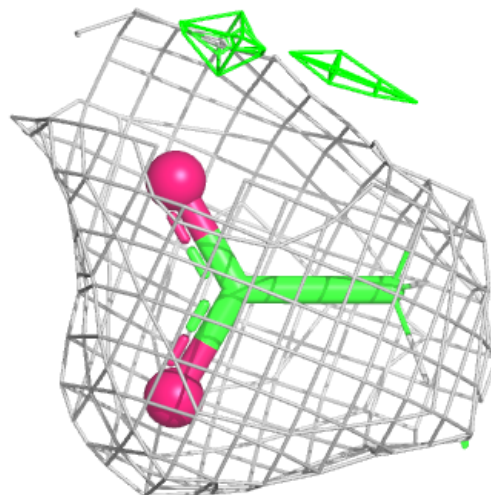
Electron density around ACT A 1301:

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



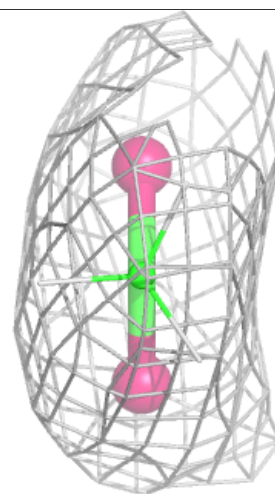
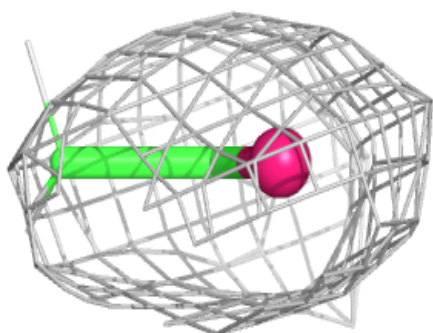
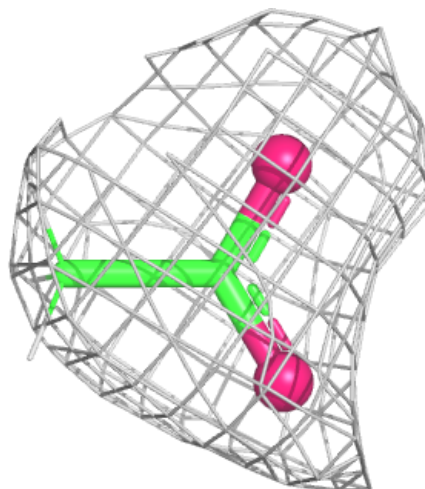
Electron density around ACT B 1303:

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



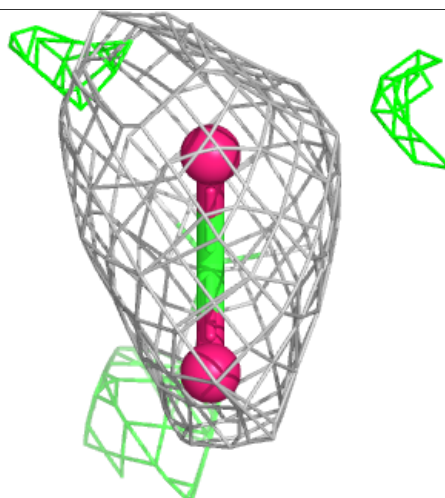
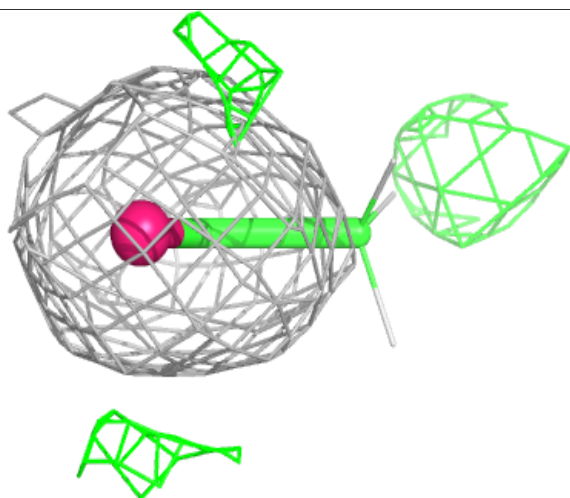
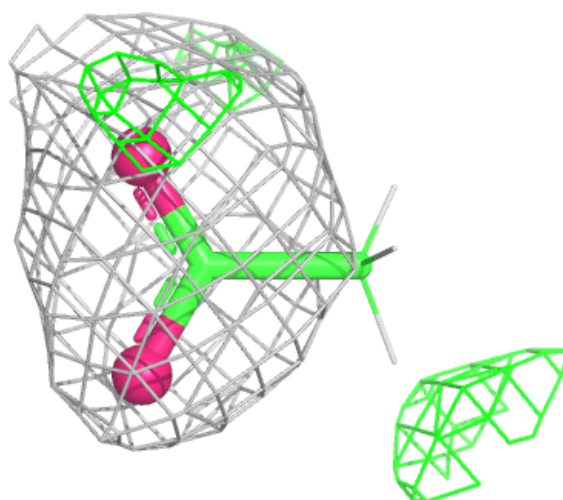
Electron density around ACT A 1304:

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



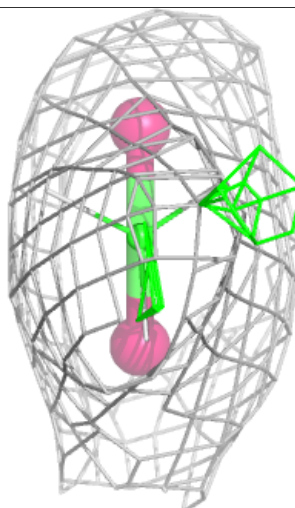
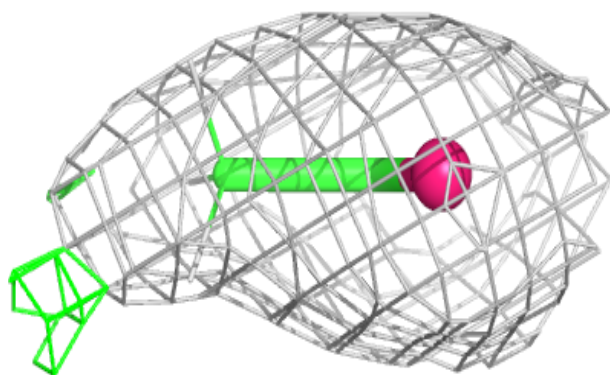
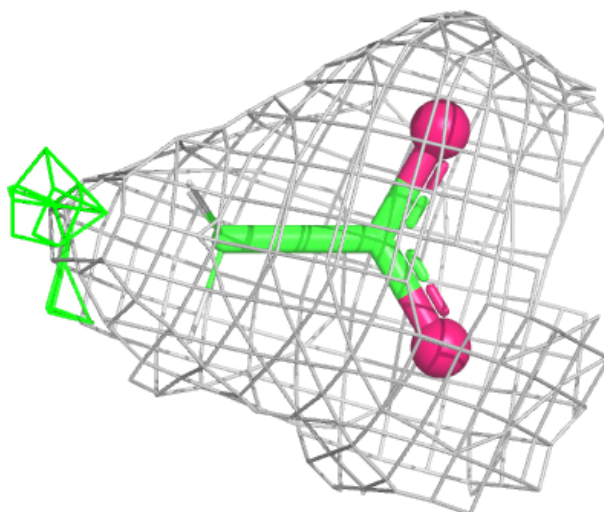
Electron density around ACT A 1305:

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



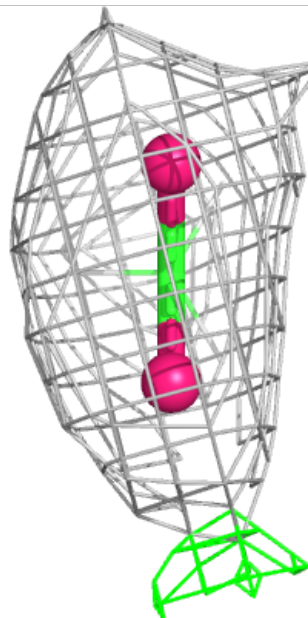
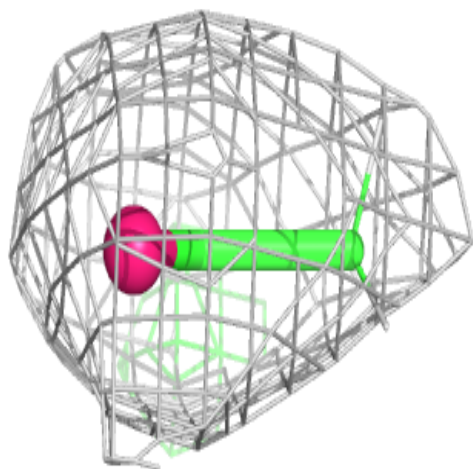
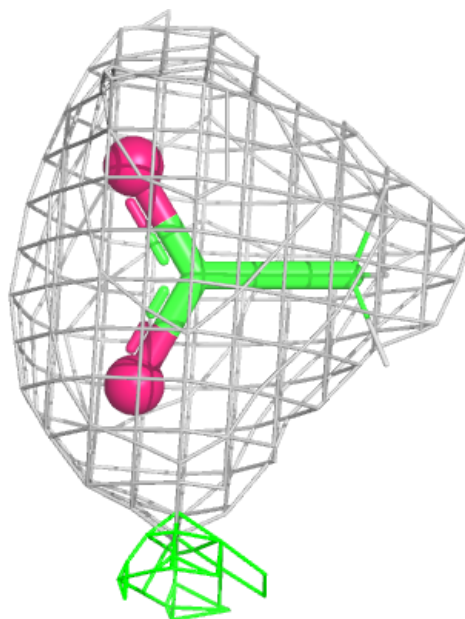
Electron density around ACT A 1303:

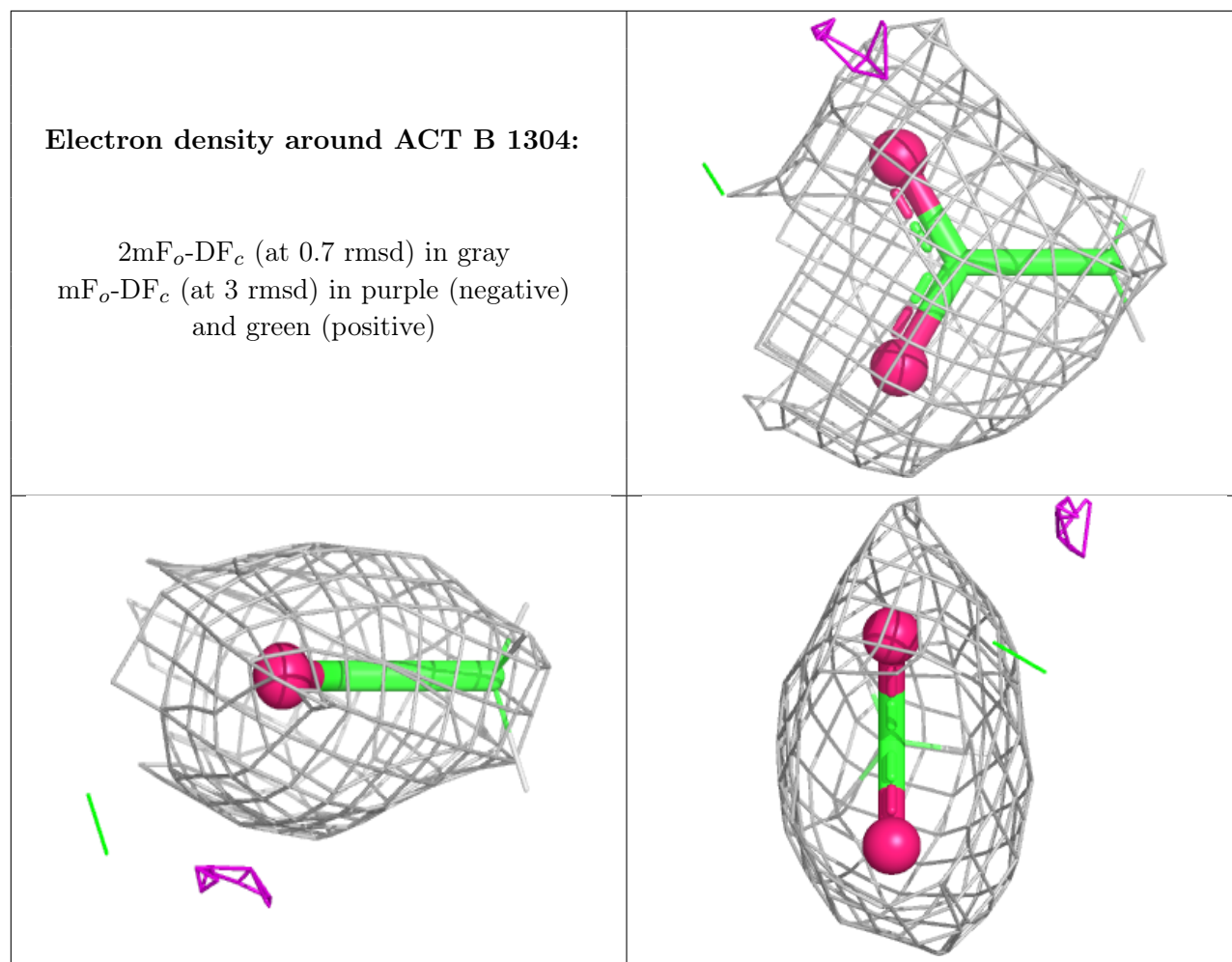
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ACT B 1302:

$2mF_o-DF_c$ (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.