Full wwPDB X-ray Structure Validation Report ⓘ

Jul 16, 2024 – 04:14 PM JST

PDB ID	:	8KE7
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:

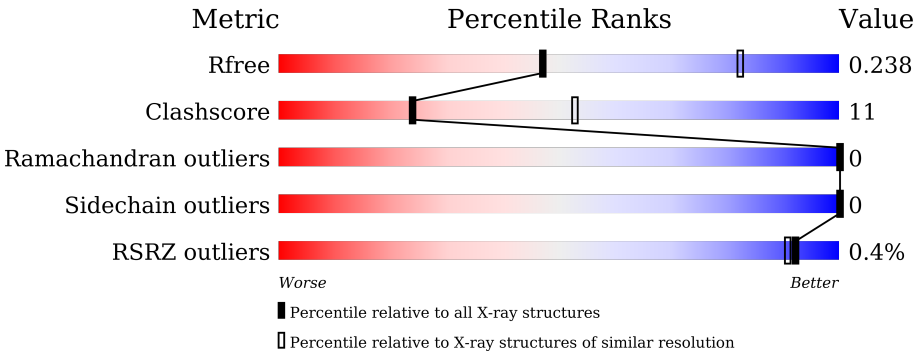
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	67% 24% 9%
1	B	803	72% 19% 9%

2 Entry composition (i)

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 5714 3654 970 1065 25	0	2	0
1	B	728	Total C H N O S 5846 3688 74 976 1082 26	0	3	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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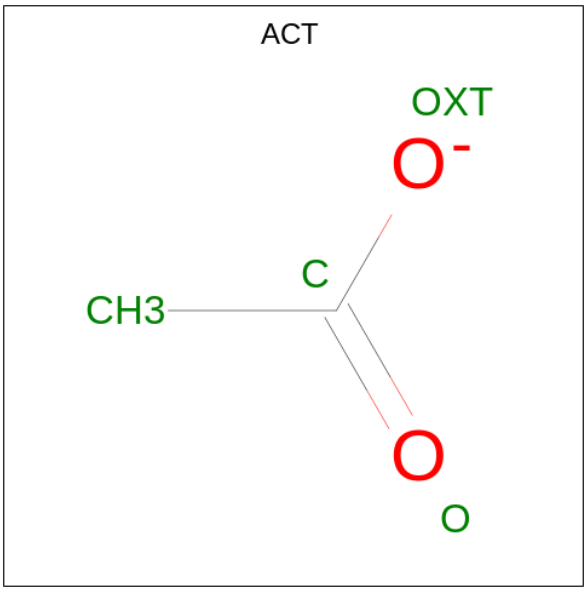
Chain	Residue	Modelled	Actual	Comment	Reference
B	440	PRO	-	expression tag	UNP Q02880
B	441	THR	-	expression tag	UNP Q02880
B	442	SER	-	expression tag	UNP Q02880
B	443	VAL	-	expression tag	UNP Q02880
B	444	ASP	-	expression tag	UNP Q02880
B	1202	GLY	-	expression tag	UNP Q02880
B	1203	ALA	-	expression 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 (three-letter code: 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 7 2 3 2	0	0
2	A	1	Total C H O 7 2 3 2	0	0
2	A	1	Total C H O 7 2 3 2	0	0
2	A	1	Total C H O 7 2 3 2	0	0
2	A	1	Total C H O 7 2 3 2	0	0
2	B	1	Total C H O 7 2 3 2	0	0
2	B	1	Total C H O 7 2 3 2	0	0
2	B	1	Total C H O 7 2 3 2	0	0
2	B	1	Total C H O 7 2 3 2	0	0

- Molecule 3 is water.

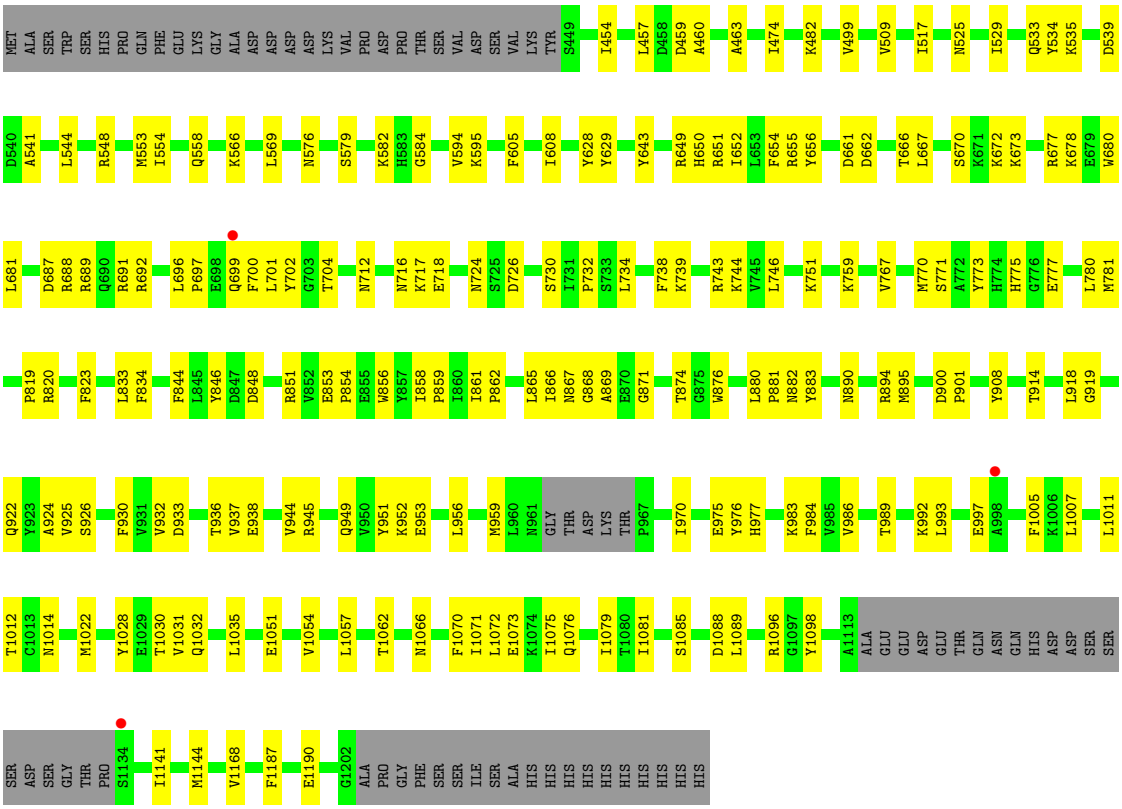
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	59	Total O 59 59	0	0
3	B	85	Total O 85 85	0	0

3 Residue-property plots (i)

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.

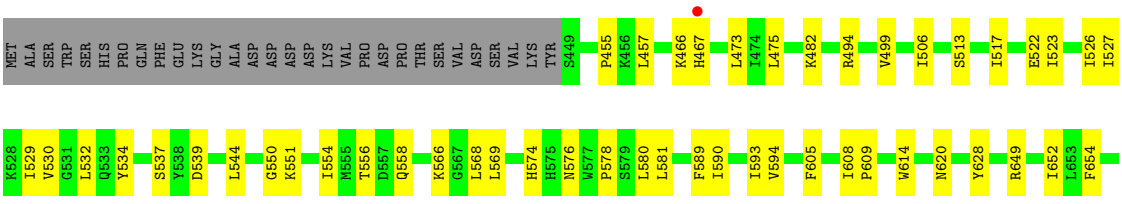
• Molecule 1: DNA topoisomerase 2-beta

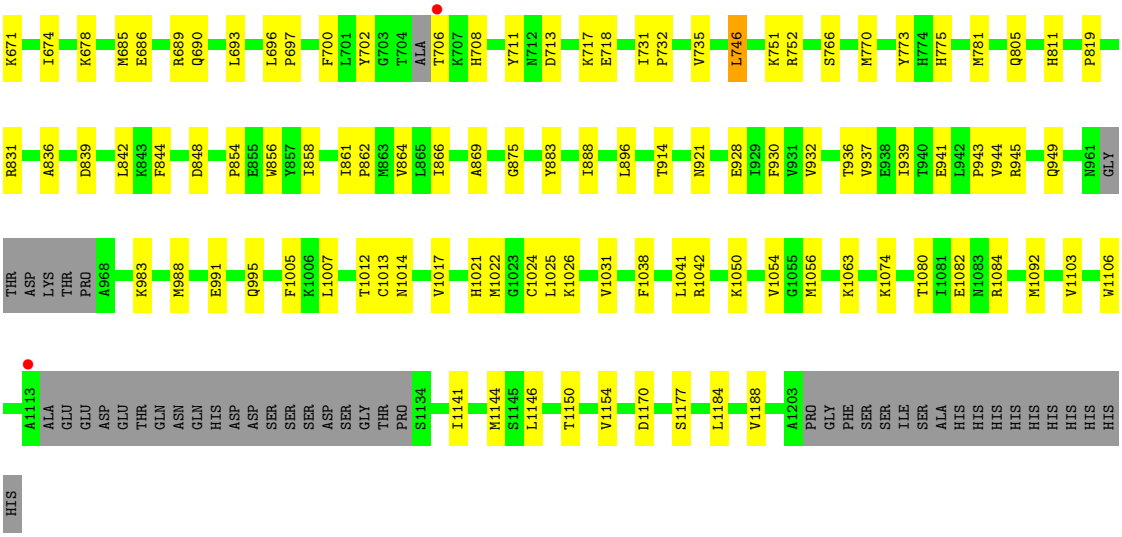
Chain A:



• Molecule 1: DNA topoisomerase 2-beta

Chain B:




K671 I674 K678 M685 E686 R689 Q690 L693 L696 P697 F700 L701 Y702 G703 T704 ALA T706 K707 H708 Y711 N712 D713 K717 E718 I731 P732 V735 L746 K751 R752 S766 M770 Y773 H774 H775 M781 Q805 H811 P819
R831 A836 D839 L842 K843 F844 D848 P854 E855 W856 Y857 I858 I861 P862 M863 V864 L865 I866 A869 G875 Y883 I888 L896 T914 N921 E928 I929 F930 V931 V932 T936 V937 E938 I939 T940 E941 L942 P943 V944 R945 Q949 N961 GLY
THR ASP LYS THR PRO A968 K983 M988 E991 Q995 F1005 K1006 L1007 T1012 C1013 N1014 V1017 H1021 M1022 G1023 C1024 L1025 K1026 V1031 F1038 L1041 R1042 K1050 V1054 G1055 M1056 K1063 K1074 T1080 I1081 E1082 N1083 R1084 M1092 V1103 W1106
A1113 ALA GLU GLU ASP GLU THR GLN ASN GLN HIS ASP ASP SER SER SER ASP SER GLY THR PRO S1134 I1141 M1144 S1145 L1146 T1150 V1154 D1170 S1177 L1184 V1188 A1203 PRO GLY PHE SER SER ILE SER ALA HIS HIS HIS HIS HIS HIS HIS HIS
HIS

4 Data and refinement statistics (i)

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) 98.2 (19.83-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.194 , 0.238 0.194 , 0.238	Depositor DCC
R_{free} test set	2000 reflections (3.42%)	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 , 32.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.27	0/5828	0.50	0/7879
1	B	0.32	1/5886 (0.0%)	0.53	3/7948 (0.0%)
All	All	0.30	1/11714 (0.0%)	0.52	3/15827 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	522	GLU	CD-OE2	9.40	1.35	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1170	ASP	CB-CG-OD1	-7.90	111.19	118.30
1	B	522	GLU	OE1-CD-OE2	6.79	131.44	123.30
1	B	746	LEU	CB-CG-CD1	-5.09	102.34	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5714	0	5519	147	0
1	B	5772	74	5651	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	253	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 11.

All (253) 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: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:1012:THR:HG22	1:A:1014:ASN:H	1.39	0.88
1:B:944:VAL:HG12	1:B:945:ARG:HG2	1.61	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:A:554:ILE:HD12	1:A:569:LEU:HD22	1.70	0.73
1:B:988:MET:HE3	1:B:1005:PHE:HZ	1.54	0.72
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
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:582:LYS:HG2	1:A:656:TYR:CD2	2.30	0.67
1:A:726:ASP:HB3	1:A:874:THR:OG1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:751:LYS:CD	1:A:770:MET:HE1	2.27	0.65
1:B:558:GLN:OE1	1:B:590:ILE:HG23	1.96	0.65
1:A:751:LYS:HD3	1:A:770:MET:HE1	1.79	0.65
1:B:593:ILE:HD12	1:B:702:TYR:O	1.97	0.64
1:A:751:LYS:CG	1:A:770:MET:HE1	2.27	0.64
1:A:1071:ILE:O	1:A:1075:ILE:HG12	1.97	0.64
1:A:751:LYS:HB3	1:A:770:MET:HE1	1.80	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: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:895:MET:CE	1:A:1035:LEU:HG	2.30	0.62
1:A:670:SER:HB3	1:A:673:LYS:HG3	1.81	0.62
1:B:1141:ILE:HA	1:B:1144:MET:HE2	1.82	0.61
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: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: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:B:988:MET:HE3	1:B:1005:PHE:CZ	2.36	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
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:867:ASN:C	1:A:882:ASN:ND2	2.57	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:ILE:O	1:A:1144:MET:HG3	2.03	0.58
1:A:1073:GLU:CD	1:A:1096:ARG:HH12	2.07	0.57
1:A:751:LYS:CB	1:A:770:MET:HE1	2.34	0.57
1:B:921:ASN:HB3	1:B:1013:CYS:HB2	1.85	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:654:PHE:C	1:A:655:ARG:HE	2.08	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:895:MET:HE3	1:A:1035:LEU:HG	1.90	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:914:THR:HG1	1:A:926:SER:HG	1.58	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:975:GLU:HG2	1:A:977:HIS:NE2	2.25	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: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:685:MET:CE	1:B:1025:LEU:HD12	2.41	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:643:TYR:HA	1:A:650:HIS:CE1	2.48	0.49
1:A:895:MET:HE1	1:A:1035:LEU:HG	1.94	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: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:B:1022:MET:HA	1:B:1022:MET:CE	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:589:PHE:C	1:B:590:ILE:HD13	2.34	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: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:A:781[B]:MET:HE2	1:A:819:PRO:HG2	1.98	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: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: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:933:ASP:OD1	1:A:933:ASP:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:993:LEU:HD23	1:A:993:LEU:C	2.39	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:667:LEU:HA	1:A:673:LYS:HD2	1.99	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: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:685:MET:HE1	1:B:1025:LEU:HD12	2.00	0.42
1:B:928:GLU:HB2	1:B:941:GLU:HB3	2.01	0.42
1:B:1022:MET:HA	1:B:1022:MET:HE2	2.02	0.42
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:672:LYS:O	1:A:673:LYS:HG2	2.20	0.42
1:A:901:PRO:HG2	1:A:1032:GLN:CD	2.40	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:B:1074:LYS:HZ1	1:B:1082:GLU:CD	2.23	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781[B]:MET:CE	1:A:819:PRO:HG2	2.51	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:A:868:GLY:N	1:A:882:ASN:ND2	2.69	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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	712	ASN
1	A	716	ASN
1	A	786	ASN
1	A	882	ASN
1	B	811	HIS
1	B	849	ASN
1	B	890	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides 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	1302	-	3,3,3	0.92	0	3,3,3	0.90	0
2	ACT	A	1303	-	3,3,3	0.92	0	3,3,3	0.85	0
2	ACT	B	1302	-	3,3,3	0.93	0	3,3,3	0.80	0
2	ACT	B	1304	-	3,3,3	0.92	0	3,3,3	0.86	0
2	ACT	A	1305	-	3,3,3	0.92	0	3,3,3	0.84	0
2	ACT	A	1304	-	3,3,3	0.95	0	3,3,3	0.80	0
2	ACT	B	1303	-	3,3,3	0.92	0	3,3,3	0.89	0
2	ACT	A	1301	-	3,3,3	0.91	0	3,3,3	0.91	0
2	ACT	B	1301	-	3,3,3	0.93	0	3,3,3	0.77	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

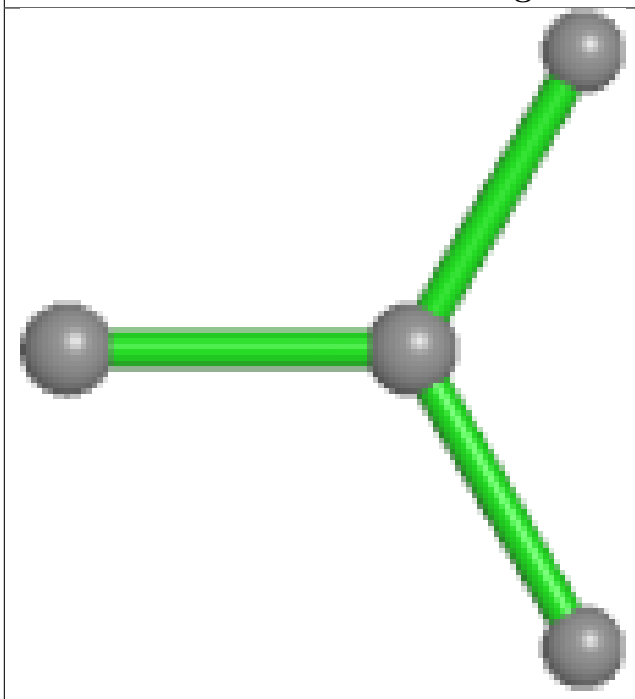
There are no torsion outliers.

There are no ring outliers.

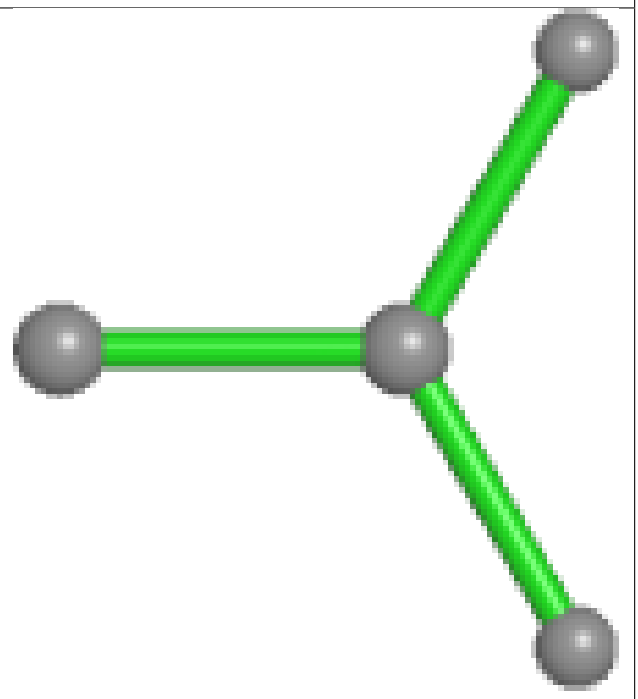
No monomer is involved in short contacts.

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 then 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.

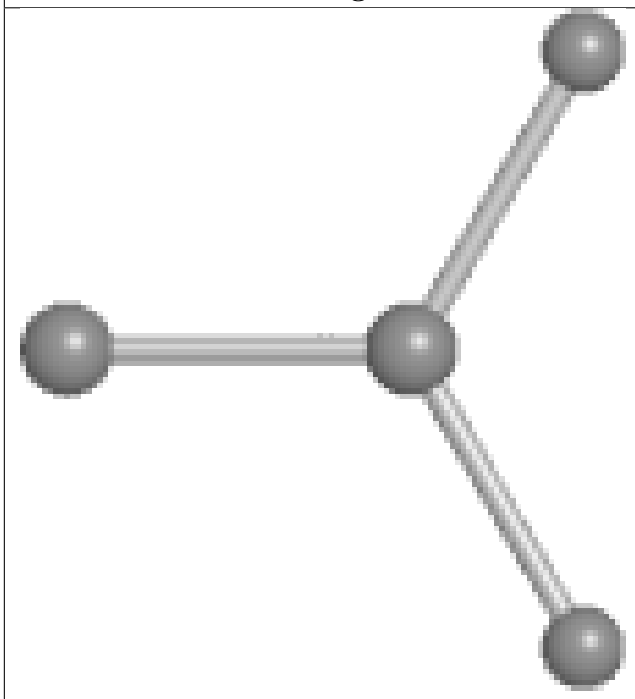
Ligand ACT A 1302



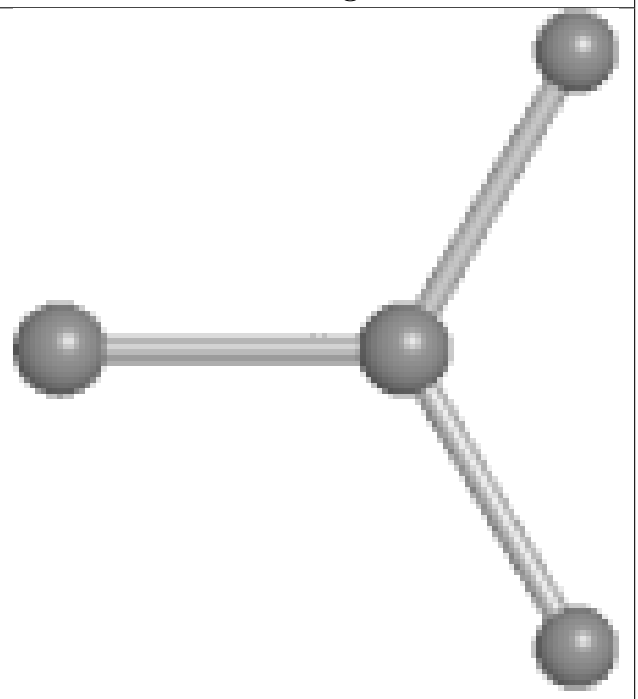
Bond lengths



Bond angles

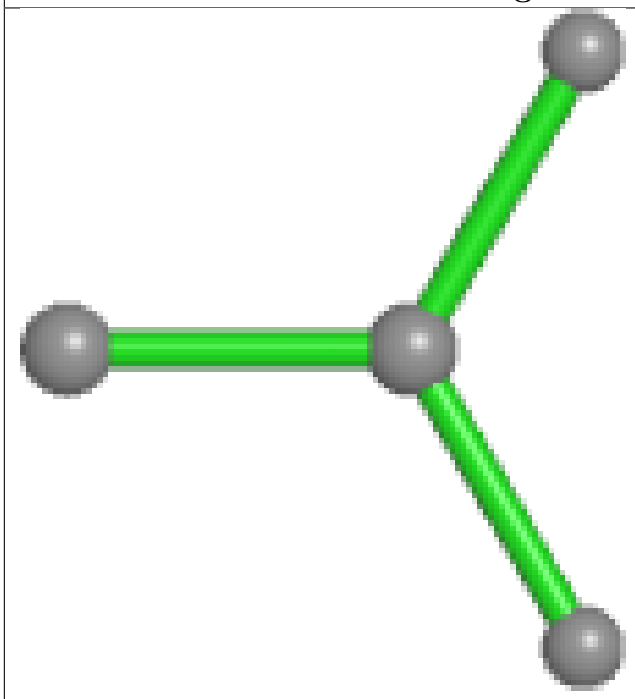


Torsions

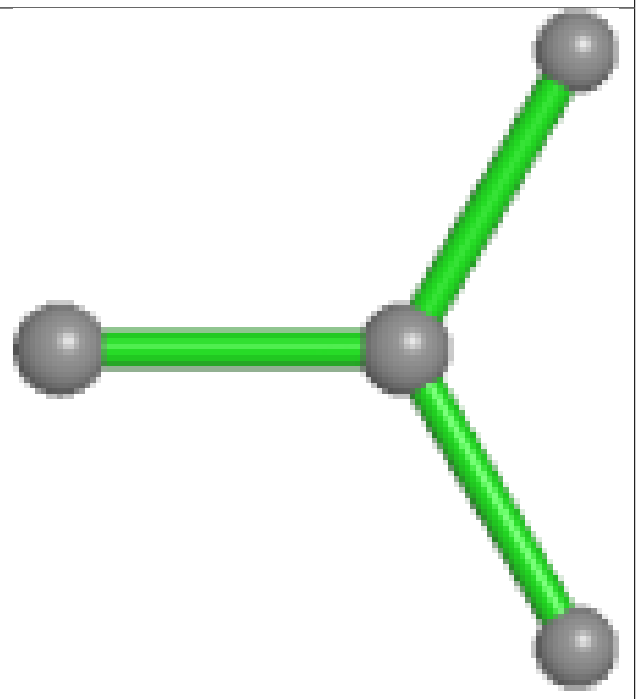


Rings

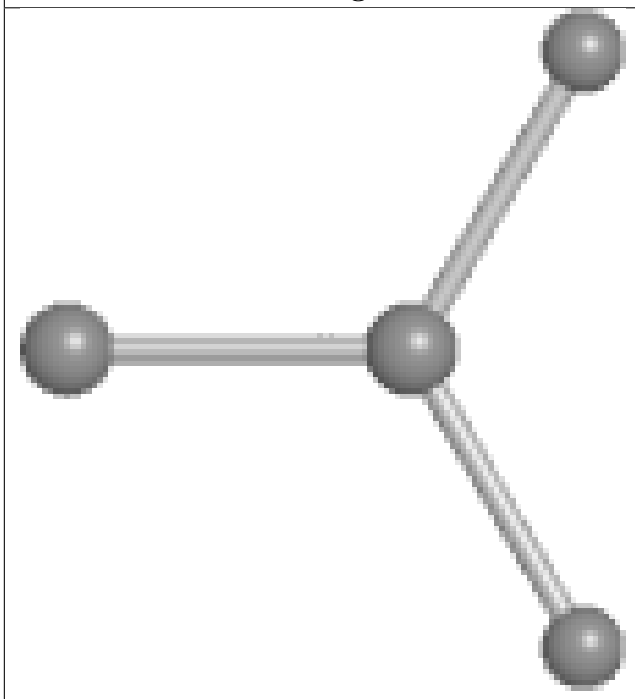
Ligand ACT A 1303



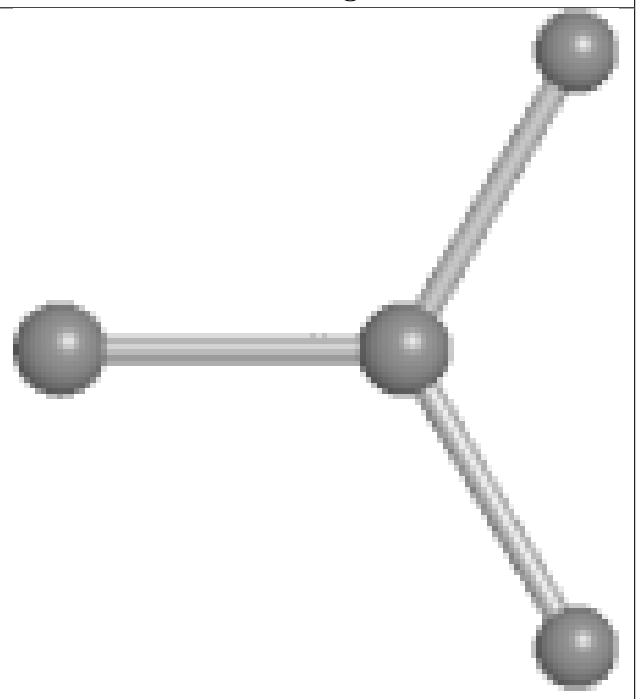
Bond lengths



Bond angles

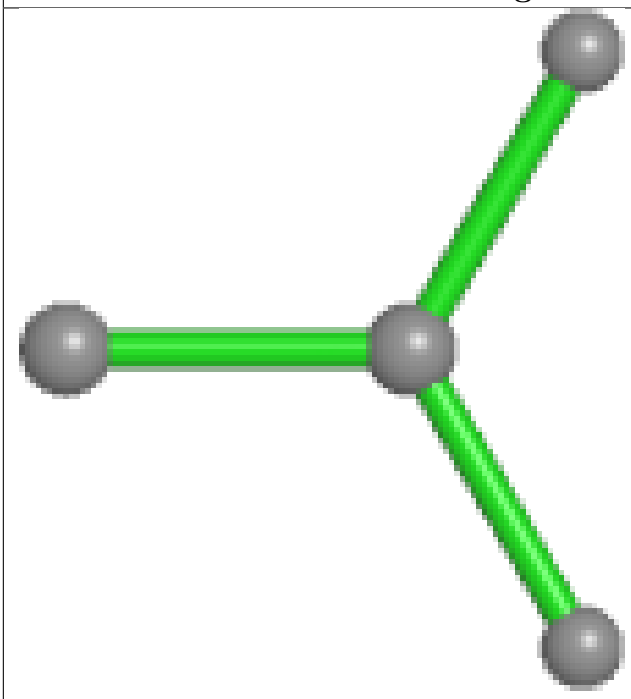


Torsions

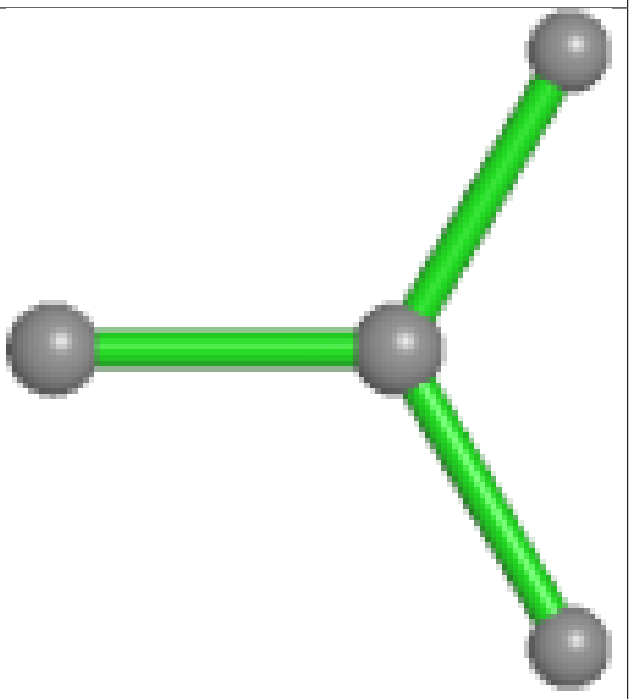


Rings

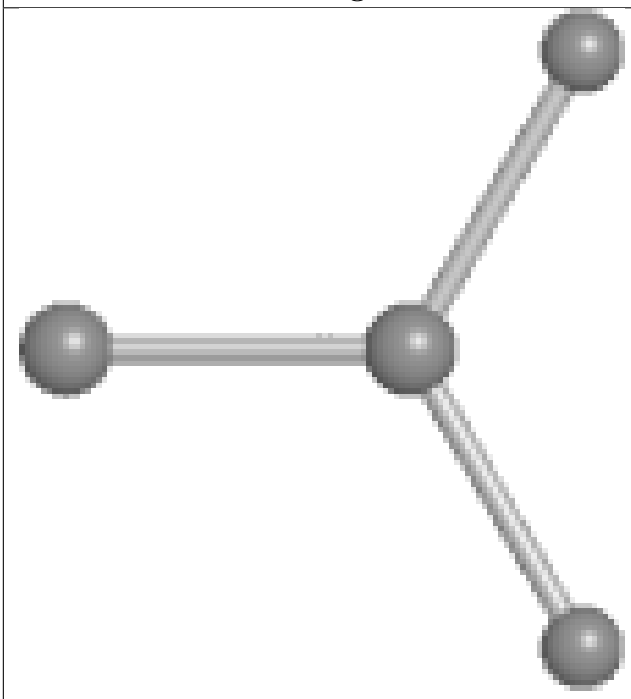
Ligand ACT B 1302



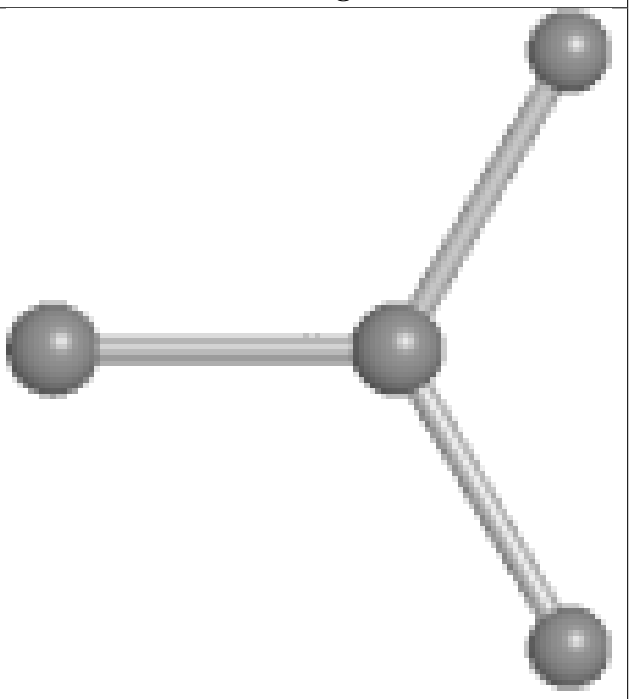
Bond lengths



Bond angles

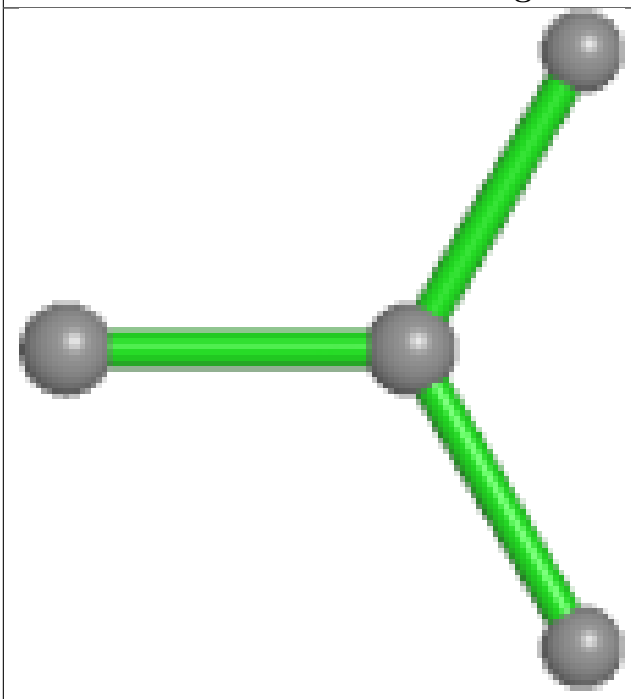


Torsions

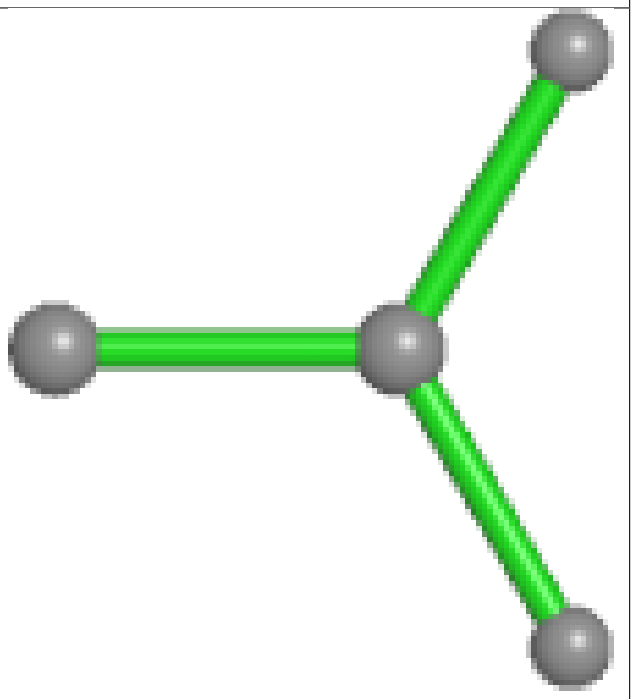


Rings

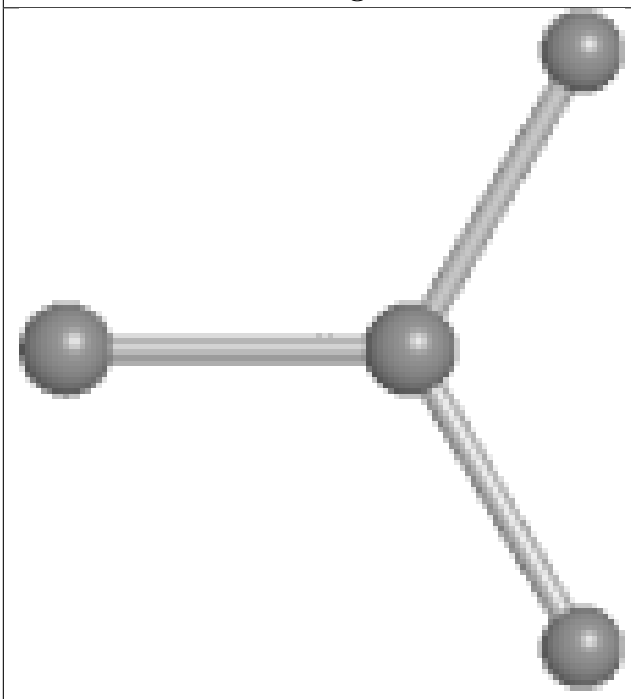
Ligand ACT B 1304



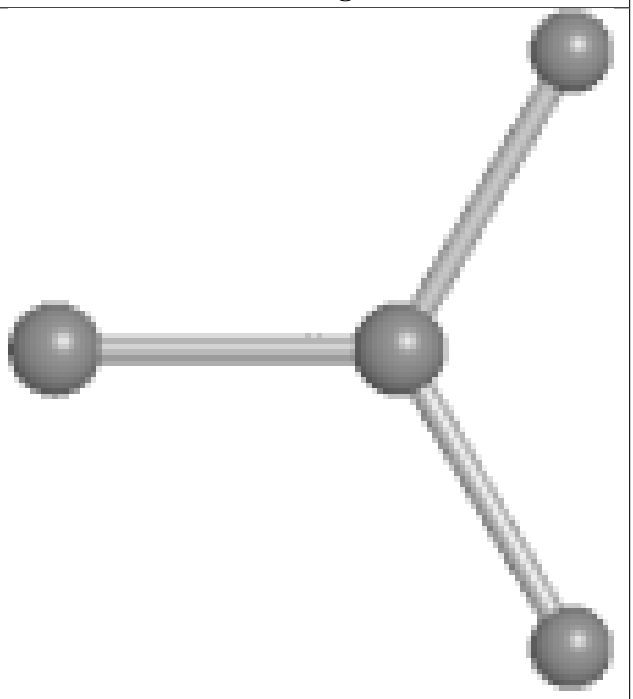
Bond lengths



Bond angles

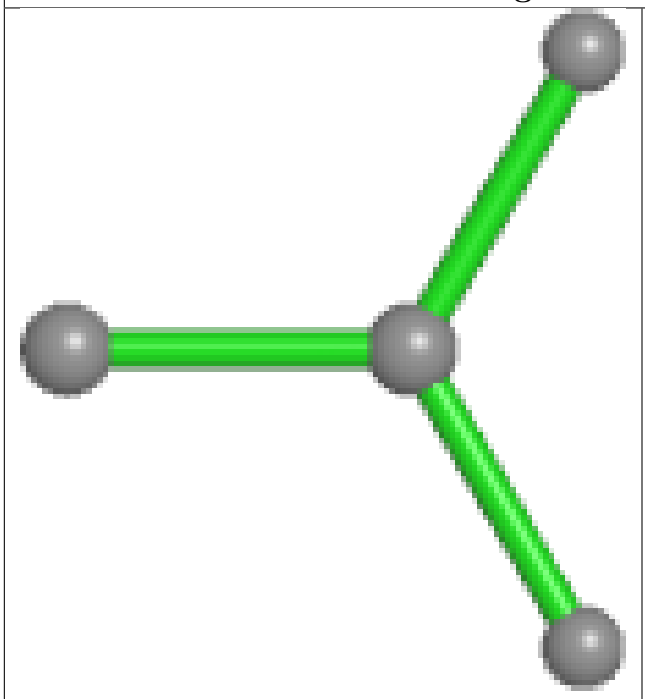


Torsions

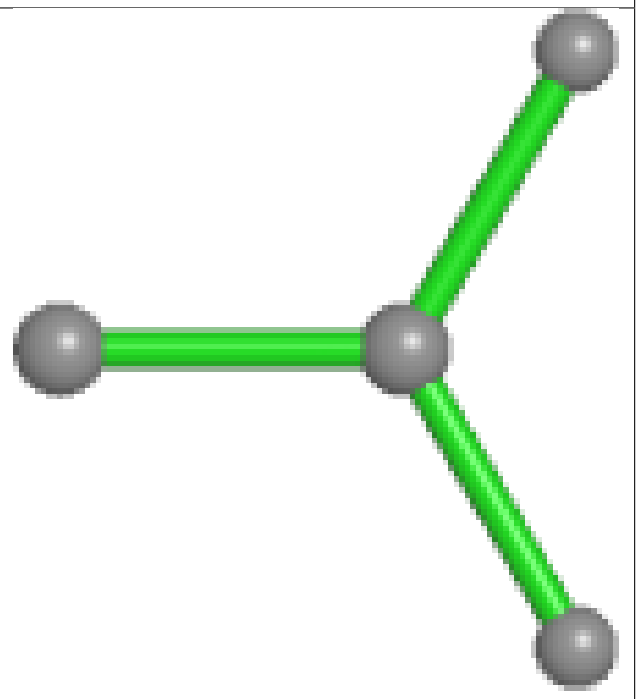


Rings

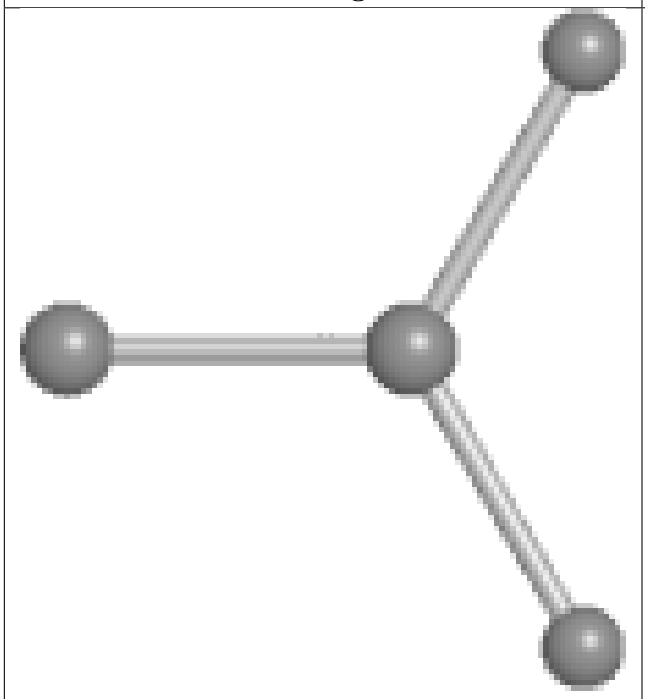
Ligand ACT A 1305



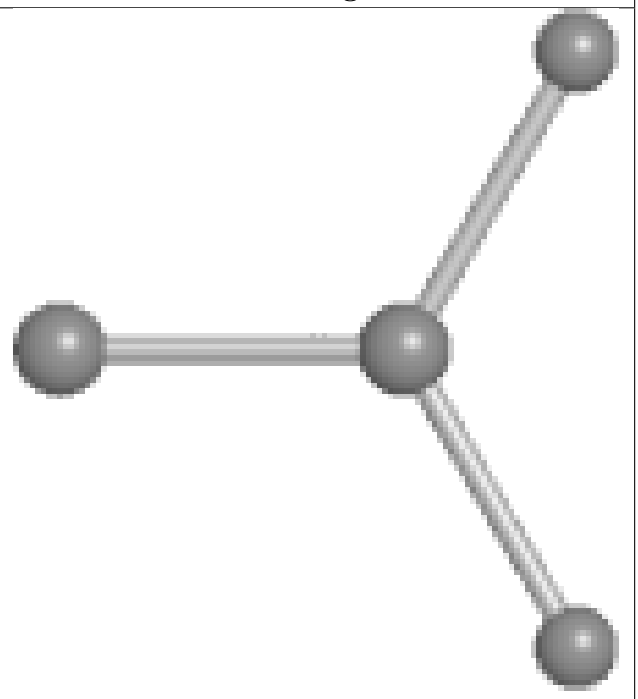
Bond lengths



Bond angles

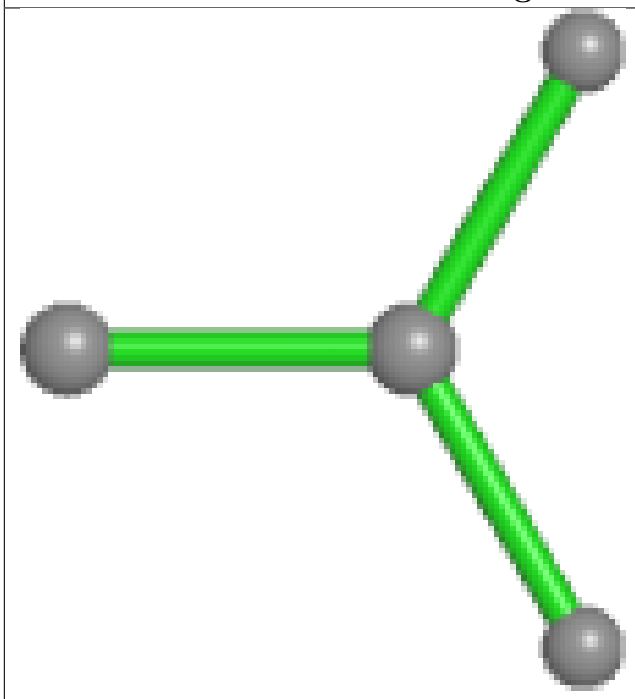


Torsions

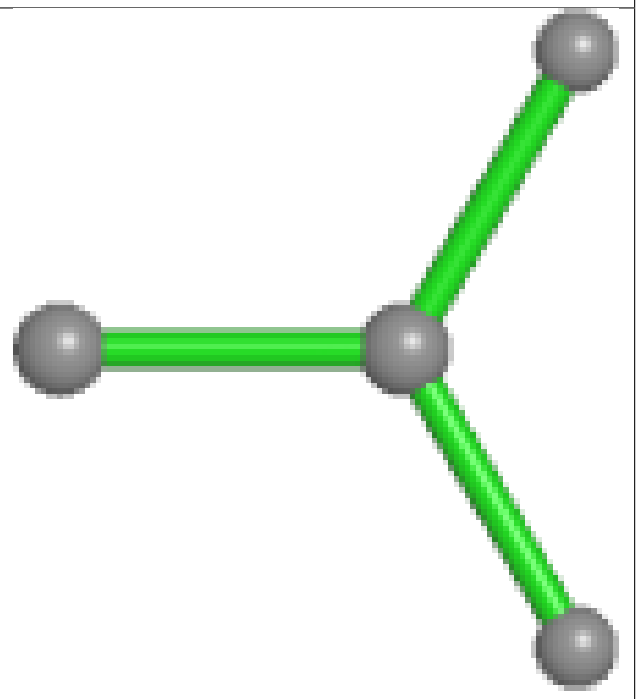


Rings

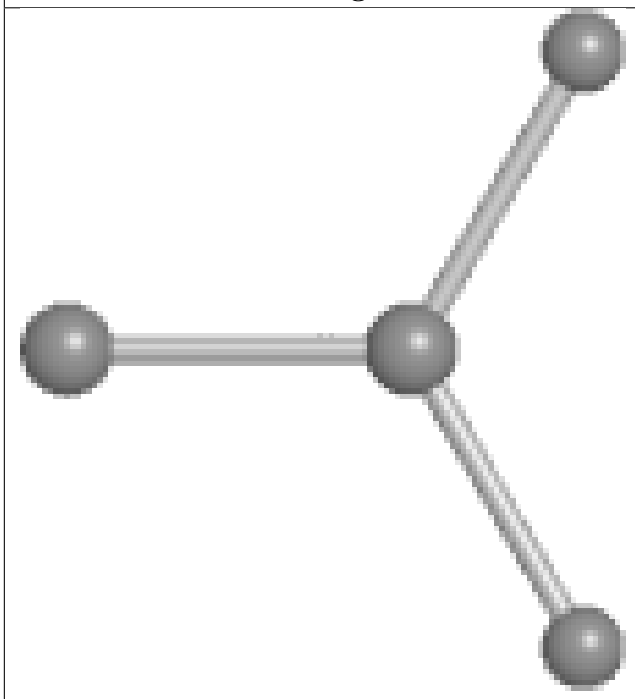
Ligand ACT A 1304



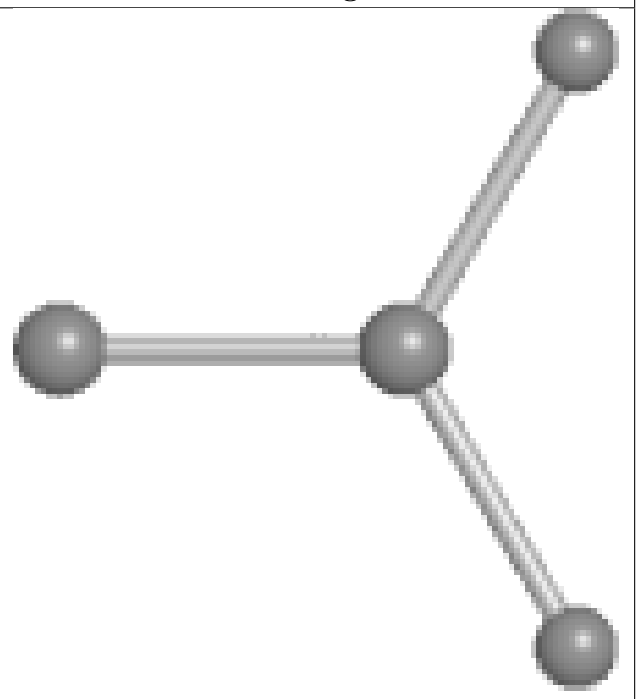
Bond lengths



Bond angles

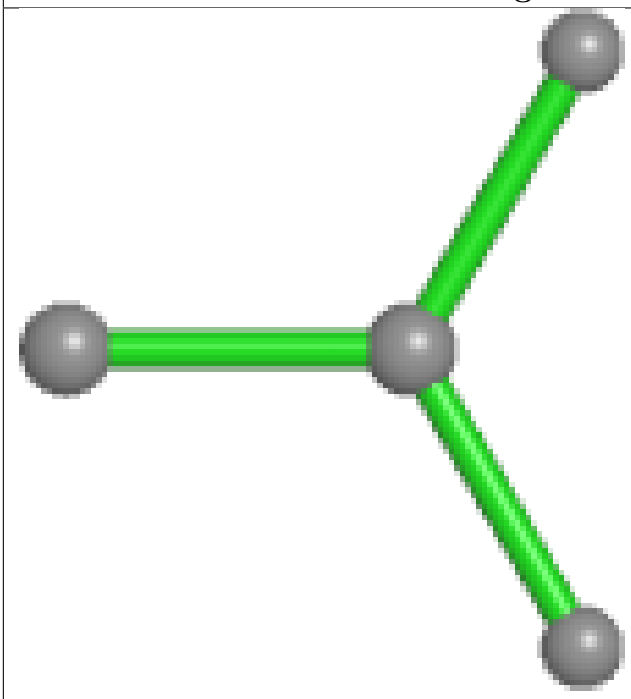


Torsions

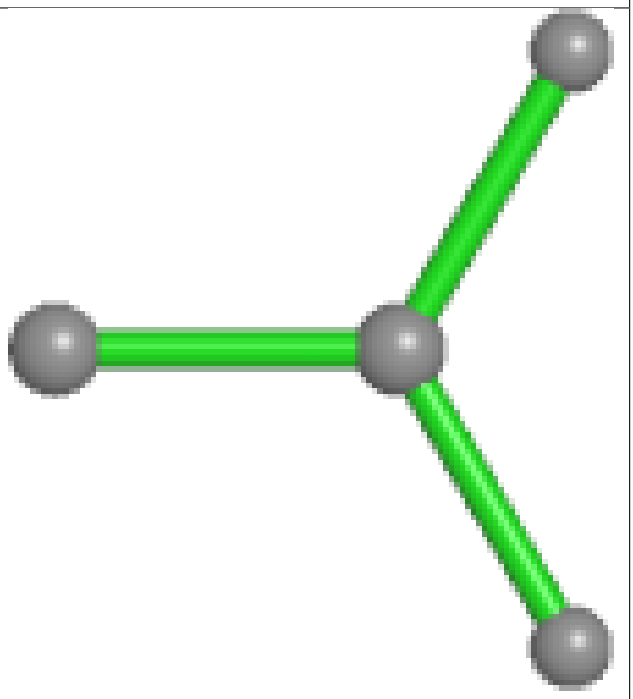


Rings

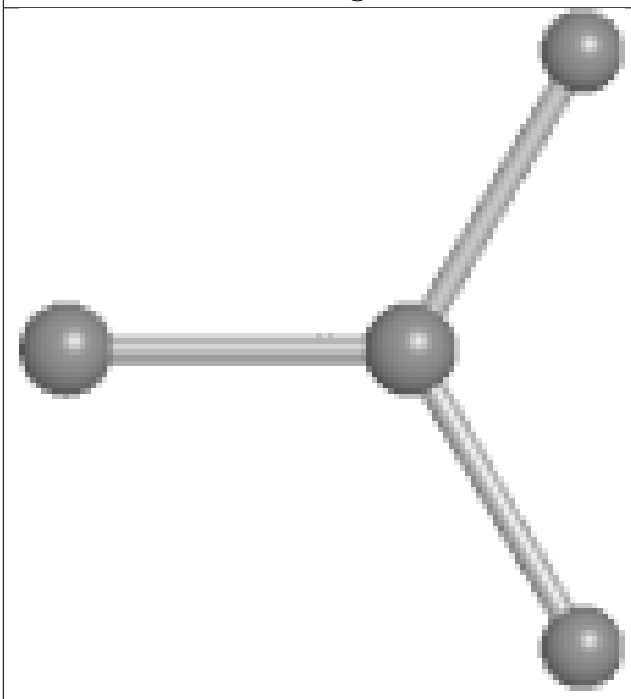
Ligand ACT B 1303



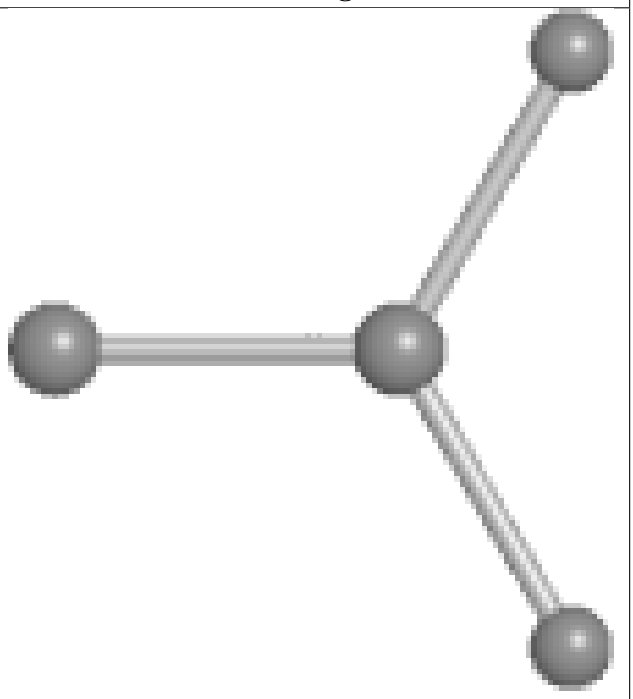
Bond lengths



Bond angles

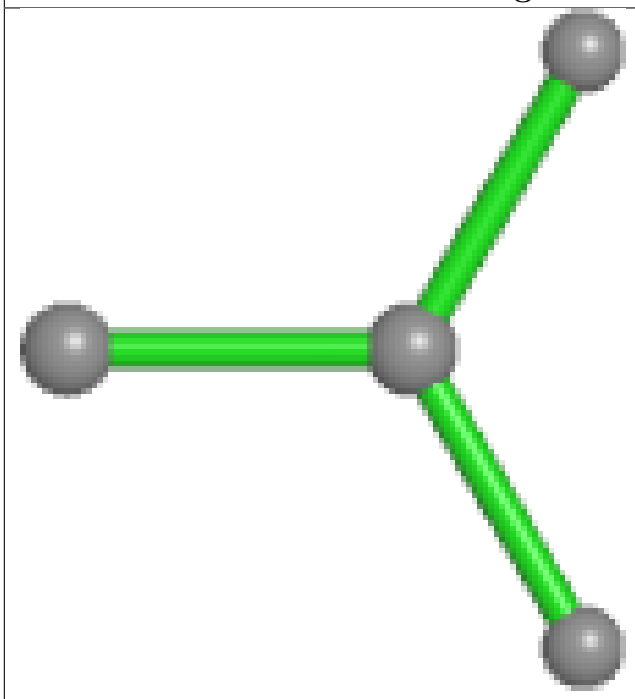


Torsions

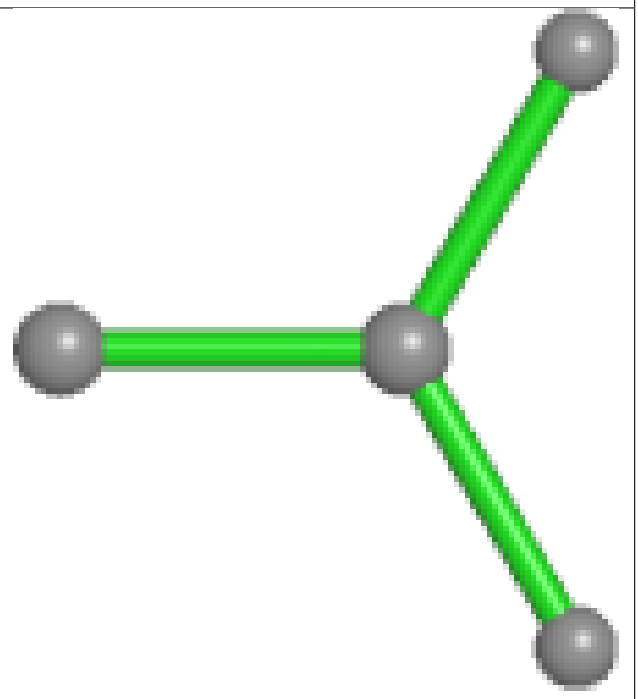


Rings

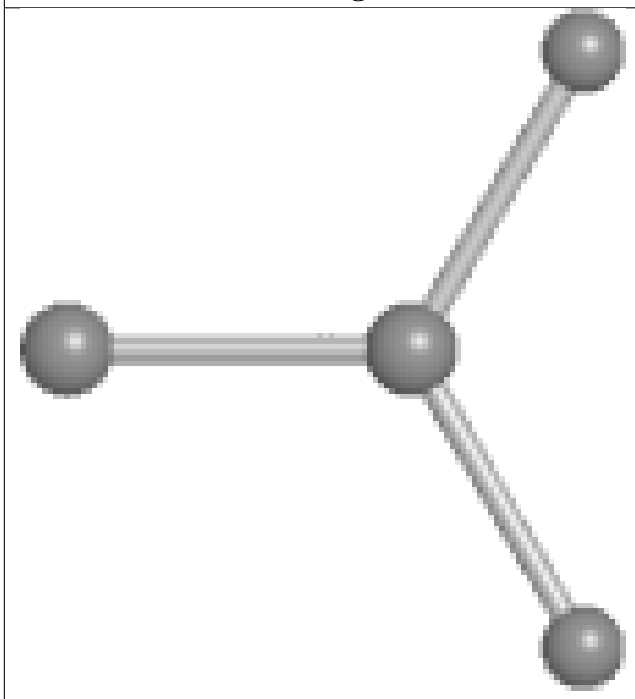
Ligand ACT A 1301



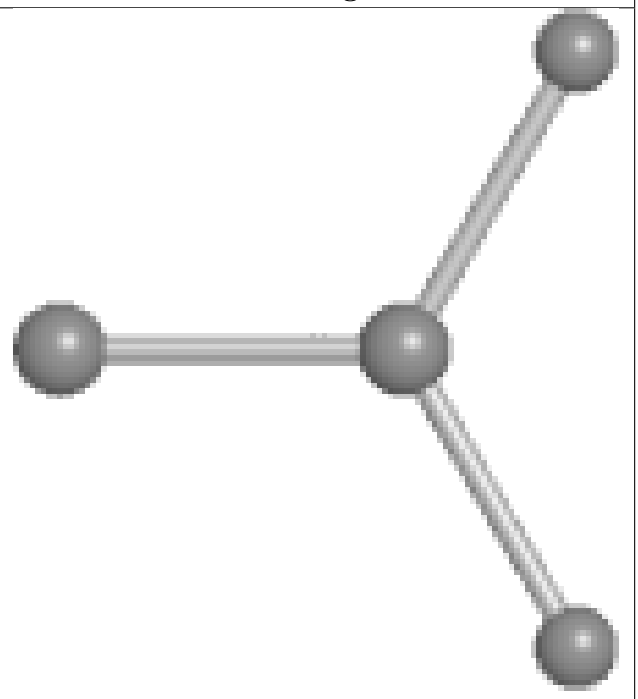
Bond lengths



Bond angles

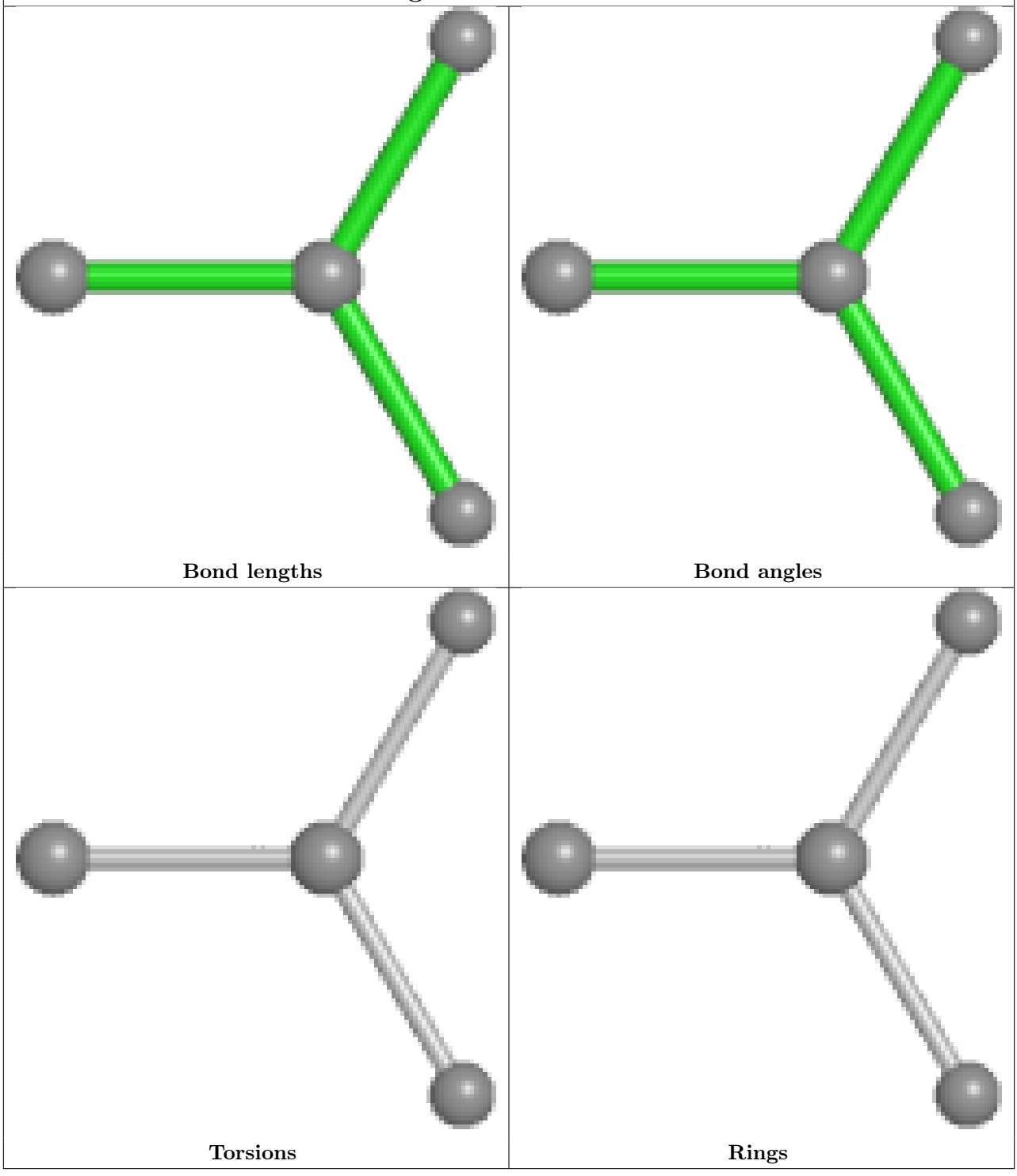


Torsions



Rings

Ligand ACT B 1301



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, 95^{th} 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%)	-0.42	3 (0%)	92	91	36, 58, 100, 123	0
1	B	728/803 (90%)	-0.47	3 (0%)	92	91	34, 56, 97, 123	0
All	All	1457/1606 (90%)	-0.44	6 (0%)	92	91	34, 58, 98, 123	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	706	THR	3.2
1	B	467	HIS	2.2
1	A	998	ALA	2.2
1	B	1113	ALA	2.1
1	A	699	GLN	2.1
1	A	1134	SER	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

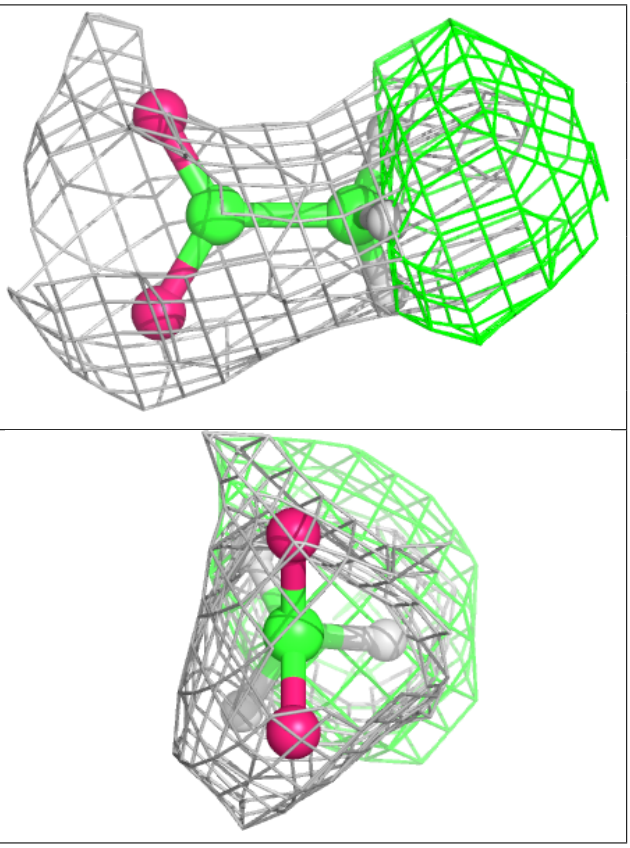
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

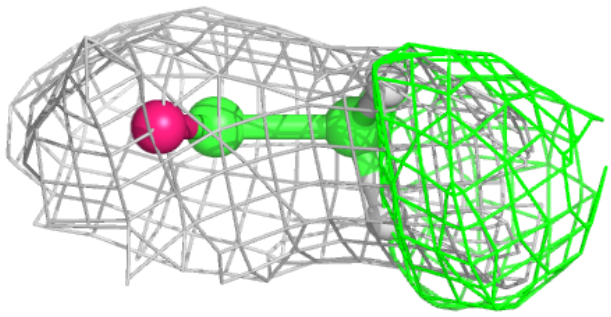
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	B	1301	4/4	0.61	0.31	83,100,104,104	0
2	ACT	A	1302	4/4	0.80	0.25	60,68,72,75	0
2	ACT	A	1301	4/4	0.80	0.35	71,76,85,85	0
2	ACT	A	1305	4/4	0.88	0.21	68,80,96,96	0
2	ACT	A	1304	4/4	0.89	0.23	64,69,83,83	0
2	ACT	B	1302	4/4	0.94	0.30	50,54,64,64	0
2	ACT	B	1303	4/4	0.94	0.16	65,68,81,81	0
2	ACT	B	1304	4/4	0.94	0.21	51,59,62,62	0
2	ACT	A	1303	4/4	0.95	0.14	49,57,59,60	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:

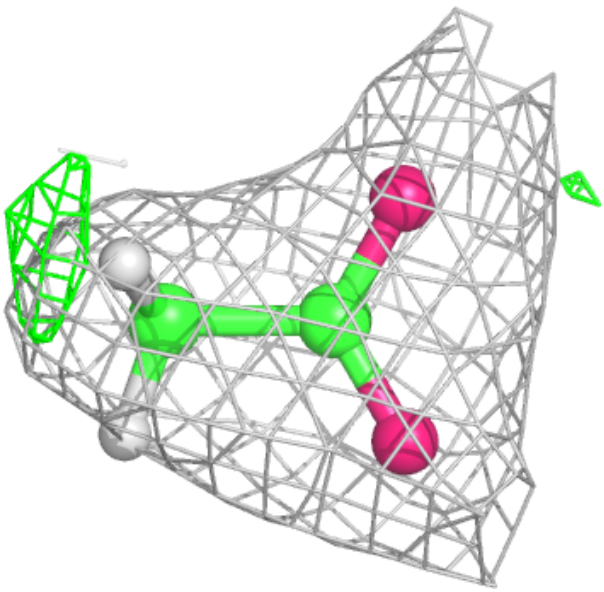
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

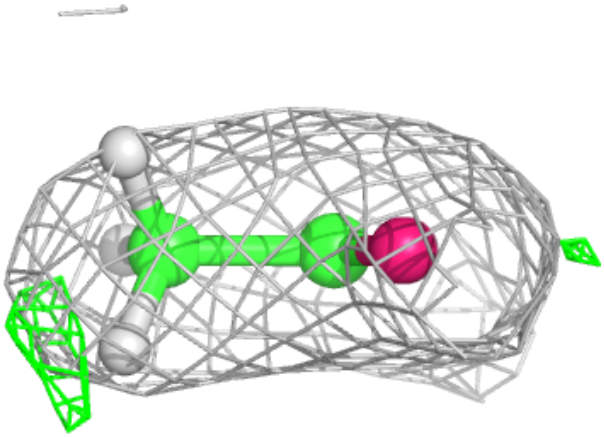


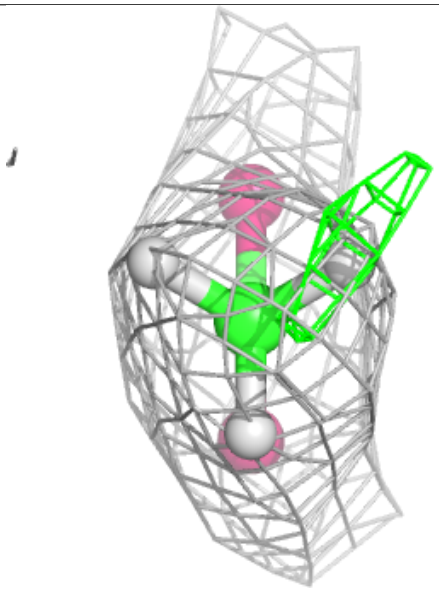


Electron density around ACT A 1302:

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

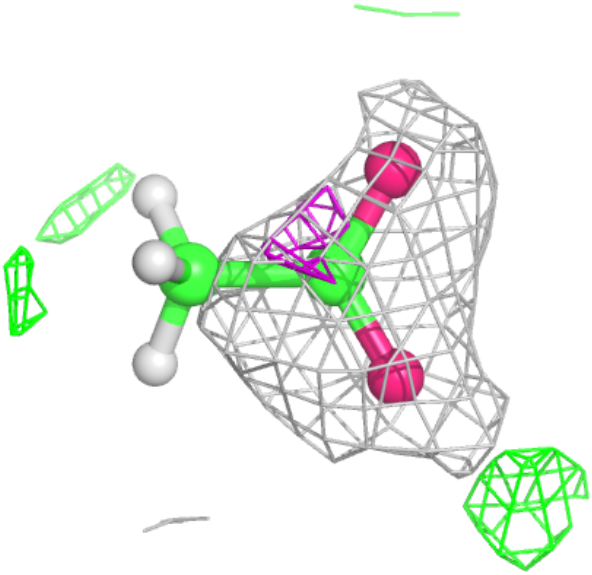


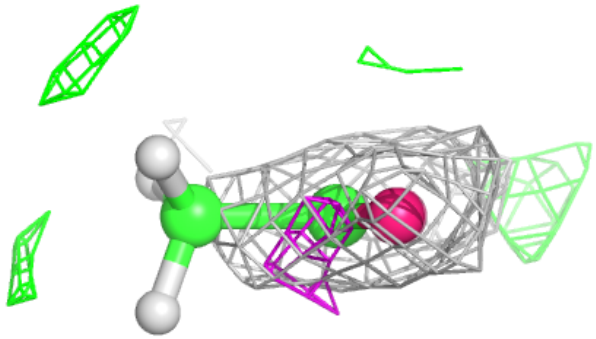


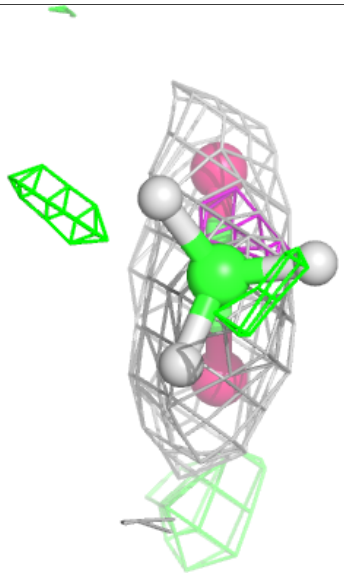


Electron density around ACT A 1301:

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

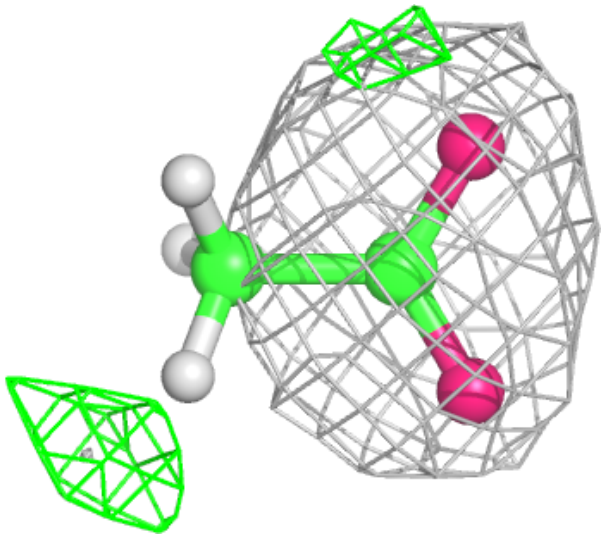


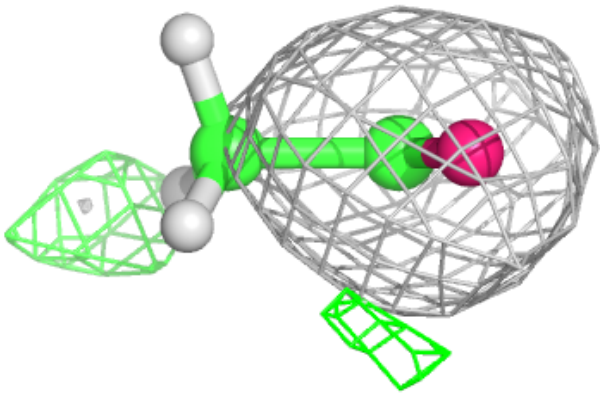


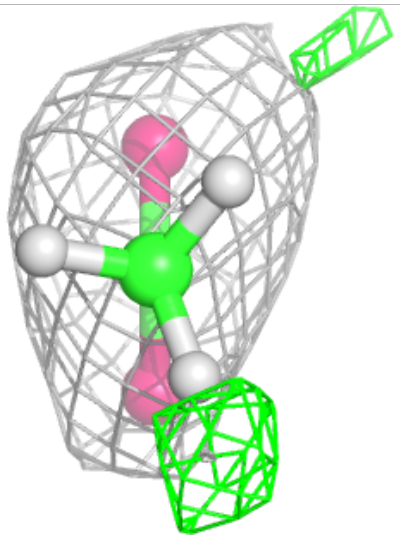


Electron density around ACT A 1305:

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

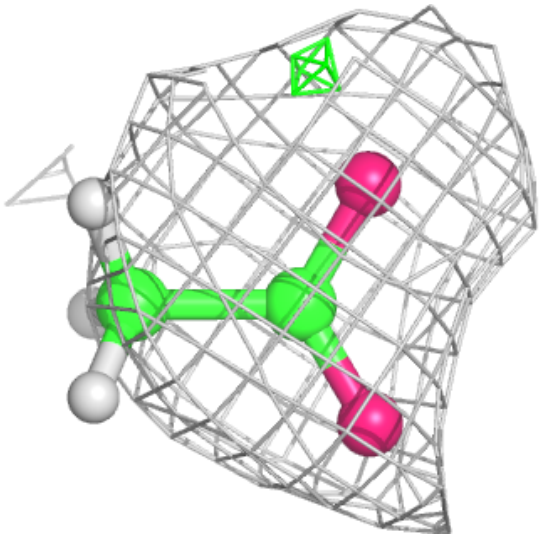


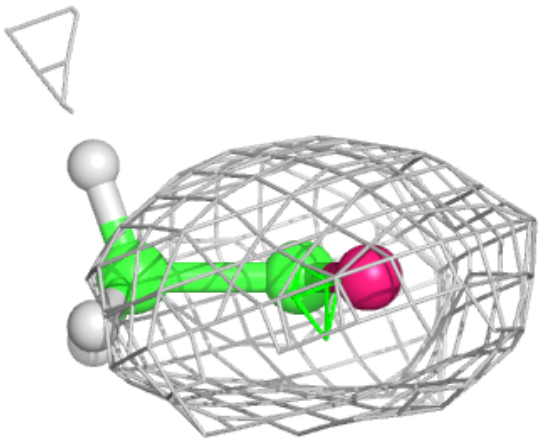


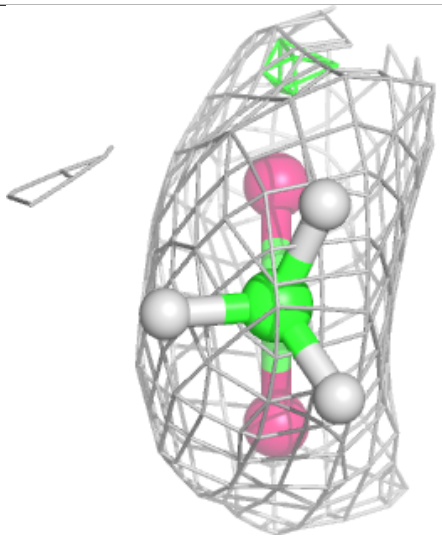


Electron density around ACT A 1304:

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

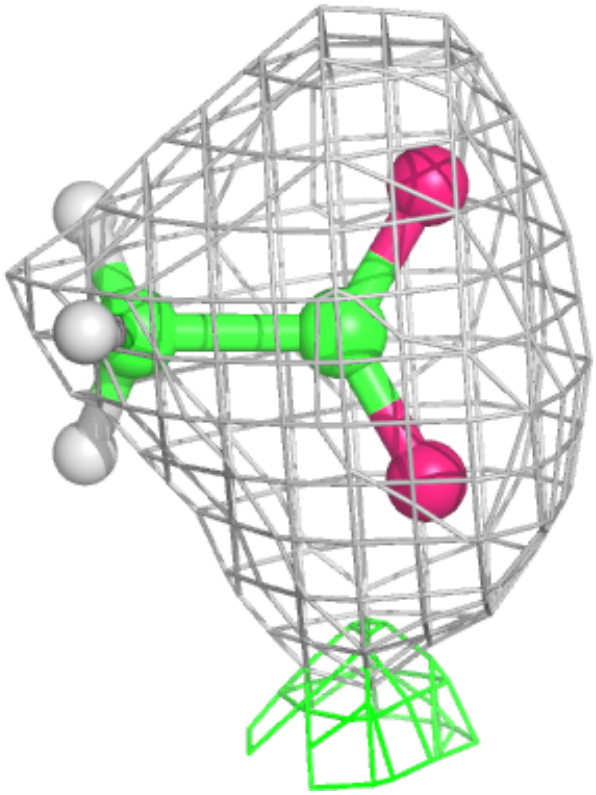


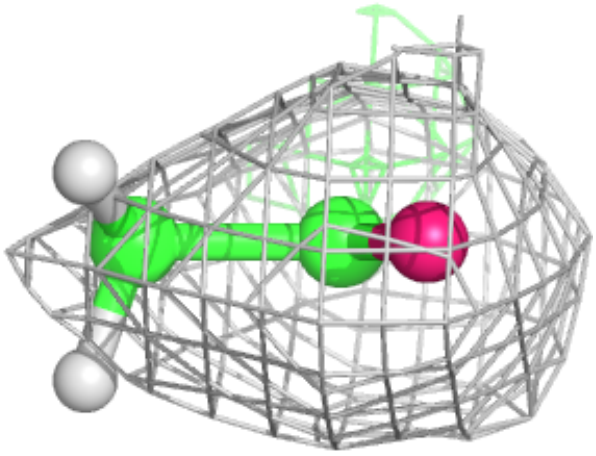


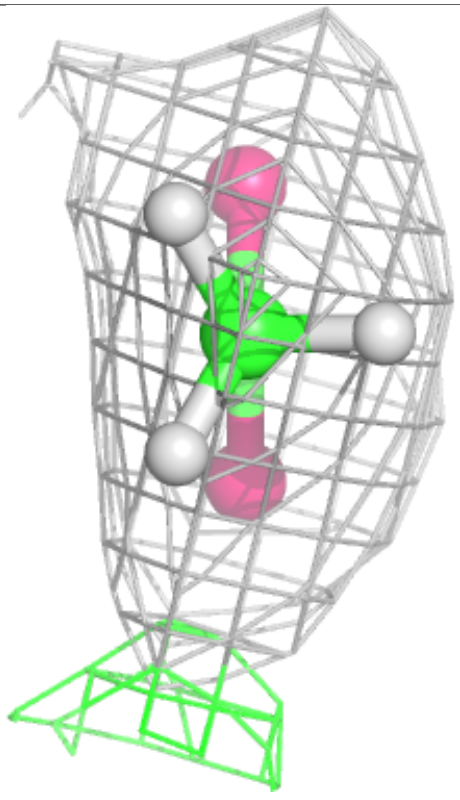


Electron density around ACT B 1302:

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

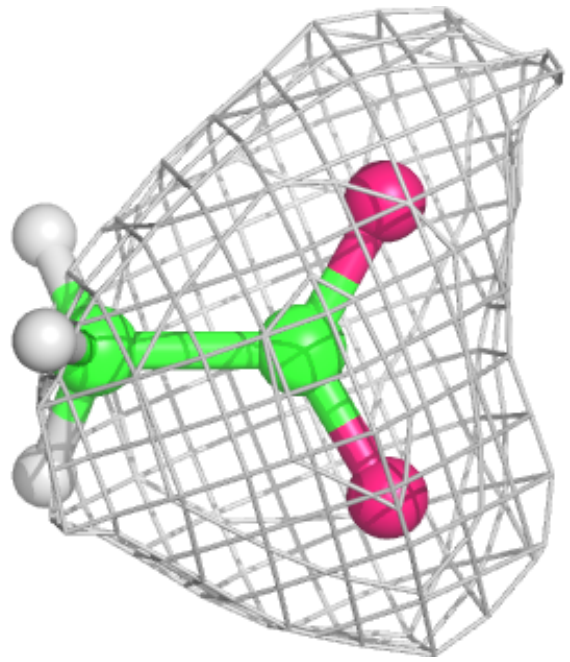


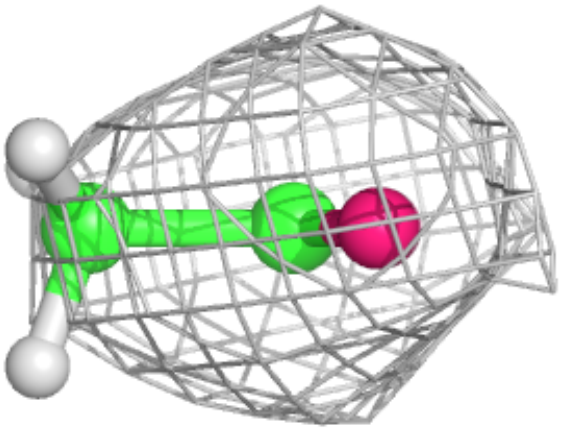


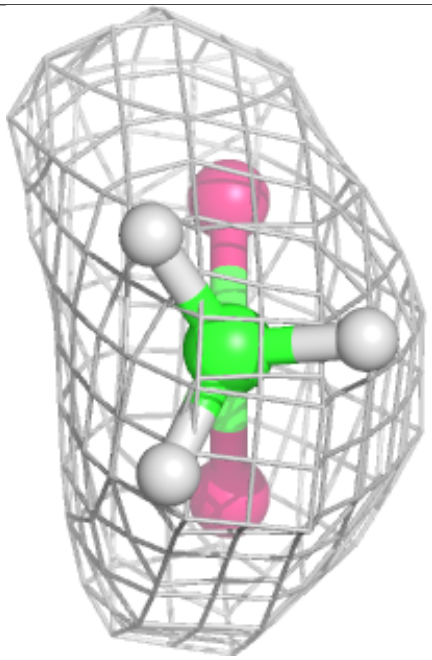


Electron density around ACT B 1303:

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

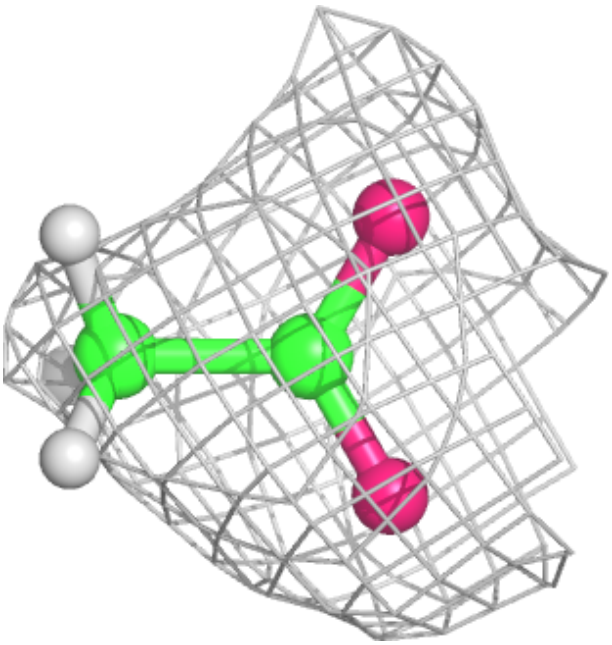


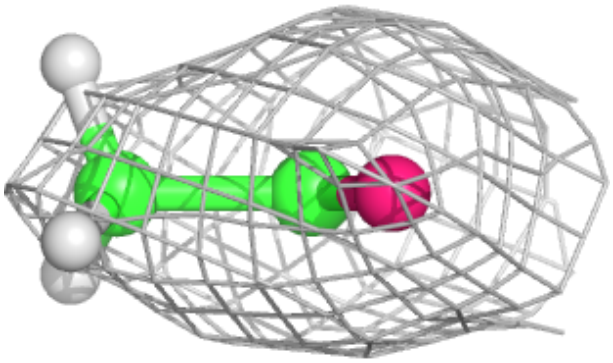


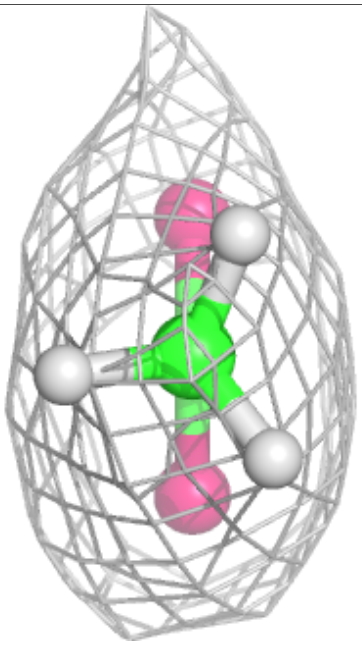


Electron density around ACT B 1304:

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

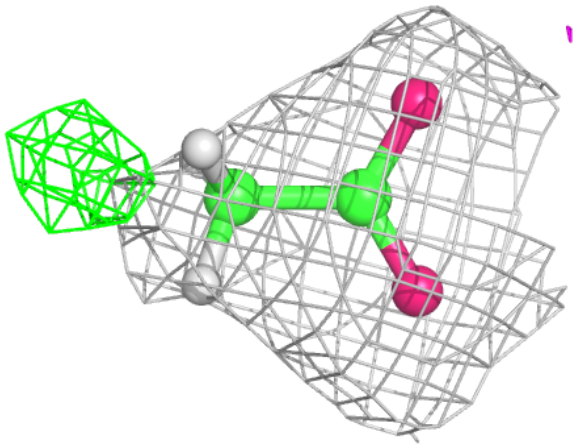


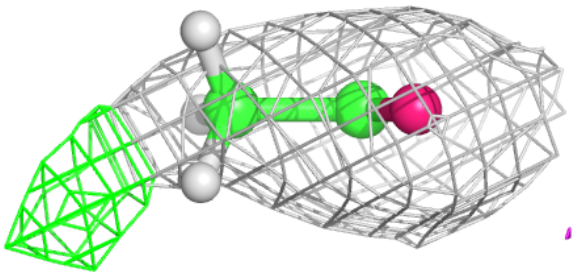


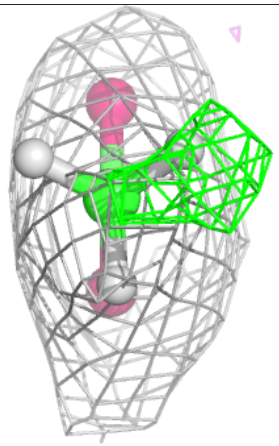


Electron density around ACT A 1303:

$2mF_o$-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

There are no such residues in this entry.