



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:17 AM UTC

PDB ID : 9HT9 / pdb_00009ht9
Title : CutC in complex with inhibitor1
Authors : Petersen, J.
Deposited on : 2024-12-19
Resolution : 1.84 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

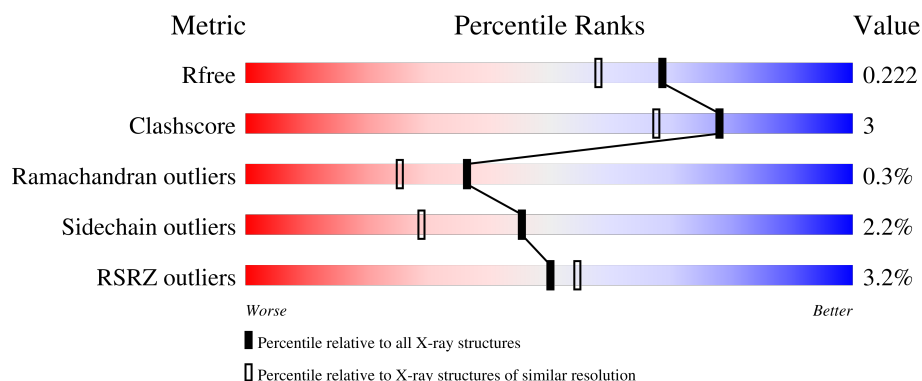
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	800	<div> <div>2%</div> <div>91%</div> <div>8%</div> <div>..</div> </div>
1	B	800	<div> <div>%</div> <div>92%</div> <div>6%</div> <div>..</div> </div>
1	C	800	<div> <div>8%</div> <div>90%</div> <div>9%</div> <div>..</div> </div>
1	D	800	<div> <div>2%</div> <div>92%</div> <div>7%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26165 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 Choline trimethylamine-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	794	Total	C	N	O	S	0	0	0
			6263	3971	1062	1185	45			
1	B	794	Total	C	N	O	S	0	0	0
			6263	3971	1062	1185	45			
1	C	794	Total	C	N	O	S	0	0	0
			6263	3971	1062	1185	45			
1	D	794	Total	C	N	O	S	0	0	0
			6263	3971	1062	1185	45			

There are 28 discrepancies between the modelled and reference sequences:

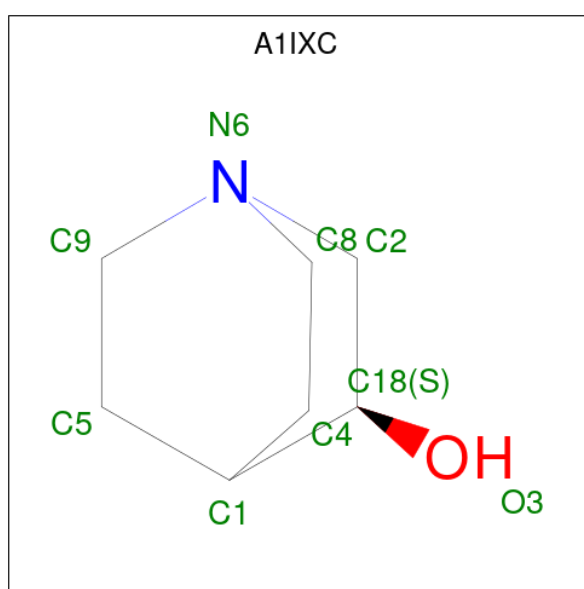
Chain	Residue	Modelled	Actual	Comment	Reference
A	47	MET	-	initiating methionine	UNP Q30W70
A	48	HIS	-	expression tag	UNP Q30W70
A	49	HIS	-	expression tag	UNP Q30W70
A	50	HIS	-	expression tag	UNP Q30W70
A	51	HIS	-	expression tag	UNP Q30W70
A	52	HIS	-	expression tag	UNP Q30W70
A	53	HIS	-	expression tag	UNP Q30W70
B	47	MET	-	initiating methionine	UNP Q30W70
B	48	HIS	-	expression tag	UNP Q30W70
B	49	HIS	-	expression tag	UNP Q30W70
B	50	HIS	-	expression tag	UNP Q30W70
B	51	HIS	-	expression tag	UNP Q30W70
B	52	HIS	-	expression tag	UNP Q30W70
B	53	HIS	-	expression tag	UNP Q30W70
C	47	MET	-	initiating methionine	UNP Q30W70
C	48	HIS	-	expression tag	UNP Q30W70
C	49	HIS	-	expression tag	UNP Q30W70
C	50	HIS	-	expression tag	UNP Q30W70
C	51	HIS	-	expression tag	UNP Q30W70
C	52	HIS	-	expression tag	UNP Q30W70
C	53	HIS	-	expression tag	UNP Q30W70

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Chain	Residue	Modelled	Actual	Comment	Reference
D	47	MET	-	initiating methionine	UNP Q30W70
D	48	HIS	-	expression tag	UNP Q30W70
D	49	HIS	-	expression tag	UNP Q30W70
D	50	HIS	-	expression tag	UNP Q30W70
D	51	HIS	-	expression tag	UNP Q30W70
D	52	HIS	-	expression tag	UNP Q30W70
D	53	HIS	-	expression tag	UNP Q30W70

- Molecule 2 is (3 {S})-1-azabicyclo[2.2.2]octan-3-ol (CCD ID: A1IXC) (formula: C₇H₁₃NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	7	1	1		
2	B	1	Total	C	N	O	0	0
			9	7	1	1		
2	C	1	Total	C	N	O	0	0
			9	7	1	1		
2	D	1	Total	C	N	O	0	0
			9	7	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	328	Total	O	0	0
			328	328		

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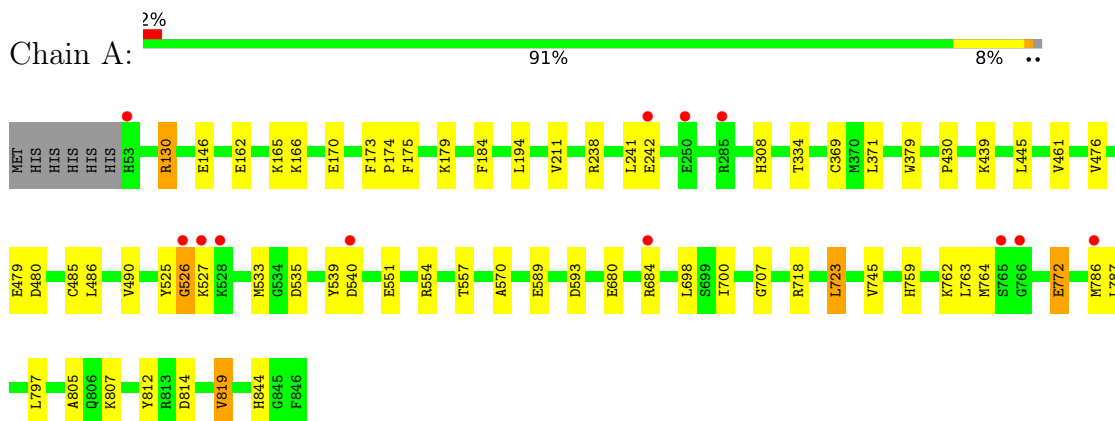
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	330	Total 330	O 330	0	0
3	C	186	Total 186	O 186	0	0
3	D	233	Total 233	O 233	0	0

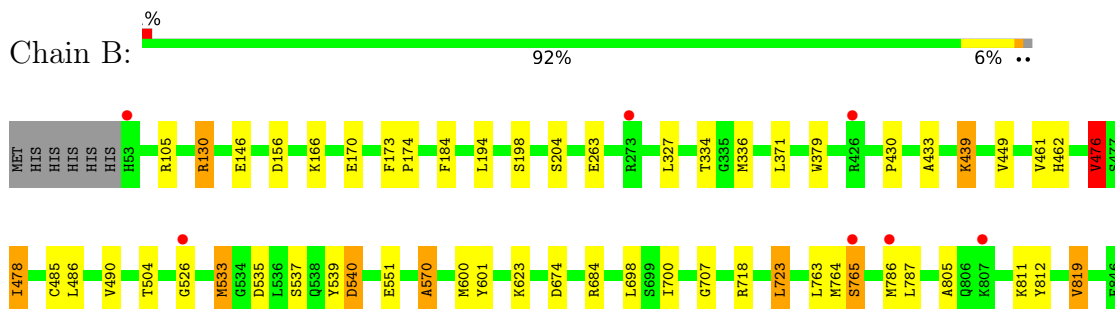
3 Residue-property plots [i](#)

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.

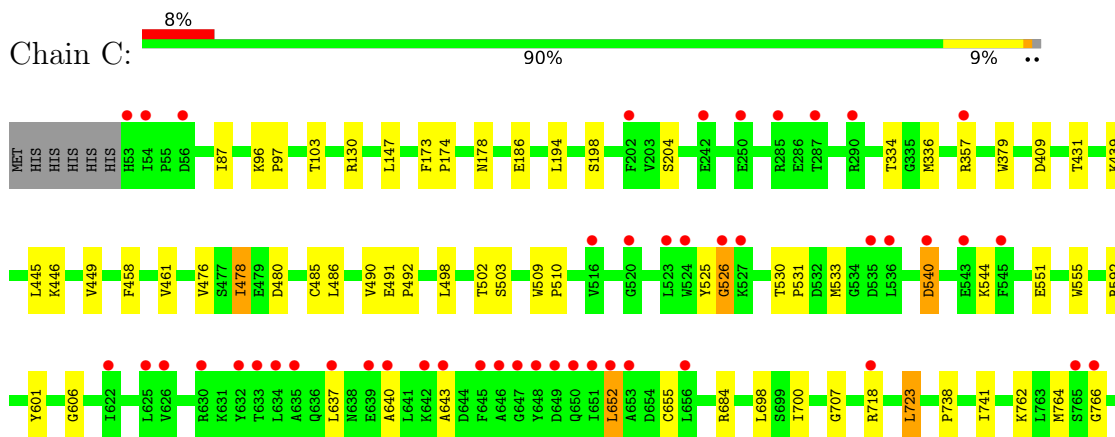
- Molecule 1: Choline trimethylamine-lyase

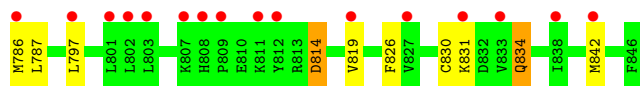


- Molecule 1: Choline trimethylamine-lyase

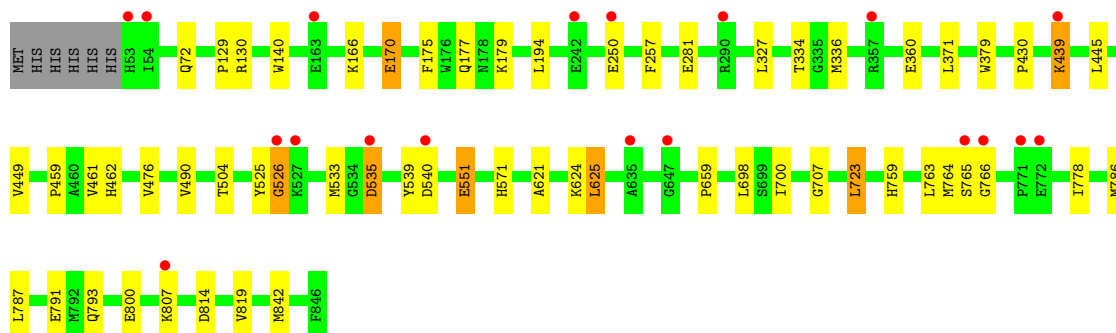
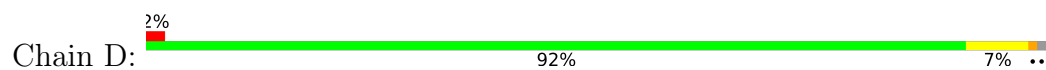


- Molecule 1: Choline trimethylamine-lyase





• Molecule 1: Choline trimethylamine-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.66Å 104.76Å 119.49Å 102.43° 108.54° 104.91°	Depositor
Resolution (Å)	107.17 – 1.84 107.17 – 1.84	Depositor EDS
% Data completeness (in resolution range)	97.0 (107.17-1.84) 97.1 (107.17-1.84)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0267 STEINER	Depositor
R, R_{free}	0.182 , 0.216 0.190 , 0.222	Depositor DCC
R_{free} test set	14479 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26165	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1IXC

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	1.11	2/6408 (0.0%)	1.35	12/8678 (0.1%)
1	B	1.11	2/6408 (0.0%)	1.35	16/8678 (0.2%)
1	C	1.07	0/6408	1.38	6/8678 (0.1%)
1	D	1.10	3/6408 (0.0%)	1.38	6/8678 (0.1%)
All	All	1.10	7/25632 (0.0%)	1.37	40/34712 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	2
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	571	HIS	CE1-NE2	5.89	1.38	1.32
1	B	146	GLU	CD-OE2	5.63	1.36	1.25
1	A	593	ASP	C-O	5.48	1.31	1.23
1	B	570	ALA	C-O	5.39	1.30	1.24
1	D	462	HIS	CE1-NE2	5.27	1.37	1.32
1	D	759	HIS	CE1-NE2	5.17	1.37	1.32
1	A	557	THR	C-O	5.00	1.29	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ARG	CG-CD-NE	-7.57	95.35	112.00
1	B	540	ASP	CB-CA-C	-7.57	98.70	110.81
1	B	539	TYR	CA-C-N	7.28	130.37	120.54
1	B	539	TYR	C-N-CA	7.28	130.37	120.54
1	A	539	TYR	CA-C-N	7.26	130.32	120.38
1	A	539	TYR	C-N-CA	7.26	130.32	120.38
1	D	540	ASP	CB-CA-C	-7.21	98.82	110.79
1	B	535	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	535	ASP	CB-CA-C	6.89	121.89	109.83
1	B	819	VAL	CB-CA-C	6.85	122.53	111.29
1	A	540	ASP	CB-CA-C	-6.64	99.39	110.68
1	D	539	TYR	CA-C-N	6.64	129.18	120.28
1	D	539	TYR	C-N-CA	6.64	129.18	120.28
1	B	684	ARG	NE-CZ-NH1	-6.63	114.87	121.50
1	B	684	ARG	NE-CZ-NH2	6.47	125.02	119.20
1	C	502	THR	CA-CB-OG1	-6.36	100.06	109.60
1	B	130	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	A	146	GLU	CB-CG-CD	6.00	122.80	112.60
1	A	772	GLU	CB-CA-C	-5.85	100.90	110.85
1	B	476	VAL	N-CA-CB	-5.81	100.32	110.49
1	A	242	GLU	CB-CG-CD	5.76	122.39	112.60
1	D	535	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	146	GLU	CB-CG-CD	5.67	122.25	112.60
1	B	504	THR	CA-CB-OG1	-5.67	101.10	109.60
1	B	130	ARG	NE-CZ-NH1	5.66	127.16	121.50
1	A	535	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	146	GLU	CB-CA-C	5.55	119.55	110.17
1	C	814	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	764	MET	CA-C-N	5.25	129.08	120.63
1	B	764	MET	C-N-CA	5.25	129.08	120.63
1	A	589	GLU	CB-CG-CD	5.23	121.49	112.60
1	C	186	GLU	CA-C-N	5.23	125.74	119.94
1	C	186	GLU	C-N-CA	5.23	125.74	119.94
1	D	504	THR	N-CA-C	-5.14	106.69	113.12
1	C	409	ASP	CA-CB-CG	-5.10	107.50	112.60
1	A	819	VAL	CB-CA-C	5.09	119.64	111.29
1	C	540	ASP	CB-CA-C	-5.09	102.40	110.84
1	D	257	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	156	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	130	ARG	NE-CZ-NH2	-5.01	114.69	119.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	526	GLY	Peptide
1	B	526	GLY	Peptide
1	C	526	GLY	Peptide
1	C	766	GLY	Peptide
1	D	526	GLY	Peptide
1	D	766	GLY	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	6263	0	6135	42	0
1	B	6263	0	6135	33	0
1	C	6263	0	6135	47	0
1	D	6263	0	6135	34	0
2	A	9	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
2	D	9	0	0	0	0
3	A	328	0	0	9	0
3	B	330	0	0	6	0
3	C	186	0	0	7	0
3	D	233	0	0	7	0
All	All	26165	0	24540	138	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 3.

All (138) 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:786:MET:SD	1:D:786:MET:SD	2.53	1.06
1:D:800:GLU:HG2	3:D:1219:HOH:O	1.56	1.02
1:B:674:ASP:HB2	3:B:1275:HOH:O	1.70	0.89
1:B:130:ARG:HD2	3:B:1140:HOH:O	1.74	0.87
1:A:130:ARG:CD	3:A:1058:HOH:O	2.26	0.81
1:D:130:ARG:HD2	3:D:1027:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:764:MET:HE2	1:D:842:MET:HG2	1.68	0.76
1:A:786:MET:SD	1:C:786:MET:SD	2.84	0.75
1:A:130:ARG:HD2	3:A:1058:HOH:O	1.85	0.73
1:B:130:ARG:CD	3:B:1140:HOH:O	2.32	0.73
1:A:130:ARG:HD3	3:A:1058:HOH:O	1.88	0.73
1:A:308:HIS:HD2	3:A:1309:HOH:O	1.72	0.72
1:B:439:LYS:CD	1:D:787:LEU:HD23	2.19	0.72
1:C:130:ARG:HD2	3:C:1018:HOH:O	1.89	0.72
1:B:439:LYS:HD3	1:D:787:LEU:HD23	1.72	0.70
1:A:787:LEU:HD23	1:C:439:LYS:HD3	1.73	0.70
1:C:684:ARG:HG3	3:C:1176:HOH:O	1.91	0.69
1:A:479:GLU:HG3	3:A:1287:HOH:O	1.93	0.69
1:D:130:ARG:CD	3:D:1027:HOH:O	2.41	0.68
1:B:600:MET:HE2	3:B:1282:HOH:O	1.92	0.68
1:A:764:MET:HE2	1:A:844:HIS:NE2	2.09	0.67
1:A:439:LYS:HD3	1:C:787:LEU:HD23	1.80	0.64
1:D:707:GLY:HA2	1:D:723:LEU:HD13	1.80	0.64
1:D:360:GLU:CG	3:D:1024:HOH:O	2.48	0.62
1:A:786:MET:HE1	1:C:786:MET:SD	2.40	0.60
1:C:592:ARG:CD	3:C:1181:HOH:O	2.50	0.60
1:C:830:CYS:O	1:C:834:GLN:HG2	2.02	0.59
1:D:175:PHE:O	1:D:179:LYS:HE2	2.03	0.58
1:C:738:PRO:HA	1:C:741:ILE:HD12	1.84	0.58
1:B:439:LYS:HD3	1:D:787:LEU:HA	1.84	0.57
1:A:166:LYS:O	1:A:170:GLU:HG2	2.04	0.57
1:C:592:ARG:HD3	3:C:1181:HOH:O	2.04	0.56
1:C:446:LYS:O	1:C:449:VAL:HG22	2.06	0.55
1:A:476:VAL:HG13	1:A:480:ASP:HB2	1.89	0.55
1:C:476:VAL:CG1	1:C:480:ASP:HB2	2.37	0.55
1:C:643:ALA:HB2	3:C:1001:HOH:O	2.05	0.55
1:D:707:GLY:CA	1:D:723:LEU:HD13	2.37	0.54
1:A:439:LYS:CD	1:C:787:LEU:HD23	2.38	0.53
1:A:680:GLU:OE2	1:A:684:ARG:HD3	2.08	0.53
1:B:184:PHE:CD1	1:B:570:ALA:HB2	2.43	0.53
1:A:684:ARG:HG3	3:A:1303:HOH:O	2.08	0.53
1:A:707:GLY:HA2	1:A:723:LEU:HD13	1.89	0.53
1:A:439:LYS:HE2	3:C:1134:HOH:O	2.08	0.52
1:A:762:LYS:HD2	1:A:797:LEU:HD11	1.91	0.52
1:B:439:LYS:HD2	1:D:787:LEU:HD23	1.90	0.52
1:C:707:GLY:HA2	1:C:723:LEU:HD13	1.91	0.52
1:B:805:ALA:HA	1:B:812:TYR:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:525:TYR:O	1:D:526:GLY:C	2.53	0.52
1:A:551:GLU:OE2	1:A:554:ARG:NH1	2.43	0.52
1:C:173:PHE:HB2	1:C:174:PRO:HD3	1.92	0.52
1:A:533:MET:HE1	1:A:551:GLU:HB3	1.92	0.51
1:A:787:LEU:HD23	1:C:439:LYS:CD	2.41	0.50
1:B:478:ILE:HD12	1:B:478:ILE:O	2.11	0.50
1:A:786:MET:CE	1:C:786:MET:SD	2.99	0.50
1:D:250:GLU:HB2	3:D:1200:HOH:O	2.12	0.49
1:D:327:LEU:HB3	1:D:336:MET:SD	2.52	0.49
1:C:476:VAL:CG1	1:C:480:ASP:CB	2.90	0.49
1:C:652:LEU:O	1:C:655:CYS:N	2.44	0.49
1:B:334:THR:HB	1:B:379:TRP:CG	2.47	0.49
1:D:791:GLU:OE2	1:D:793:GLN:NE2	2.42	0.49
1:B:707:GLY:HA2	1:B:723:LEU:HD13	1.95	0.49
1:A:175:PHE:O	1:A:179:LYS:HE2	2.12	0.48
1:D:360:GLU:HG2	3:D:1024:HOH:O	2.11	0.48
1:B:433:ALA:HB1	1:B:486:LEU:HD13	1.96	0.48
1:B:439:LYS:HD2	1:D:787:LEU:CD2	2.43	0.48
1:D:334:THR:HB	1:D:379:TRP:CG	2.49	0.48
1:B:439:LYS:CD	1:D:787:LEU:CD2	2.92	0.48
1:C:592:ARG:HD2	3:C:1181:HOH:O	2.10	0.47
1:A:525:TYR:O	1:A:526:GLY:C	2.57	0.47
1:C:826:PHE:CZ	1:C:834:GLN:HB2	2.50	0.47
1:A:707:GLY:CA	1:A:723:LEU:HD13	2.44	0.47
1:B:786:MET:SD	1:D:786:MET:CE	3.03	0.47
1:C:530:THR:HG22	1:C:555:TRP:CZ3	2.50	0.47
1:C:762:LYS:HD2	1:C:797:LEU:HD11	1.96	0.47
1:C:533:MET:HE1	1:C:551:GLU:HB3	1.96	0.47
1:C:764:MET:HE2	1:C:842:MET:SD	2.55	0.47
1:B:533:MET:HE1	1:B:551:GLU:HB3	1.97	0.46
1:B:674:ASP:CB	3:B:1275:HOH:O	2.44	0.46
1:C:831:LYS:O	1:C:834:GLN:HG3	2.16	0.46
1:D:360:GLU:CD	3:D:1024:HOH:O	2.58	0.46
1:A:797:LEU:HD12	1:A:797:LEU:C	2.41	0.45
1:D:371:LEU:HD22	1:D:430:PRO:HD2	1.97	0.45
1:A:211:VAL:HG12	3:A:1084:HOH:O	2.16	0.45
1:C:540:ASP:HB2	1:C:544:LYS:HD2	1.99	0.45
1:A:485:CYS:C	1:A:486:LEU:HG	2.42	0.45
1:B:166:LYS:O	1:B:170:GLU:HG3	2.17	0.45
1:A:173:PHE:HB2	1:A:174:PRO:HD3	1.99	0.44
1:D:140:TRP:CZ2	1:D:177:GLN:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:HIS:CE1	1:B:486:LEU:HD22	2.53	0.44
1:C:96:LYS:N	1:C:97:PRO:CD	2.81	0.44
1:B:786:MET:SD	1:D:786:MET:HE1	2.58	0.44
1:C:498:LEU:HA	1:C:601:TYR:HB2	2.00	0.44
1:D:166:LYS:O	1:D:170:GLU:HG2	2.18	0.43
1:B:787:LEU:HA	1:D:439:LYS:HD3	1.99	0.43
1:C:431:THR:HA	1:C:458:PHE:CE1	2.54	0.43
1:A:745:VAL:HG21	1:A:759:HIS:CE1	2.53	0.43
1:B:198:SER:HA	1:B:204:SER:O	2.18	0.43
1:A:764:MET:HE2	1:A:844:HIS:CD2	2.53	0.43
1:B:811:LYS:HB3	1:B:811:LYS:HE2	1.87	0.43
1:A:476:VAL:HG13	1:A:480:ASP:CB	2.49	0.43
1:B:173:PHE:HB2	1:B:174:PRO:HD3	2.01	0.43
1:B:623:LYS:HD3	3:B:1119:HOH:O	2.18	0.43
1:C:476:VAL:HG12	1:C:480:ASP:HB2	2.01	0.42
1:B:485:CYS:C	1:B:486:LEU:HG	2.42	0.42
1:A:805:ALA:HA	1:A:812:TYR:CD2	2.54	0.42
1:C:525:TYR:O	1:C:526:GLY:C	2.61	0.42
1:A:371:LEU:HD22	1:A:430:PRO:HD2	2.01	0.42
1:B:105:ARG:HD3	1:B:263:GLU:OE2	2.20	0.42
1:C:530:THR:HB	1:C:531:PRO:CD	2.50	0.42
1:D:72:GLN:HG3	1:D:129:PRO:HB2	2.02	0.42
1:D:445:LEU:HD23	1:D:778:ILE:HG23	2.01	0.42
1:B:371:LEU:HD22	1:B:430:PRO:HD2	2.02	0.42
1:D:764:MET:HE2	1:D:842:MET:CG	2.43	0.42
1:C:198:SER:HA	1:C:204:SER:O	2.20	0.42
1:C:334:THR:HB	1:C:379:TRP:CG	2.54	0.42
1:B:476:VAL:HG22	1:B:601:TYR:CE2	2.55	0.41
1:A:184:PHE:CD1	1:A:570:ALA:HB2	2.54	0.41
1:A:334:THR:HB	1:A:379:TRP:CG	2.55	0.41
1:A:308:HIS:HE1	3:A:1306:HOH:O	2.02	0.41
1:A:787:LEU:CD2	1:C:439:LYS:HD3	2.48	0.41
1:C:87:ILE:CD1	1:C:103:THR:HA	2.51	0.41
1:A:211:VAL:HG12	1:A:211:VAL:O	2.21	0.41
1:A:369:CYS:HB3	3:A:1261:HOH:O	2.20	0.41
1:D:533:MET:HE3	1:D:551:GLU:HB3	2.03	0.41
1:A:533:MET:HE1	1:A:551:GLU:CB	2.50	0.41
1:D:624:LYS:HD2	1:D:659:PRO:HD3	2.02	0.41
1:A:162:GLU:OE2	1:A:165:LYS:NZ	2.53	0.41
1:B:327:LEU:HB3	1:B:336:MET:SD	2.60	0.41
1:C:478:ILE:O	1:C:478:ILE:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LEU:HD23	1:C:147:LEU:HA	1.83	0.40
1:C:336:MET:HB2	1:C:336:MET:HE3	1.74	0.40
1:D:621:ALA:O	1:D:625:LEU:HB2	2.21	0.40
1:C:485:CYS:C	1:C:486:LEU:HG	2.47	0.40
1:C:503:SER:HA	1:C:606:GLY:O	2.21	0.40
1:C:533:MET:CE	1:C:551:GLU:HB3	2.51	0.40
1:C:491:GLU:HA	1:C:492:PRO:HD2	2.00	0.40
1:C:509:TRP:N	1:C:510:PRO:CD	2.85	0.40
1:C:637:LEU:O	1:C:640:ALA:HB3	2.22	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	792/800 (99%)	773 (98%)	17 (2%)	2 (0%)	36	25
1	B	792/800 (99%)	768 (97%)	21 (3%)	3 (0%)	30	18
1	C	792/800 (99%)	765 (97%)	24 (3%)	3 (0%)	30	18
1	D	792/800 (99%)	769 (97%)	21 (3%)	2 (0%)	36	25
All	All	3168/3200 (99%)	3075 (97%)	83 (3%)	10 (0%)	36	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	652	LEU
1	C	700	ILE
1	D	700	ILE
1	A	700	ILE
1	B	700	ILE
1	D	490	VAL

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Mol	Chain	Res	Type
1	A	490	VAL
1	B	765	SER
1	B	490	VAL
1	C	490	VAL

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	669/676 (99%)	656 (98%)	13 (2%)	50	34
1	B	669/676 (99%)	654 (98%)	15 (2%)	45	29
1	C	669/676 (99%)	657 (98%)	12 (2%)	51	35
1	D	669/676 (99%)	651 (97%)	18 (3%)	39	22
All	All	2676/2704 (99%)	2618 (98%)	58 (2%)	45	29

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	LEU
1	A	241	LEU
1	A	445	LEU
1	A	461	VAL
1	A	527	LYS
1	A	698	LEU
1	A	718	ARG
1	A	723	LEU
1	A	763	LEU
1	A	772	GLU
1	A	807	LYS
1	A	814	ASP
1	A	819	VAL
1	B	194	LEU
1	B	439	LYS
1	B	449	VAL
1	B	461	VAL

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Mol	Chain	Res	Type
1	B	476	VAL
1	B	478	ILE
1	B	533	MET
1	B	537	SER
1	B	540	ASP
1	B	698	LEU
1	B	718	ARG
1	B	723	LEU
1	B	763	LEU
1	B	765	SER
1	B	819	VAL
1	C	178	ASN
1	C	194	LEU
1	C	357	ARG
1	C	445	LEU
1	C	461	VAL
1	C	478	ILE
1	C	698	LEU
1	C	718	ARG
1	C	723	LEU
1	C	814	ASP
1	C	819	VAL
1	C	834	GLN
1	D	170	GLU
1	D	194	LEU
1	D	281	GLU
1	D	439	LYS
1	D	449	VAL
1	D	459	PRO
1	D	461	VAL
1	D	476	VAL
1	D	535	ASP
1	D	551	GLU
1	D	625	LEU
1	D	698	LEU
1	D	723	LEU
1	D	763	LEU
1	D	765	SER
1	D	807	LYS
1	D	814	ASP
1	D	819	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	218	ASN
1	A	308	HIS
1	A	508	GLN
1	A	806	GLN
1	A	808	HIS
1	B	68	ASN
1	B	116	GLN
1	B	188	GLN
1	B	218	ASN
1	B	806	GLN
1	C	68	ASN
1	C	116	GLN
1	C	218	ASN
1	C	408	HIS
1	C	493	GLN
1	C	636	GLN
1	C	808	HIS
1	D	68	ASN
1	D	144	GLN
1	D	218	ASN
1	D	308	HIS
1	D	508	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1IXC	C	901	-	10,10,10	1.07	1 (10%)	12,14,14	1.25	2 (16%)
2	A1IXC	B	901	-	10,10,10	1.73	3 (30%)	12,14,14	1.09	1 (8%)
2	A1IXC	D	901	-	10,10,10	1.49	1 (10%)	12,14,14	1.28	1 (8%)
2	A1IXC	A	901	-	10,10,10	1.39	1 (10%)	12,14,14	1.41	1 (8%)

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	A1IXC	C	901	-	-	-	0/3/2/2
2	A1IXC	B	901	-	-	-	0/3/2/2
2	A1IXC	D	901	-	-	-	0/3/2/2
2	A1IXC	A	901	-	-	-	0/3/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	A1IXC	C2-N6	3.43	1.52	1.46
2	B	901	A1IXC	C2-C18	2.83	1.56	1.52
2	A	901	A1IXC	C2-C18	2.83	1.56	1.52
2	C	901	A1IXC	C2-C18	2.27	1.55	1.52
2	B	901	A1IXC	C2-N6	2.13	1.50	1.46
2	B	901	A1IXC	C9-N6	2.04	1.52	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	A1IXC	C5-C1-C4	-3.03	104.25	109.43
2	D	901	A1IXC	C5-C9-N6	-2.95	106.30	111.08
2	B	901	A1IXC	C5-C1-C18	-2.78	102.58	108.86
2	C	901	A1IXC	C5-C9-N6	-2.38	107.22	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	A1IXC	C8-N6-C2	2.07	112.97	109.53

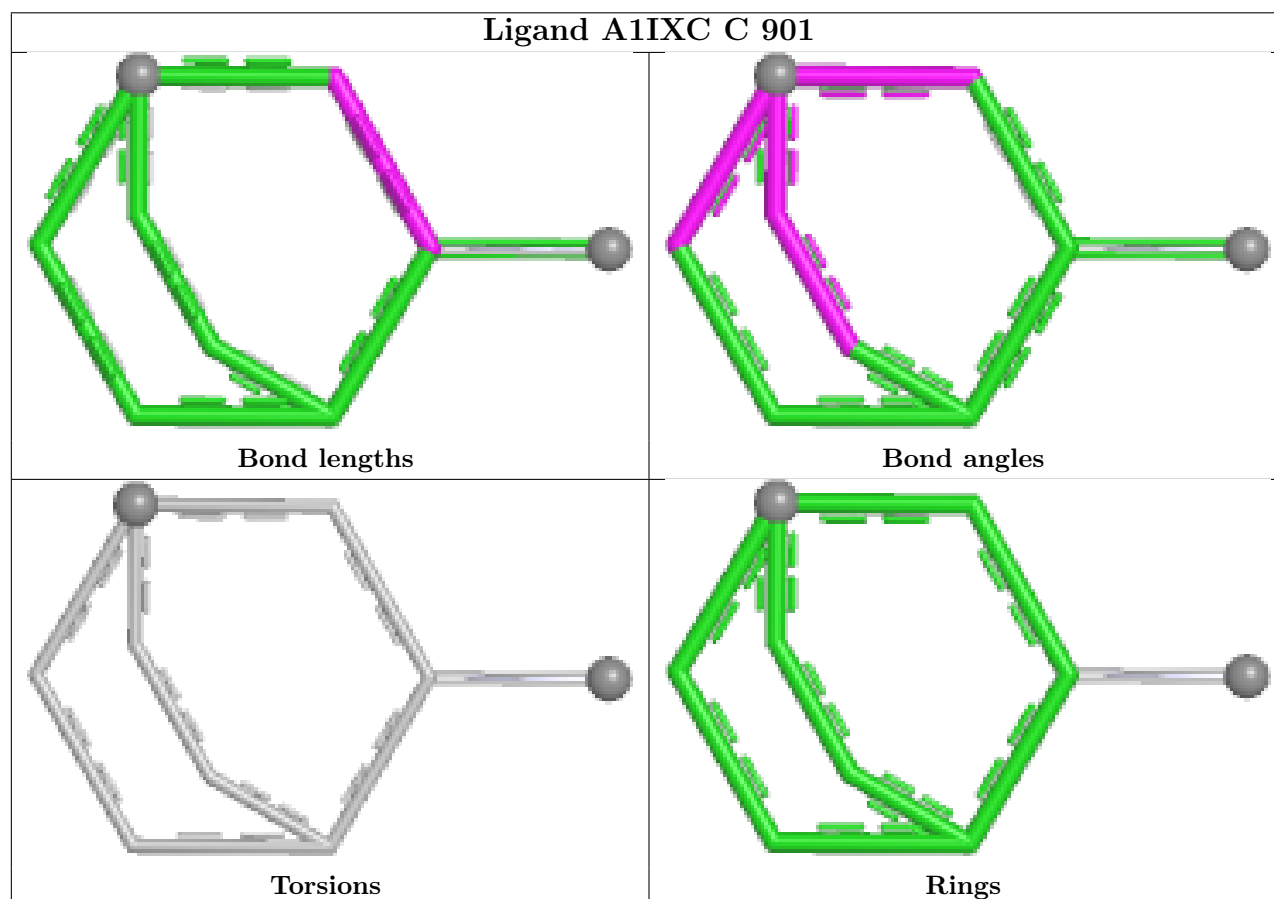
There are no chirality outliers.

There are no torsion outliers.

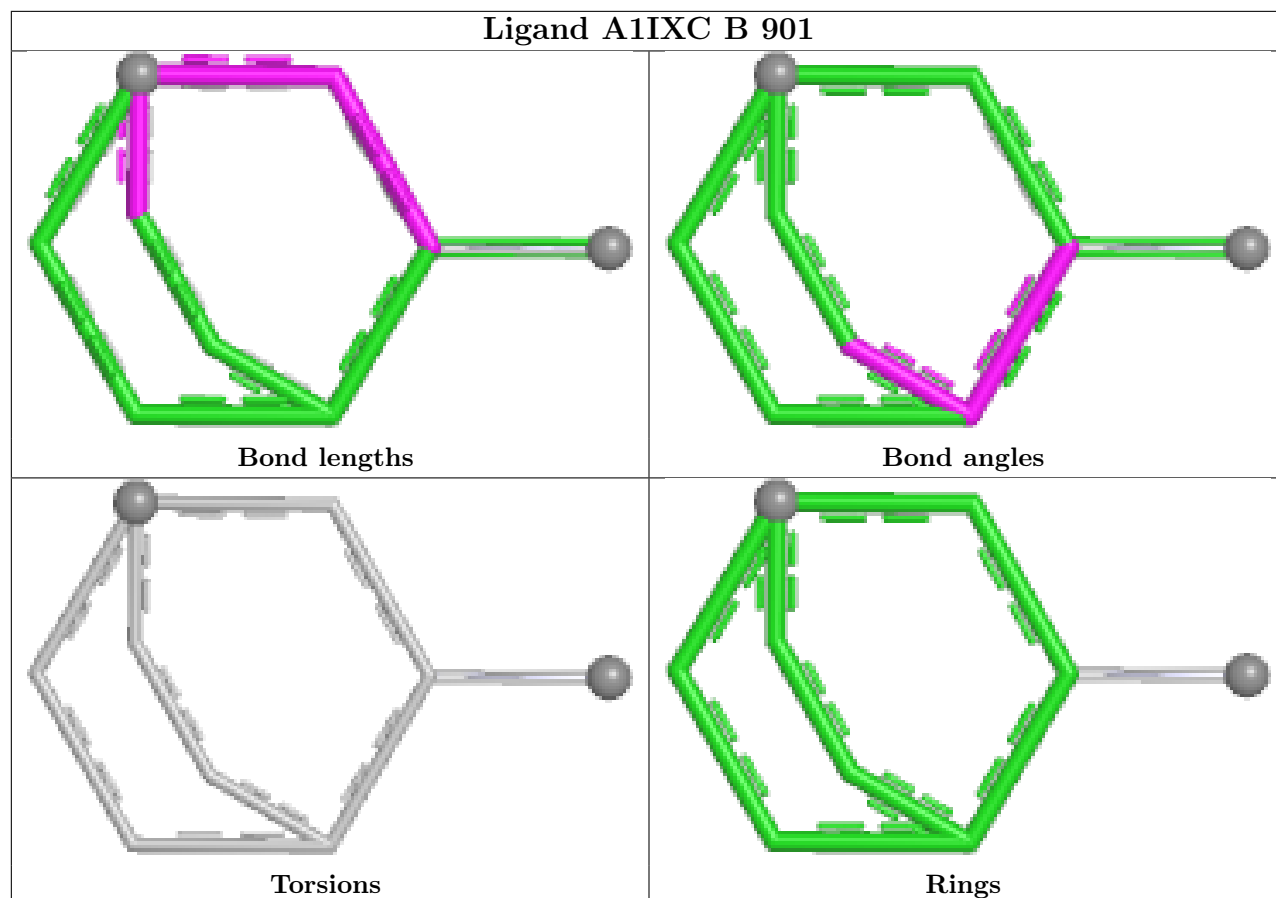
There are no ring outliers.

No monomer is involved in short contacts.

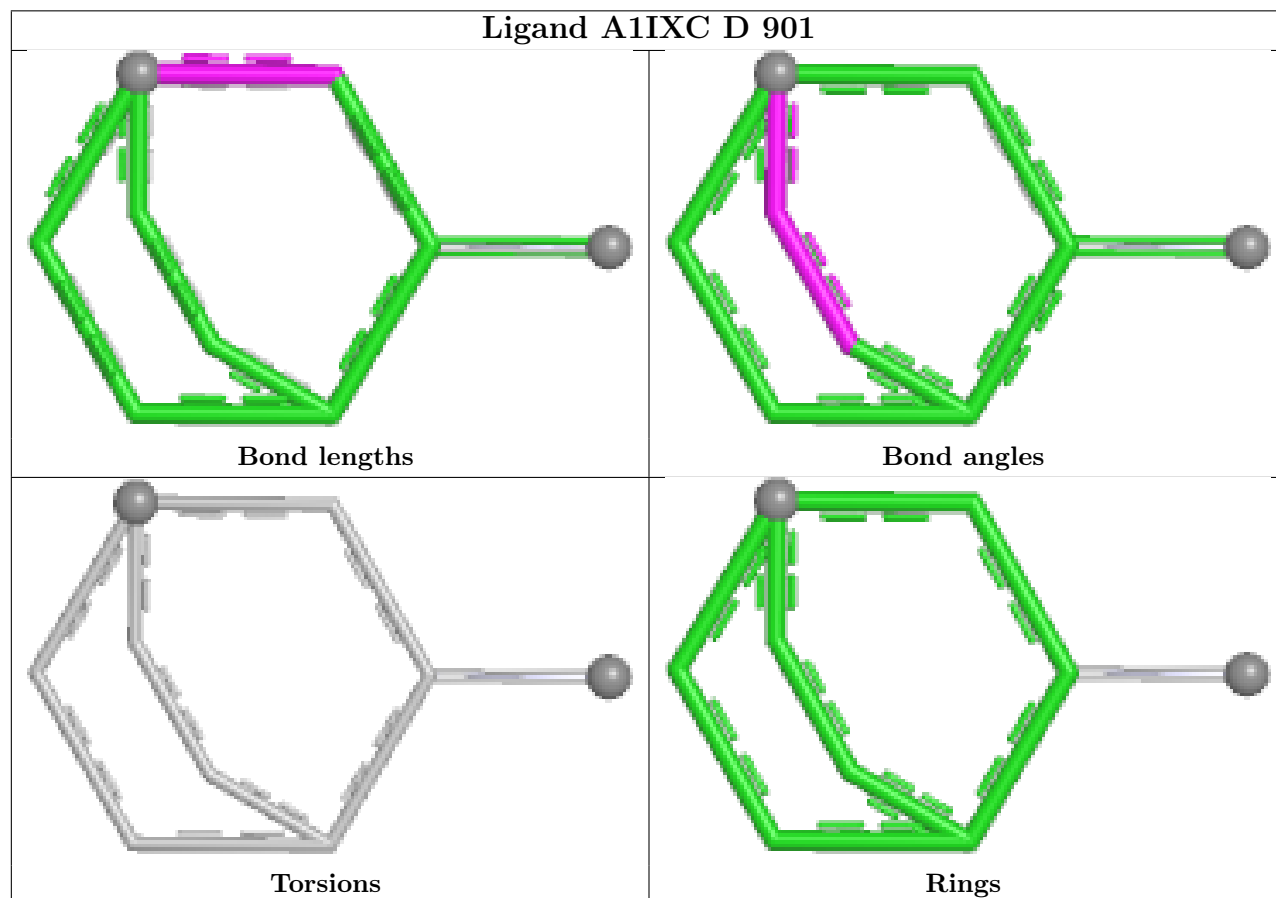
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

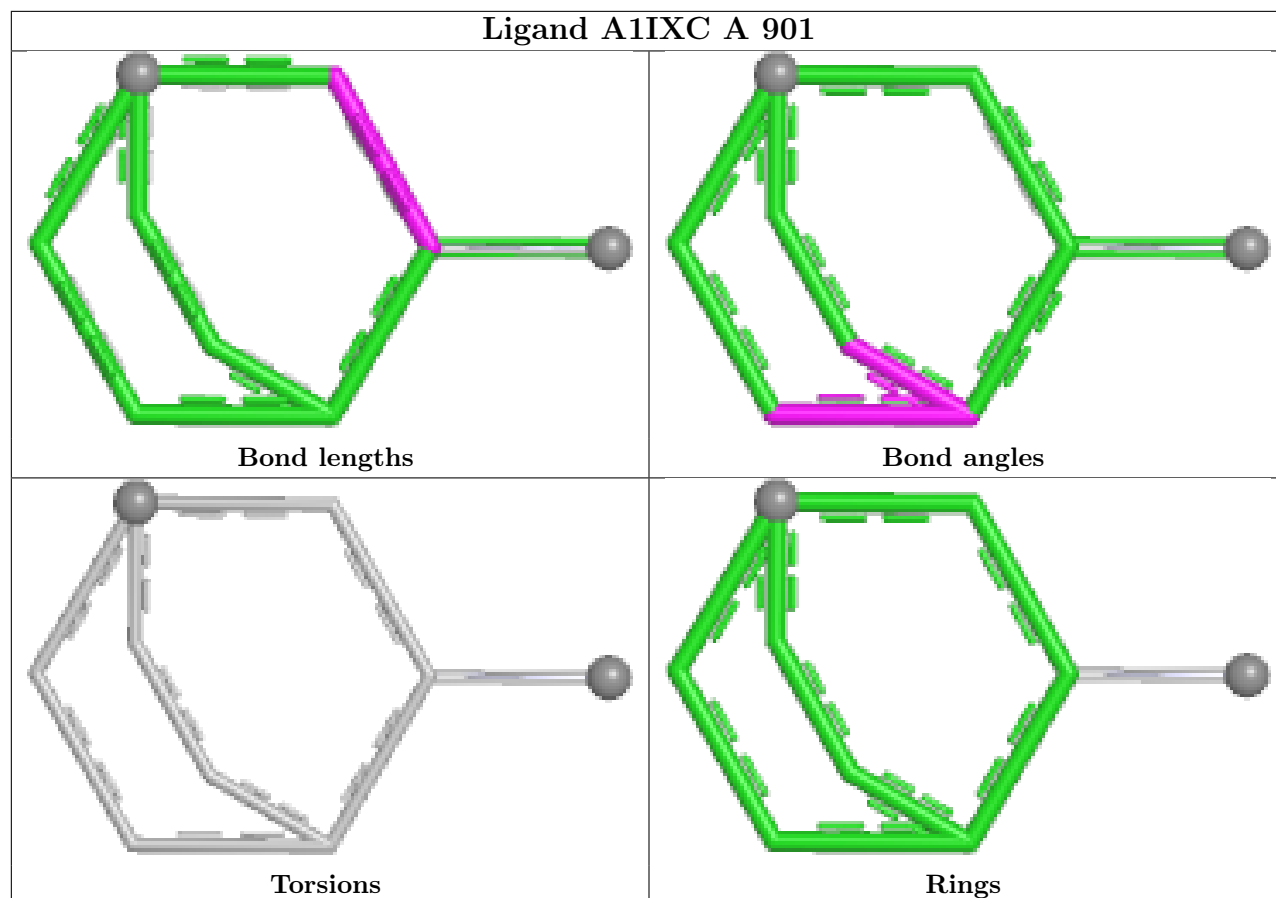


Ligand A1IXC B 901



Ligand A1IXC D 901





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	794/800 (99%)	-0.13	12 (1%) 72 79	13, 20, 33, 54	0
1	B	794/800 (99%)	-0.16	7 (0%) 81 87	12, 20, 33, 52	0
1	C	794/800 (99%)	0.44	63 (7%) 18 19	17, 27, 50, 74	0
1	D	794/800 (99%)	0.14	19 (2%) 59 66	16, 24, 39, 58	0
All	All	3176/3200 (99%)	0.07	101 (3%) 50 54	12, 22, 41, 74	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	526	GLY	5.2
1	D	53	HIS	4.7
1	A	285	ARG	4.6
1	A	526	GLY	4.6
1	A	53	HIS	4.1
1	C	827	VAL	4.1
1	C	53	HIS	4.1
1	C	766	GLY	4.1
1	D	54	ILE	4.0
1	C	646	ALA	3.8
1	C	625	LEU	3.7
1	C	526	GLY	3.7
1	C	647	GLY	3.7
1	C	635	ALA	3.7
1	C	54	ILE	3.7
1	B	765	SER	3.6
1	D	766	GLY	3.6
1	C	634	LEU	3.6
1	C	653	ALA	3.6
1	C	645	PHE	3.5
1	B	53	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	648	TYR	3.3
1	C	811	LYS	3.3
1	B	807	LYS	3.2
1	D	526	GLY	3.2
1	C	535	ASP	3.2
1	C	523	LEU	3.2
1	C	803	LEU	3.2
1	C	812	TYR	3.2
1	B	786	MET	3.1
1	A	765	SER	3.1
1	D	250	GLU	3.1
1	D	357	ARG	3.0
1	D	242	GLU	2.9
1	C	652	LEU	2.9
1	A	766	GLY	2.9
1	C	807	LYS	2.9
1	C	786	MET	2.9
1	D	807	LYS	2.8
1	D	772	GLU	2.8
1	D	540	ASP	2.8
1	A	684	ARG	2.8
1	A	540	ASP	2.7
1	C	718	ARG	2.7
1	B	273	ARG	2.6
1	D	290	ARG	2.6
1	C	651	ILE	2.6
1	B	426	ARG	2.6
1	C	242	GLU	2.6
1	C	630	ARG	2.5
1	C	802	LEU	2.5
1	C	643	ALA	2.5
1	C	632	TYR	2.5
1	C	649	ASP	2.5
1	A	242	GLU	2.4
1	C	543	GLU	2.4
1	C	626	VAL	2.4
1	D	647	GLY	2.4
1	A	786	MET	2.4
1	C	797	LEU	2.4
1	D	635	ALA	2.4
1	C	809	PRO	2.4
1	C	808	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	842	MET	2.3
1	C	516	VAL	2.3
1	C	357	ARG	2.3
1	A	528	LYS	2.3
1	C	831	LYS	2.3
1	A	250	GLU	2.3
1	C	524	TRP	2.3
1	C	801	LEU	2.3
1	C	633	THR	2.3
1	D	527	LYS	2.3
1	C	650	GLN	2.3
1	C	833	VAL	2.3
1	C	640	ALA	2.2
1	D	771	PRO	2.2
1	C	656	LEU	2.2
1	C	56	ASP	2.2
1	C	819	VAL	2.2
1	C	536	LEU	2.2
1	C	540	ASP	2.2
1	D	765	SER	2.1
1	C	637	LEU	2.1
1	C	202	PHE	2.1
1	C	838	ILE	2.1
1	A	527	LYS	2.1
1	D	439	LYS	2.1
1	D	163	GLU	2.1
1	C	622	ILE	2.1
1	C	527	LYS	2.1
1	C	639	GLU	2.1
1	C	642	LYS	2.1
1	D	535	ASP	2.1
1	C	545	PHE	2.0
1	C	765	SER	2.0
1	C	520	GLY	2.0
1	C	290	ARG	2.0
1	C	250	GLU	2.0
1	C	287	THR	2.0
1	C	285	ARG	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 [i](#)

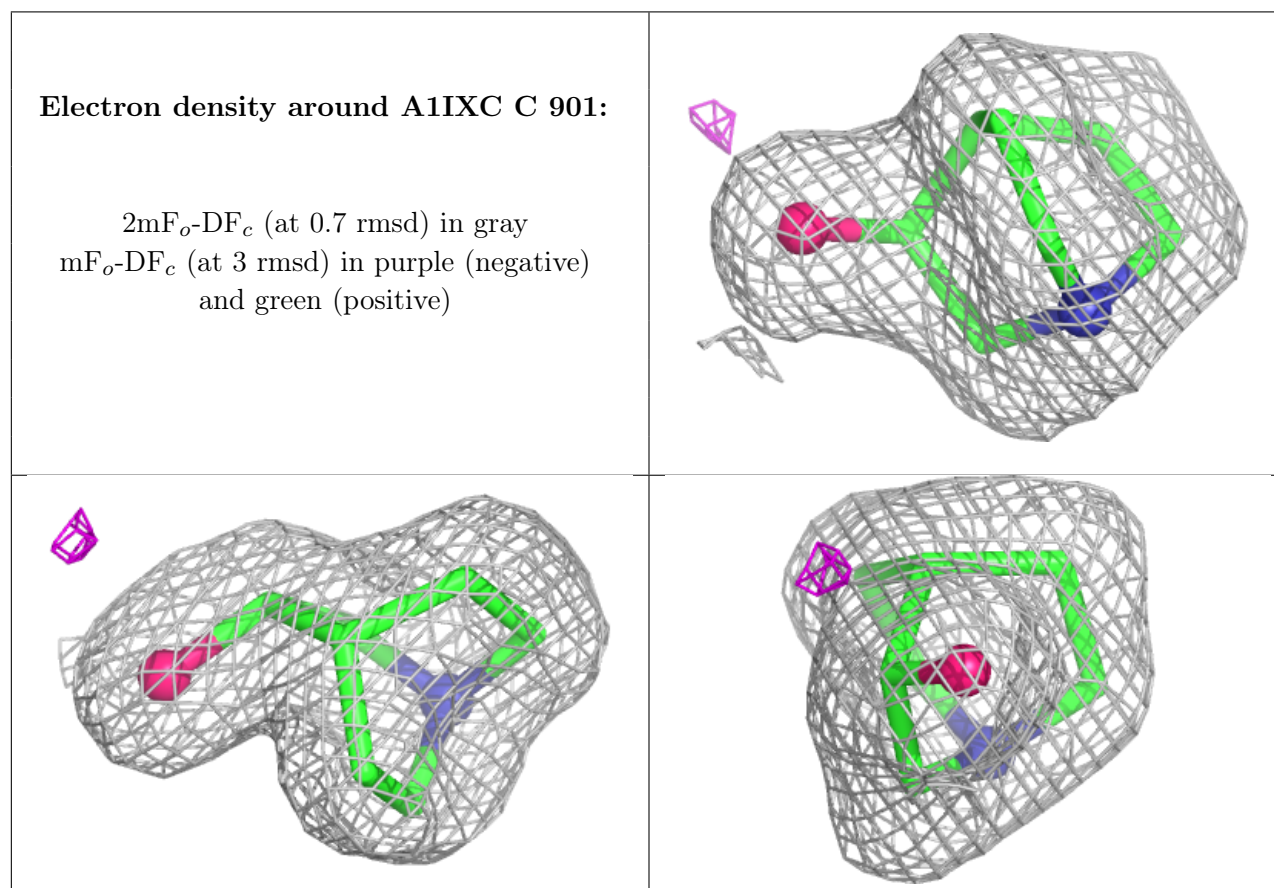
There are no oligosaccharides in this entry.

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.

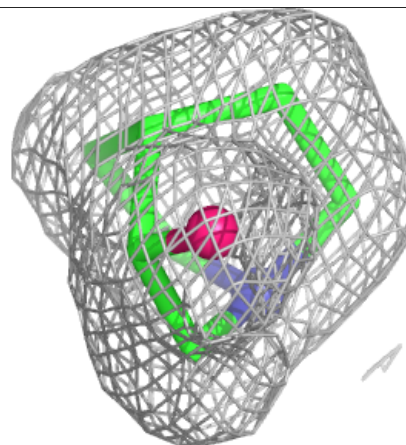
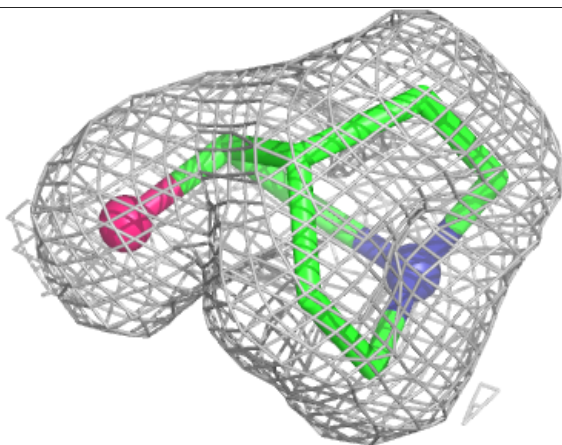
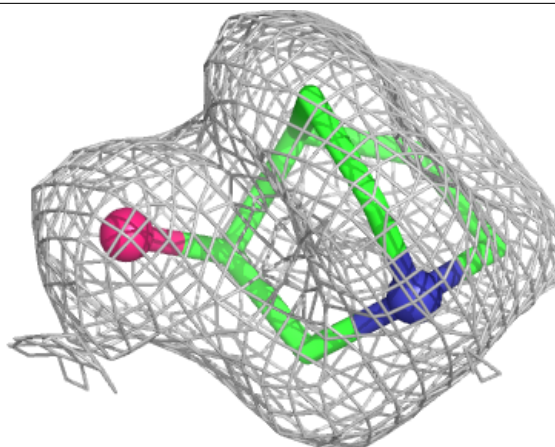
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1IXC	C	901	9/9	0.96	0.06	20,21,22,23	0
2	A1IXC	D	901	9/9	0.96	0.06	16,17,18,19	0
2	A1IXC	A	901	9/9	0.97	0.06	14,15,15,16	0
2	A1IXC	B	901	9/9	0.97	0.05	13,14,14,16	0

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.



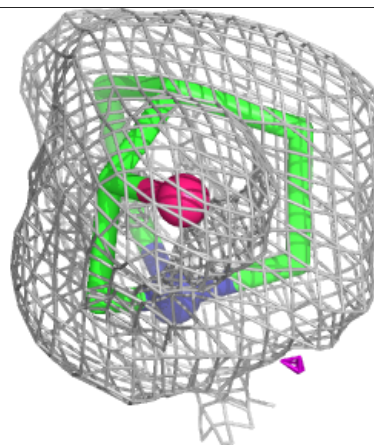
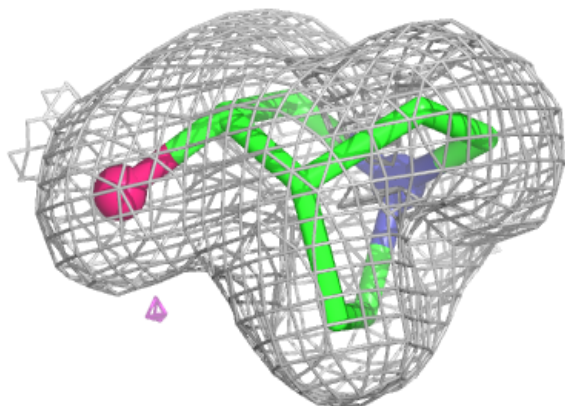
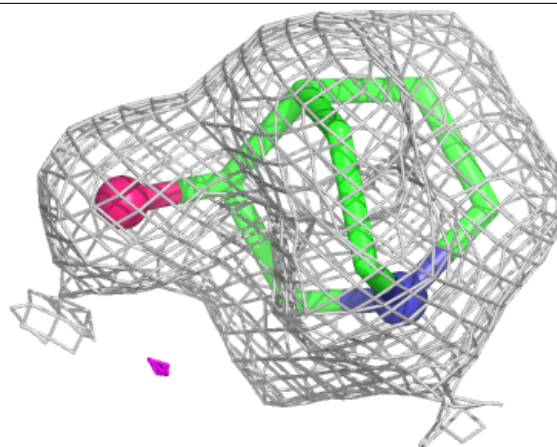
Electron density around A1IXC D 901:

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



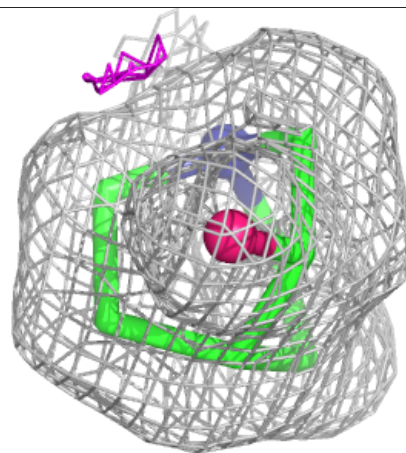
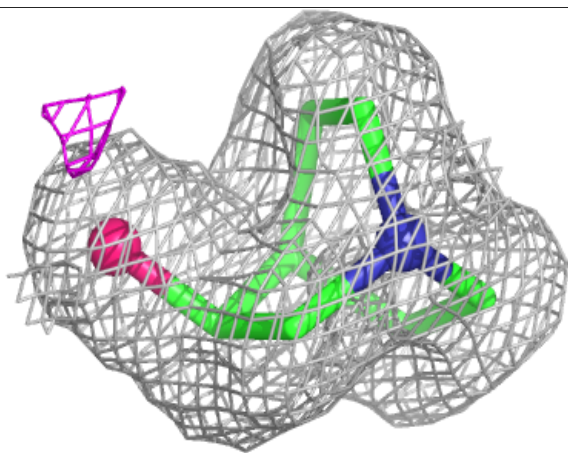
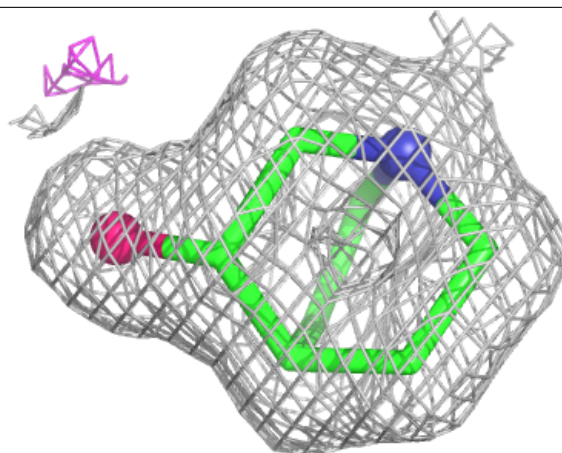
Electron density around A1IXC A 901:

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



Electron density around A1IXC B 901:

$2mF_o-DF_c$ (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.