



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:22 AM UTC

PDB ID : 9HTB / pdb\_00009htb  
Title : CutC in complex with inhibitor2  
Authors : Petersen, J.  
Deposited on : 2024-12-19  
Resolution : 1.58 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](mailto: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>.

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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

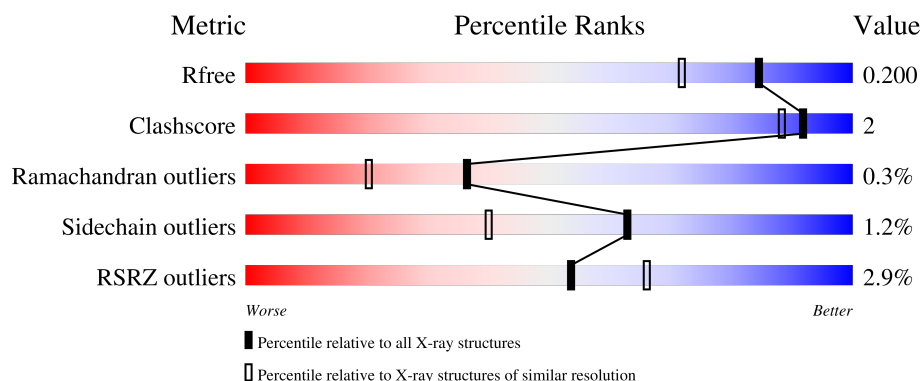
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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  $\geq 3$ , 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> <div></div> <div>95%</div> <div>5%</div> <div>..</div> </div> </div>
1	B	800	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>..</div> </div> </div>
1	C	800	<div> <div>5%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>.</div> </div> </div>
1	D	800	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>5%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27112 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	1	0
			6266	3973	1062	1186	45			
1	B	794	Total	C	N	O	S	0	2	0
			6270	3977	1062	1186	45			
1	C	794	Total	C	N	O	S	0	2	0
			6271	3979	1062	1185	45			
1	D	794	Total	C	N	O	S	0	2	0
			6270	3977	1062	1186	45			

There are 28 discrepancies between the modelled and reference sequences:

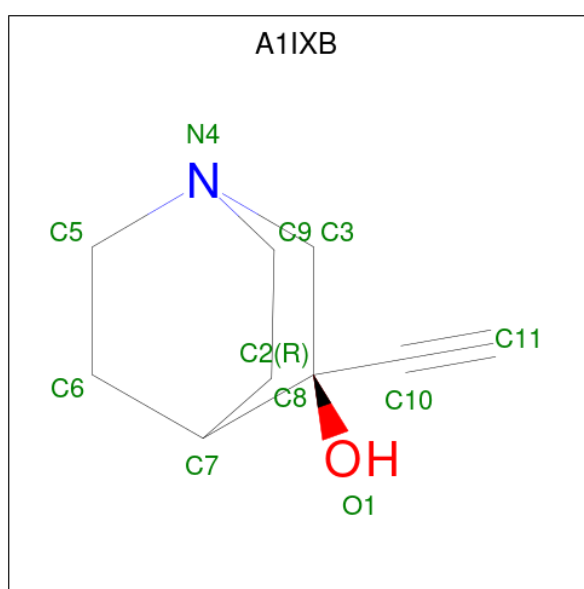
Chain	Residue	Modelled	Actual	Comment	Reference
A	47	MET	-	initiating methionine	UNP Q30W70
A	48	HIS	-	expression tag	UNP Q30W70
A	49	HIS	-	expression tag	UNP Q30W70
A	50	HIS	-	expression tag	UNP Q30W70
A	51	HIS	-	expression tag	UNP Q30W70
A	52	HIS	-	expression tag	UNP Q30W70
A	53	HIS	-	expression tag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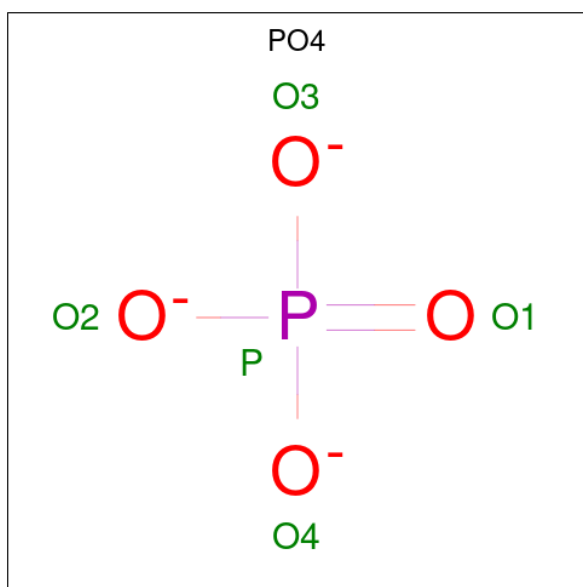
Chain	Residue	Modelled	Actual	Comment	Reference
D	47	MET	-	initiating methionine	UNP Q30W70
D	48	HIS	-	expression tag	UNP Q30W70
D	49	HIS	-	expression tag	UNP Q30W70
D	50	HIS	-	expression tag	UNP Q30W70
D	51	HIS	-	expression tag	UNP Q30W70
D	52	HIS	-	expression tag	UNP Q30W70
D	53	HIS	-	expression tag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

- Molecule 2 is (3 {R})-3-ethynyl-1-azabicyclo[2.2.2]octan-3-ol (CCD ID: A1IXB) (formula: C<sub>9</sub>H<sub>13</sub>NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	9	1	1		
2	B	1	Total	C	N	O	0	0
			11	9	1	1		
2	C	1	Total	C	N	O	0	0
			11	9	1	1		
2	D	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).

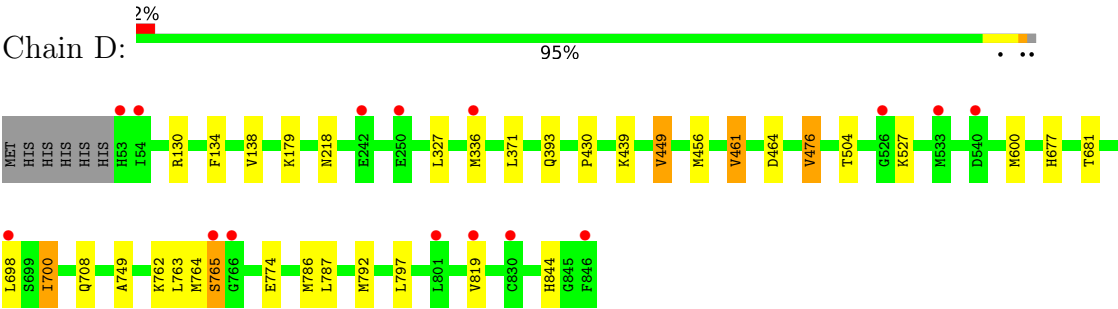


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	527	Total	O	0	0
			527	527		
4	B	561	Total	O	0	0
			561	561		
4	C	437	Total	O	0	0
			437	437		
4	D	461	Total	O	0	0
			461	461		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.86Å 104.90Å 119.72Å 102.55° 108.39° 104.81°	Depositor
Resolution (Å)	107.45 – 1.58 107.45 – 1.58	Depositor EDS
% Data completeness (in resolution range)	78.2 (107.45-1.58) 78.2 (107.45-1.58)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 1.58Å)	Xtriage
Refinement program	BUSTER 2.11.8 (8-JUN-2022) PACIOREK	Depositor
R, $R_{free}$	0.182 , 0.207 0.175 , 0.200	Depositor DCC
$R_{free}$ test set	18498 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	27112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, A1IXB

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	0.84	2/6414 (0.0%)	0.98	13/8686 (0.1%)
1	B	0.86	3/6421 (0.0%)	0.98	12/8696 (0.1%)
1	C	0.77	3/6422 (0.0%)	0.96	8/8698 (0.1%)
1	D	0.78	2/6421 (0.0%)	0.97	8/8696 (0.1%)
All	All	0.81	10/25678 (0.0%)	0.97	41/34776 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	533	MET	SD-CE	-7.93	1.59	1.79
1	C	134	PHE	C-N	5.76	1.41	1.33
1	D	600	MET	SD-CE	-5.67	1.65	1.79
1	D	134	PHE	C-N	5.53	1.41	1.34
1	A	134	PHE	C-N	5.53	1.40	1.33
1	A	533	MET	SD-CE	5.51	1.93	1.79
1	B	134	PHE	C-N	5.51	1.41	1.34
1	C	700	ILE	CA-C	5.30	1.59	1.52
1	B	533	MET	CA-C	5.29	1.59	1.52
1	B	336	MET	CA-C	-5.23	1.46	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	527	LYS	N-CA-C	8.06	120.22	108.86
1	C	527	LYS	N-CA-C	7.90	120.00	108.86
1	D	527	LYS	N-CA-C	7.90	119.99	108.86
1	A	527	LYS	N-CA-C	7.83	119.90	108.86
1	D	476	VAL	N-CA-CB	-7.36	99.16	111.38
1	B	476	VAL	N-CA-CB	-7.31	99.25	111.38
1	A	476	VAL	N-CA-CB	-7.19	99.44	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	476	VAL	N-CA-CB	-7.02	99.73	111.38
1	C	504	THR	N-CA-C	-6.89	104.87	113.55
1	C	138	VAL	N-CA-C	-6.67	105.25	111.45
1	B	764	MET	CA-C-N	6.37	133.70	121.54
1	B	764	MET	C-N-CA	6.37	133.70	121.54
1	A	504	THR	N-CA-C	-6.26	105.66	113.55
1	B	504	THR	N-CA-C	-6.18	105.77	113.55
1	D	504	THR	N-CA-C	-6.07	105.90	113.55
1	A	461	VAL	N-CA-CB	6.07	118.27	110.99
1	A	559	ASN	CA-CB-CG	-5.78	106.82	112.60
1	C	393	GLN	N-CA-C	5.77	117.82	109.04
1	D	138	VAL	N-CA-C	-5.62	106.23	111.45
1	D	393	GLN	N-CA-C	5.59	117.54	109.04
1	A	764	MET	CA-C-N	5.50	132.05	121.54
1	A	764	MET	C-N-CA	5.50	132.05	121.54
1	C	182	ASP	CA-CB-CG	5.49	118.08	112.60
1	A	393	GLN	N-CA-C	5.42	117.28	109.04
1	D	749	ALA	N-CA-C	-5.33	98.61	107.99
1	B	138	VAL	N-CA-C	-5.31	106.51	111.45
1	C	749	ALA	N-CA-C	-5.31	98.65	107.99
1	A	765	SER	N-CA-C	5.28	122.04	110.80
1	B	749	ALA	N-CA-C	-5.27	98.72	107.99
1	A	791	GLU	CB-CG-CD	5.23	121.50	112.60
1	A	749	ALA	N-CA-C	-5.22	98.80	107.99
1	D	464	ASP	N-CA-C	5.21	116.95	111.28
1	B	763	LEU	CD1-CG-CD2	5.19	122.22	110.80
1	B	795	ASN	N-CA-C	-5.19	101.25	109.76
1	B	765	SER	N-CA-C	5.16	121.80	110.80
1	D	765	SER	N-CA-C	5.16	121.78	110.80
1	B	393	GLN	N-CA-C	5.14	116.85	109.04
1	C	795	ASN	N-CA-C	-5.07	101.44	109.76
1	A	464	ASP	N-CA-C	5.03	116.77	111.28
1	B	182	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	460	ALA	N-CA-C	-5.00	101.80	109.76

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	6266	0	6140	20	0
1	B	6270	0	6149	24	0
1	C	6271	0	6153	25	0
1	D	6270	0	6149	22	0
2	A	11	0	0	3	0
2	B	11	0	0	3	0
2	C	11	0	0	1	0
2	D	11	0	0	1	0
3	D	5	0	0	0	0
4	A	527	0	0	4	0
4	B	561	0	0	5	0
4	C	437	0	0	2	0
4	D	461	0	0	2	0
All	All	27112	0	24591	77	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 2.

All (77) 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:A:787:LEU:HD23	1:C:439:LYS:HD3	1.50	0.92
1:B:333:GLN:HG3	1:B:336:MET:HE1	1.52	0.91
1:A:439:LYS:HD3	1:C:787:LEU:HD23	1.51	0.90
1:A:764:MET:HE2	1:A:844:HIS:NE2	1.96	0.80
1:D:764:MET:HE2	1:D:844:HIS:NE2	1.97	0.80
1:C:764:MET:HE2	1:C:844:HIS:NE2	1.99	0.77
1:B:698:LEU:HD12	2:B:901:A1IXB:C11	2.17	0.75
1:B:700:ILE:HD11	2:B:901:A1IXB:C11	2.16	0.75
1:A:528:LYS:NZ	4:A:1001:HOH:O	2.20	0.74
1:B:439:LYS:HD3	1:D:787:LEU:HD23	1.67	0.73
1:C:700:ILE:HD11	2:C:901:A1IXB:C11	2.21	0.69
1:B:439:LYS:HD3	1:D:787:LEU:CD2	2.22	0.68
1:A:139:ALA:CB	1:A:211:VAL:HG13	2.24	0.67
1:B:130:ARG:HD2	4:B:1129:HOH:O	2.00	0.61
1:A:764:MET:HE2	1:A:844:HIS:CD2	2.36	0.61
1:A:130:ARG:HD2	4:A:1066:HOH:O	2.02	0.59
1:C:179:LYS:NZ	1:D:179:LYS:HZ2	1.99	0.59
1:D:764:MET:HE2	1:D:844:HIS:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:LYS:HD2	1:A:797:LEU:HD11	1.85	0.58
1:D:762:LYS:HD2	1:D:797:LEU:HD11	1.85	0.58
1:D:130:ARG:HD2	4:D:1031:HOH:O	2.04	0.57
1:B:762:LYS:HD2	1:B:797:LEU:HD11	1.87	0.57
1:C:762:LYS:HD2	1:C:797:LEU:HD11	1.87	0.56
1:A:787:LEU:CD2	1:C:439:LYS:HD3	2.30	0.55
1:C:764:MET:HE2	1:C:844:HIS:CD2	2.41	0.55
1:B:550:LYS:HE2	4:B:1484:HOH:O	2.05	0.55
1:D:700:ILE:HD11	2:D:901:A1IXB:C11	2.37	0.55
1:C:179:LYS:HZ1	1:D:179:LYS:HZ2	1.55	0.55
1:C:677:HIS:O	1:C:681:THR:HG23	2.07	0.54
1:B:528:LYS:NZ	4:B:1002:HOH:O	2.37	0.54
1:B:461[B]:VAL:CG2	1:B:792:MET:HG2	2.37	0.54
1:C:179:LYS:NZ	1:D:179:LYS:NZ	2.55	0.54
1:D:677:HIS:O	1:D:681:THR:HG23	2.08	0.53
1:A:698:LEU:HD12	2:A:901:A1IXB:C11	2.38	0.53
1:A:677:HIS:O	1:A:681:THR:HG23	2.11	0.51
1:B:677:HIS:O	1:B:681:THR:HG23	2.10	0.51
1:A:700:ILE:HD11	2:A:901:A1IXB:C11	2.41	0.50
1:C:446:LYS:O	1:C:449:VAL:HG22	2.10	0.50
1:D:708:GLN:HG3	4:D:1143:HOH:O	2.11	0.50
1:C:130:ARG:HD2	4:C:1148:HOH:O	2.10	0.50
1:A:439:LYS:HD3	1:C:787:LEU:CD2	2.33	0.48
1:D:449:VAL:HG21	1:D:774:GLU:HG3	1.94	0.48
1:A:327:LEU:HB3	1:A:336:MET:SD	2.54	0.48
1:C:327:LEU:HB3	1:C:336:MET:SD	2.55	0.47
1:D:461[B]:VAL:CG2	1:D:792:MET:HG2	2.45	0.47
1:B:787:LEU:HD23	1:D:439:LYS:HD3	1.96	0.46
1:D:327:LEU:HB3	1:D:336:MET:SD	2.56	0.46
1:A:211:VAL:HG12	1:A:211:VAL:O	2.16	0.46
1:C:449:VAL:HG21	1:C:774:GLU:HG3	1.97	0.46
1:B:708:GLN:HG3	4:B:1391:HOH:O	2.17	0.45
1:C:179:LYS:HZ2	1:D:179:LYS:NZ	2.15	0.44
1:C:216:ASP:HA	1:C:487:MET:SD	2.57	0.44
1:B:169:ARG:HD3	4:B:1471:HOH:O	2.16	0.44
1:A:708:GLN:HG3	4:A:1257:HOH:O	2.17	0.44
1:B:336:MET:HB2	1:B:336:MET:HE3	1.73	0.43
1:B:786:MET:SD	1:D:786:MET:SD	3.16	0.43
1:C:708:GLN:HG3	4:C:1317:HOH:O	2.18	0.43
1:B:698:LEU:CD1	2:B:901:A1IXB:C11	2.92	0.43
1:C:371:LEU:HD22	1:C:430:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:MET:HE3	1:D:456:MET:HB3	1.92	0.43
1:C:461[B]:VAL:CG2	1:C:792:MET:HG2	2.49	0.42
1:B:767:LEU:O	1:B:773:GLY:HA3	2.20	0.42
1:A:698:LEU:CD1	2:A:901:A1IXB:C11	2.97	0.42
1:B:509:TRP:CD1	1:B:675:LEU:HD11	2.55	0.41
1:C:456:MET:HB3	1:C:456:MET:HE3	1.81	0.41
1:B:487:MET:HE3	1:B:487:MET:HB3	1.96	0.41
1:B:787:LEU:CD2	1:D:439:LYS:HD3	2.50	0.41
1:A:130:ARG:CD	4:A:1066:HOH:O	2.66	0.41
1:B:371:LEU:HD22	1:B:430:PRO:HD2	2.02	0.41
1:A:179:LYS:NZ	1:B:179:LYS:HZ2	2.19	0.41
1:B:771:PRO:HD2	1:B:772:GLU:OE2	2.21	0.41
1:D:371:LEU:HD22	1:D:430:PRO:HD2	2.03	0.41
1:A:334:THR:HB	1:A:379:TRP:CG	2.56	0.41
1:C:764:MET:CE	1:C:844:HIS:NE2	2.78	0.41
1:C:509:TRP:CD1	1:C:675:LEU:HD11	2.56	0.40
1:C:811:LYS:HB3	1:C:811:LYS:HE2	1.95	0.40
1:D:764:MET:CE	1:D:844:HIS:NE2	2.78	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	793/800 (99%)	776 (98%)	15 (2%)	2 (0%)	36	20
1	B	794/800 (99%)	775 (98%)	16 (2%)	3 (0%)	30	12
1	C	794/800 (99%)	775 (98%)	17 (2%)	2 (0%)	36	20
1	D	794/800 (99%)	775 (98%)	17 (2%)	2 (0%)	36	20
All	All	3175/3200 (99%)	3101 (98%)	65 (2%)	9 (0%)	36	20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	765	SER
1	C	765	SER
1	D	765	SER
1	A	765	SER
1	A	700	ILE
1	B	490	VAL
1	B	700	ILE
1	C	700	ILE
1	D	700	ILE

### 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	670/676 (99%)	662 (99%)	8 (1%)	63	40
1	B	671/676 (99%)	660 (98%)	11 (2%)	55	28
1	C	671/676 (99%)	663 (99%)	8 (1%)	63	40
1	D	671/676 (99%)	663 (99%)	8 (1%)	63	40
All	All	2683/2704 (99%)	2648 (99%)	35 (1%)	63	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	461	VAL
1	A	476	VAL
1	A	533	MET
1	A	698	LEU
1	A	763	LEU
1	A	772	GLU
1	A	819	VAL
1	B	218	ASN
1	B	336	MET
1	B	449	VAL
1	B	461[A]	VAL
1	B	461[B]	VAL

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Mol	Chain	Res	Type
1	B	476	VAL
1	B	533	MET
1	B	698	LEU
1	B	763	LEU
1	B	801	LEU
1	B	819	VAL
1	C	218	ASN
1	C	461[A]	VAL
1	C	461[B]	VAL
1	C	476	VAL
1	C	540	ASP
1	C	698	LEU
1	C	763	LEU
1	C	819	VAL
1	D	218	ASN
1	D	449	VAL
1	D	461[A]	VAL
1	D	461[B]	VAL
1	D	476	VAL
1	D	698	LEU
1	D	763	LEU
1	D	819	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	72	GLN
1	A	116	GLN
1	A	144	GLN
1	A	188	GLN
1	A	308	HIS
1	A	438	ASN
1	A	808	HIS
1	B	68	ASN
1	B	72	GLN
1	B	116	GLN
1	B	308	HIS
1	B	808	HIS
1	C	68	ASN
1	C	72	GLN
1	C	116	GLN

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Mol	Chain	Res	Type
1	C	144	GLN
1	C	218	ASN
1	C	302	ASN
1	C	308	HIS
1	C	438	ASN
1	C	508	GLN
1	C	808	HIS
1	D	68	ASN
1	D	116	GLN
1	D	218	ASN
1	D	302	ASN
1	D	308	HIS
1	D	397	ASN
1	D	508	GLN
1	D	808	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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	A1IXB	A	901	-	11,12,12	1.56	1 (9%)	12,18,18	1.52	3 (25%)
2	A1IXB	B	901	-	11,12,12	1.47	1 (9%)	12,18,18	1.23	1 (8%)
2	A1IXB	C	901	-	11,12,12	1.64	1 (9%)	12,18,18	1.48	1 (8%)
2	A1IXB	D	901	-	11,12,12	1.42	2 (18%)	12,18,18	1.74	3 (25%)
3	PO4	D	902	-	4,4,4	0.31	0	6,6,6	0.37	0

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	A1IXB	B	901	-	-	0/0/24/24	0/3/2/2
2	A1IXB	D	901	-	-	0/0/24/24	0/3/2/2
2	A1IXB	C	901	-	-	0/0/24/24	0/3/2/2
2	A1IXB	A	901	-	-	0/0/24/24	0/3/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	A1IXB	C3-C2	3.04	1.58	1.54
2	D	901	A1IXB	C3-C2	2.24	1.57	1.54
2	D	901	A1IXB	C2-C10	-2.20	1.46	1.48
2	A	901	A1IXB	C3-C2	2.17	1.57	1.54
2	B	901	A1IXB	C2-C10	-2.17	1.46	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	A1IXB	C8-C7-C2	-4.76	106.77	109.46
2	C	901	A1IXB	C6-C7-C2	-3.73	107.35	109.46
2	A	901	A1IXB	C8-C7-C2	-2.73	107.92	109.46
2	A	901	A1IXB	C6-C7-C8	-2.46	104.28	109.08
2	D	901	A1IXB	C6-C7-C2	-2.45	108.07	109.46
2	A	901	A1IXB	C9-N4-C3	-2.11	106.31	109.46
2	D	901	A1IXB	O1-C2-C7	-2.05	104.97	109.38
2	B	901	A1IXB	C6-C7-C2	-2.05	108.30	109.46

There are no chirality outliers.

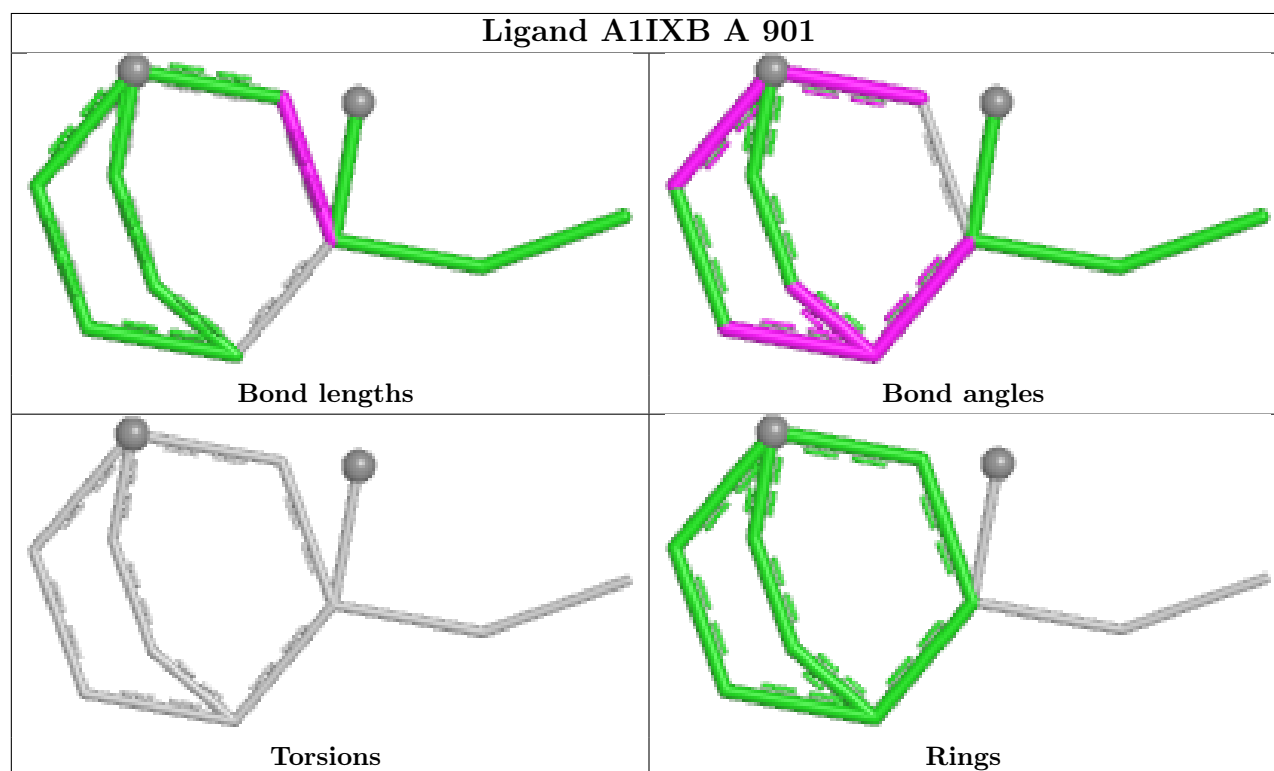
There are no torsion outliers.

There are no ring outliers.

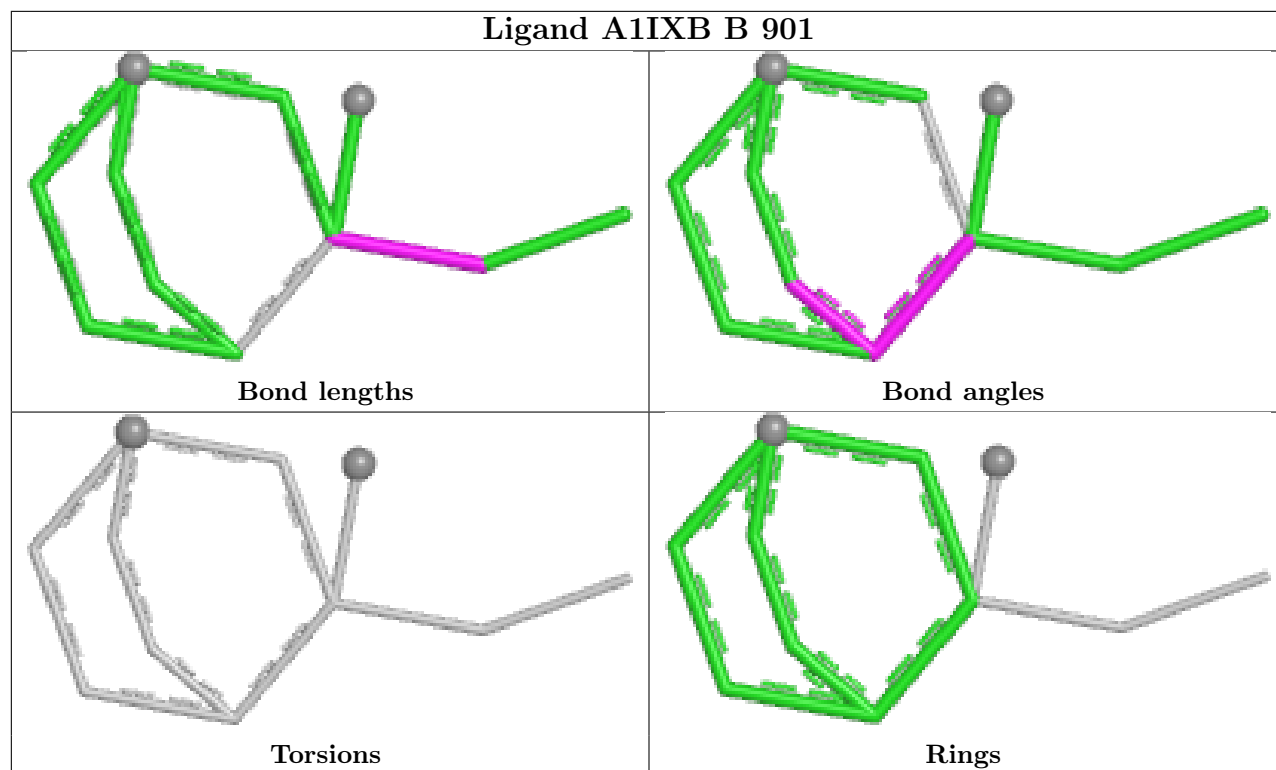
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	A1IXB	3	0
2	B	901	A1IXB	3	0
2	C	901	A1IXB	1	0
2	D	901	A1IXB	1	0

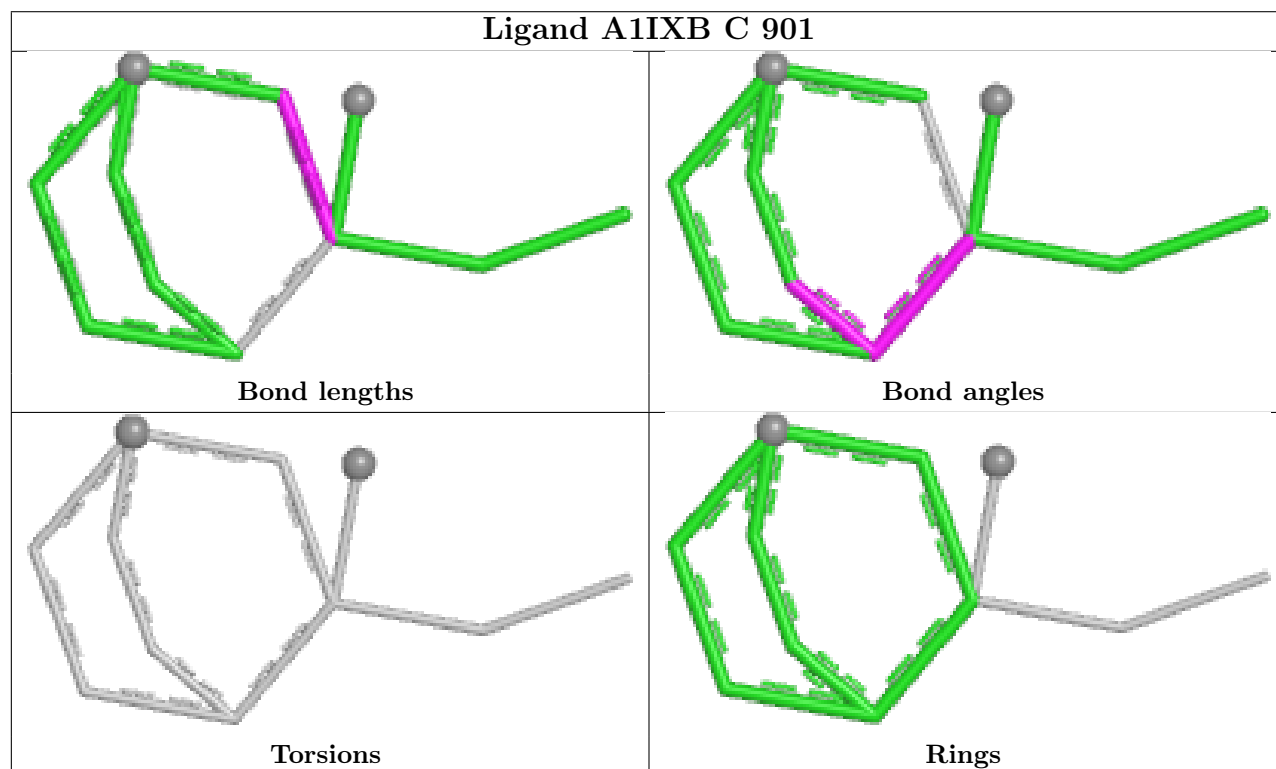
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

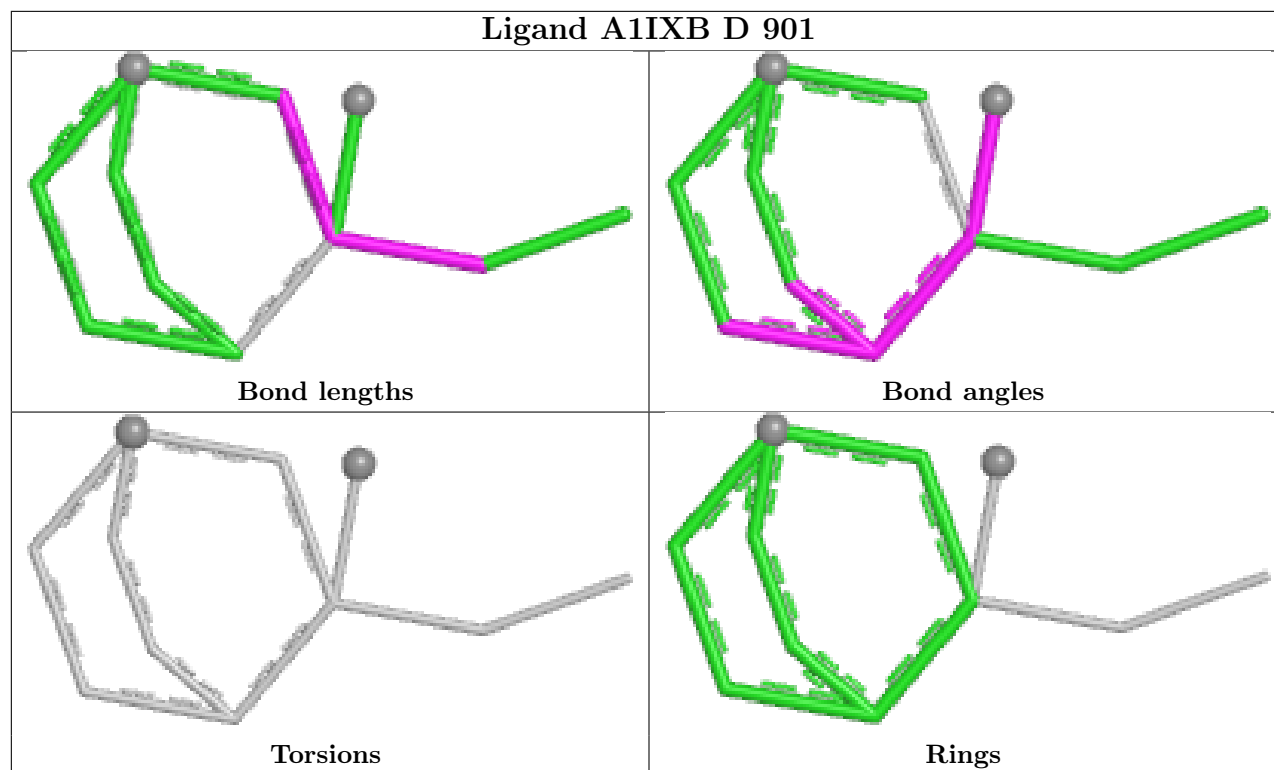


## Ligand A1IXB B 901



## Ligand A1IXB C 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	794/800 (99%)	-0.02	17 (2%) 63 73	9, 18, 32, 45	1 (0%)
1	B	794/800 (99%)	-0.05	16 (2%) 65 74	8, 17, 31, 43	2 (0%)
1	C	794/800 (99%)	0.39	43 (5%) 31 42	12, 24, 44, 59	2 (0%)
1	D	794/800 (99%)	0.21	15 (1%) 66 75	12, 22, 39, 50	2 (0%)
All	All	3176/3200 (99%)	0.13	91 (2%) 53 66	8, 20, 38, 59	7 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	HIS	5.9
1	C	698	LEU	5.0
1	C	54	ILE	4.9
1	D	53	HIS	4.9
1	C	526	GLY	4.7
1	D	526	GLY	4.6
1	C	540	ASP	4.2
1	B	53	HIS	3.9
1	D	846	PHE	3.8
1	D	698	LEU	3.8
1	B	526	GLY	3.7
1	A	698	LEU	3.6
1	A	53	HIS	3.6
1	C	645	PHE	3.6
1	A	526	GLY	3.5
1	C	846	PHE	3.5
1	D	765	SER	3.5
1	B	698	LEU	3.5
1	D	54	ILE	3.3
1	B	765	SER	3.1
1	C	625	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	827	VAL	3.0
1	C	766	GLY	2.9
1	B	533	MET	2.9
1	C	657	ALA	2.8
1	A	535	ASP	2.8
1	C	535	ASP	2.7
1	D	540	ASP	2.7
1	A	846	PHE	2.7
1	C	631	LYS	2.7
1	A	540	ASP	2.7
1	A	54	ILE	2.7
1	C	523	LEU	2.6
1	C	819	VAL	2.6
1	C	352	ASP	2.6
1	A	238	ARG	2.6
1	C	800	GLU	2.6
1	C	765	SER	2.6
1	A	765	SER	2.5
1	C	634	LEU	2.4
1	C	633	THR	2.4
1	D	819	VAL	2.4
1	D	336	MET	2.4
1	C	637	LEU	2.4
1	C	803	LEU	2.4
1	C	653	ALA	2.3
1	B	819	VAL	2.3
1	B	807	LYS	2.3
1	C	651	ILE	2.3
1	C	656	LEU	2.3
1	D	242	GLU	2.3
1	C	632	TYR	2.3
1	C	297	LYS	2.3
1	A	336	MET	2.3
1	C	646	ALA	2.3
1	C	769	ASP	2.3
1	D	533	MET	2.3
1	B	535	ASP	2.2
1	B	846	PHE	2.2
1	A	733	ALA	2.2
1	A	211	VAL	2.2
1	A	328	VAL	2.2
1	C	767	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	533	MET	2.2
1	A	408	HIS	2.2
1	C	844	HIS	2.2
1	B	830	CYS	2.2
1	D	830	CYS	2.2
1	D	766	GLY	2.2
1	C	328[A]	VAL	2.2
1	C	811	LYS	2.1
1	B	766	GLY	2.1
1	B	54	ILE	2.1
1	B	734	ASP	2.1
1	C	650	GLN	2.1
1	C	647	GLY	2.1
1	D	250	GLU	2.1
1	B	540	ASP	2.1
1	C	336	MET	2.1
1	C	287	THR	2.0
1	A	285	ARG	2.0
1	C	843	LEU	2.0
1	D	801	LEU	2.0
1	A	242	GLU	2.0
1	C	648	TYR	2.0
1	B	786	MET	2.0
1	C	288	ASP	2.0
1	C	845	GLY	2.0
1	C	630	ARG	2.0
1	B	242	GLU	2.0
1	C	525	TYR	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.

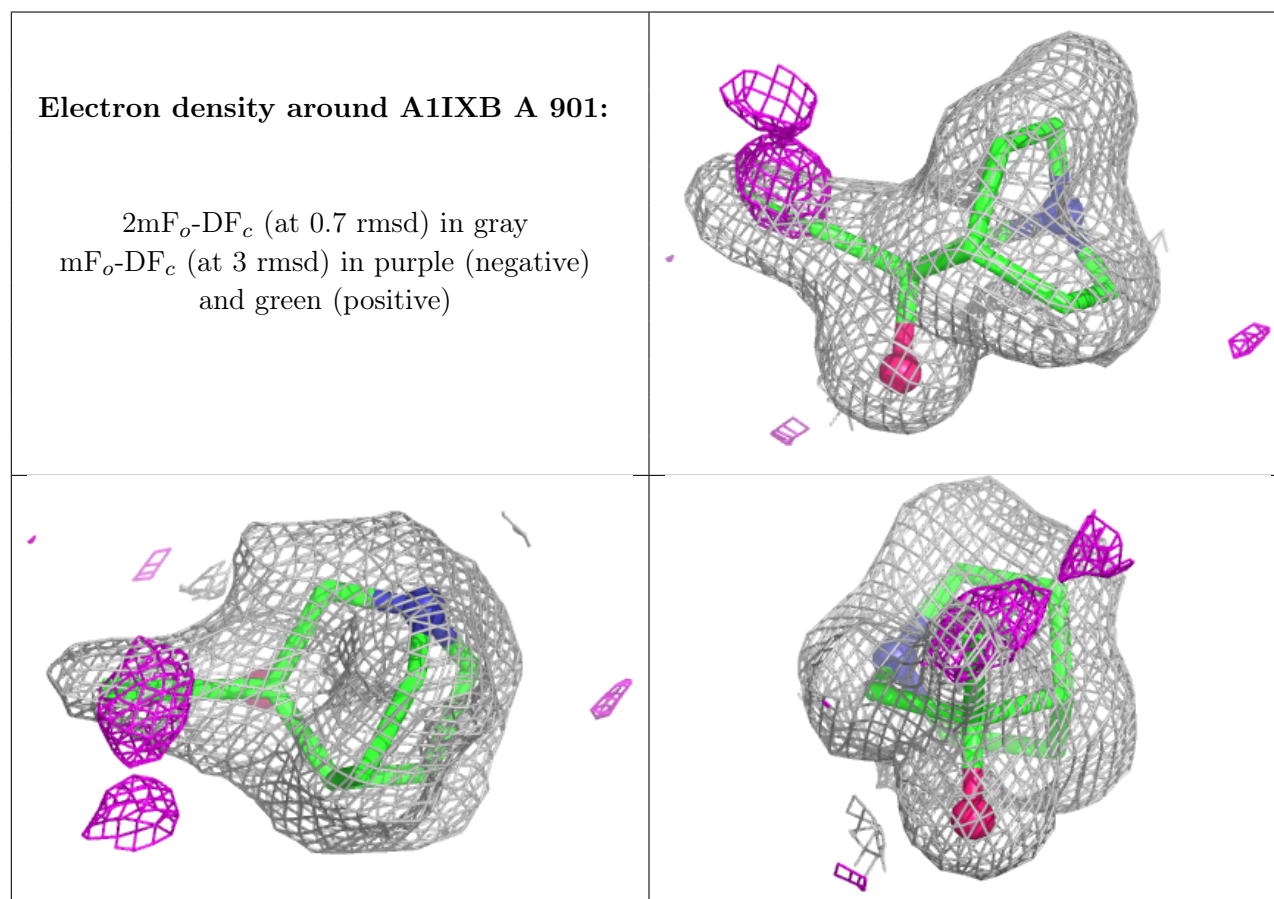
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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.

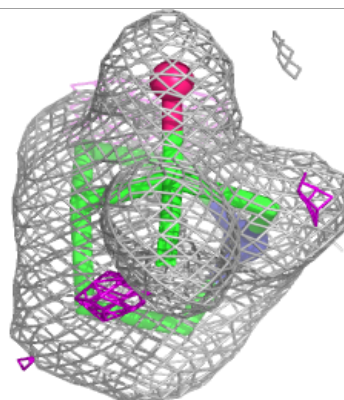
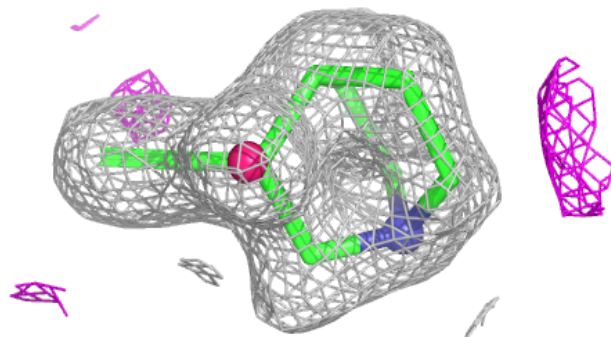
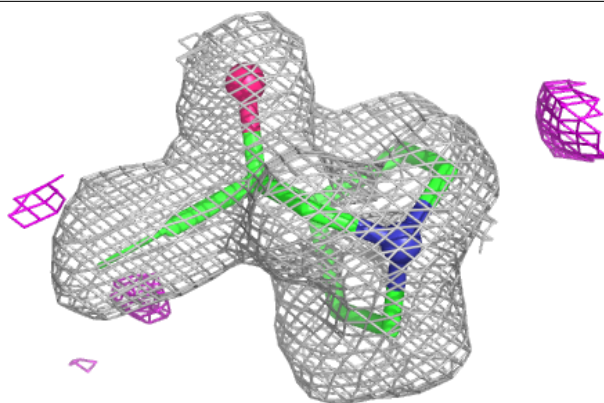
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	A1IXB	A	901	11/11	0.92	0.09	18,20,24,25	0
2	A1IXB	B	901	11/11	0.92	0.08	20,21,25,25	0
2	A1IXB	C	901	11/11	0.93	0.08	26,27,29,29	0
2	A1IXB	D	901	11/11	0.95	0.08	24,25,28,29	0
3	PO4	D	902	5/5	0.96	0.07	32,32,33,34	0

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.

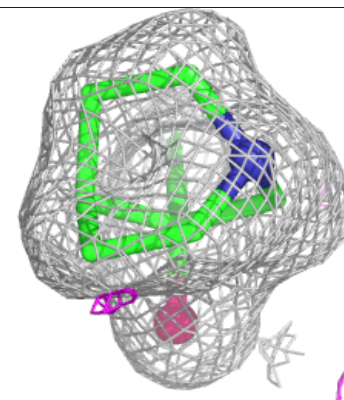
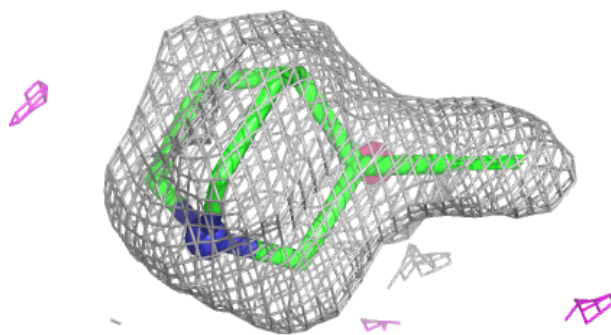
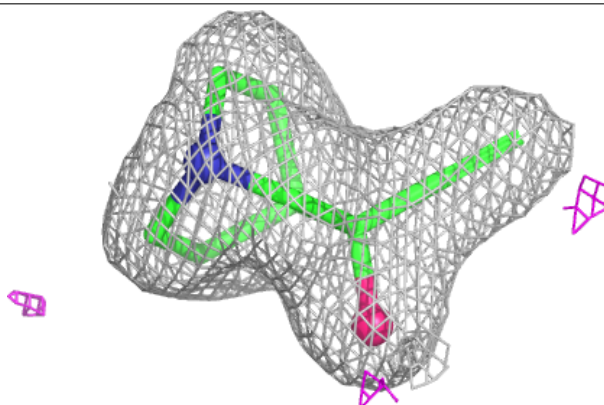


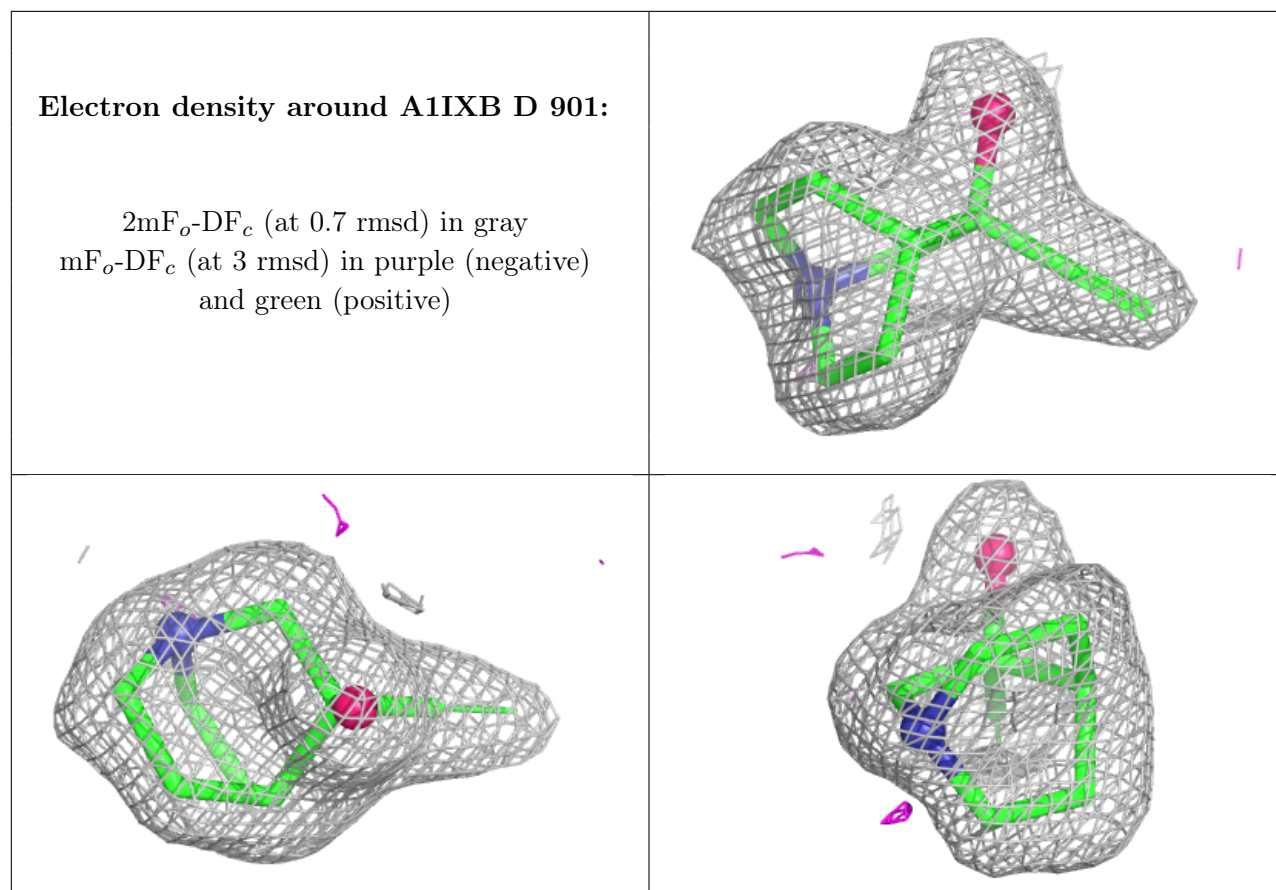
**Electron density around A1IXB B 901:**

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

**Electron density around A1IXB C 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 ⓘ

There are no such residues in this entry.