



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 05:58 AM EDT

PDB ID : 7SVM
Title : DPP8 IN COMPLEX WITH LIGAND ICeD-2
Authors : Lammens, A.; Hollenstein, K.; Klein, D.J.
Deposited on : 2021-11-19
Resolution : 2.69 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 : 2.35.1
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) : 2.35.1

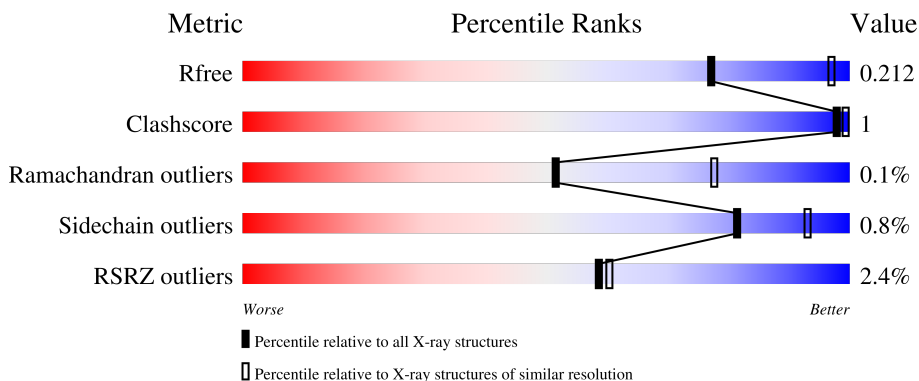
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	898	 2% 91% 5%
1	B	898	 2% 91% 5%
1	C	898	 2% 90% 6%

2 Entry composition [i](#)

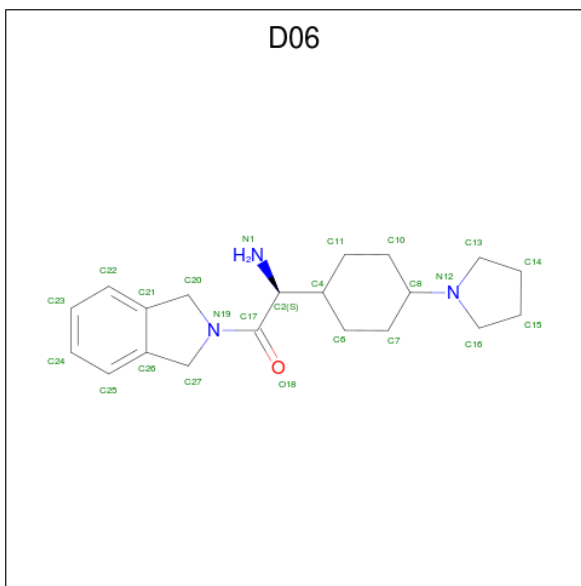
There are 4 unique types of molecules in this entry. The entry contains 21621 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	852	Total 6937	C 4454	N 1166	O 1288	S 29	119	1	0
1	B	852	Total 6953	C 4464	N 1168	O 1290	S 31	117	3	0
1	C	843	Total 6876	C 4413	N 1160	O 1275	S 28	96	2	0

- Molecule 2 is (2S)-2-amino-1-(1,3-dihydro-2H-isoindol-2-yl)-2-[(1r,4S)-4-(pyrrolidin-1-yl)cyclohexyl]ethan-1-one (three-letter code: D06) (formula: C₂₀H₂₉N₃O) (labeled as "Ligand of Interest" by depositor).



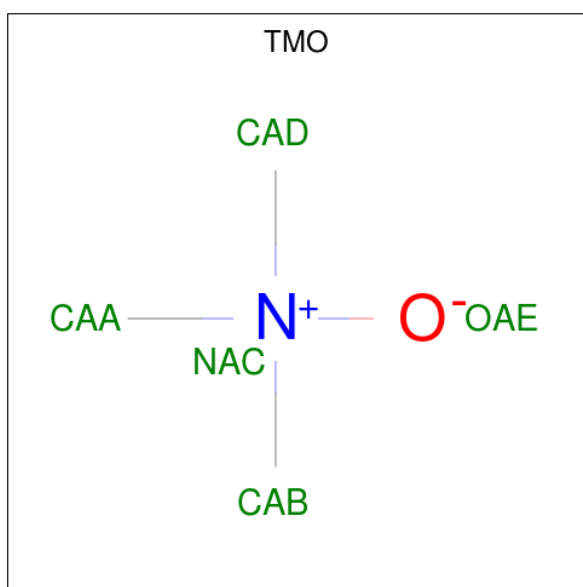
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 24	C 20	N 3	O 1	0	0
2	A	1	Total 24	C 20	N 3	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 24	C 20	N 3	O 1	0	0
2	A	1	Total 24	C 20	N 3	O 1	0	0
2	A	1	Total 24	C 20	N 3	O 1	0	0
2	A	1	Total 24	C 20	N 3	O 1	0	0
2	A	1	Total 24	C 20	N 3	O 1	0	0
2	B	1	Total 24	C 20	N 3	O 1	0	0
2	B	1	Total 24	C 20	N 3	O 1	0	0
2	B	1	Total 24	C 20	N 3	O 1	0	0
2	C	1	Total 24	C 20	N 3	O 1	0	0
2	C	1	Total 24	C 20	N 3	O 1	0	0
2	C	1	Total 24	C 20	N 3	O 1	0	0

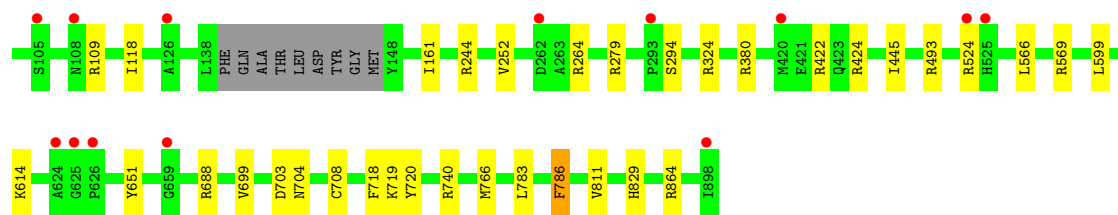
- Molecule 3 is trimethylamine oxide (three-letter code: TMO) (formula: C₃H₉NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total	O	0	0
			162	162		
4	B	141	Total	O	0	0
			141	141		
4	C	170	Total	O	0	0
			170	170		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	162.29Å 244.94Å 261.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	135.29 – 2.69 48.05 – 2.69	Depositor EDS
% Data completeness (in resolution range)	96.1 (135.29-2.69) 96.2 (48.05-2.69)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.176 , 0.216 0.181 , 0.212	Depositor DCC
R_{free} test set	833 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21621	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TMO, D06

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	0.67	4/7130 (0.1%)	0.90	17/9671 (0.2%)
1	B	0.68	5/7146 (0.1%)	0.91	18/9691 (0.2%)
1	C	0.67	2/7066 (0.0%)	0.87	13/9582 (0.1%)
All	All	0.68	11/21342 (0.1%)	0.90	48/28944 (0.2%)

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
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	244	ARG	NE-CZ	13.07	1.50	1.33
1	A	147	MET	SD-CE	8.99	2.28	1.77
1	B	349	MET	SD-CE	8.71	2.26	1.77
1	A	891	ARG	NE-CZ	8.55	1.44	1.33
1	B	424	ARG	CD-NE	7.89	1.59	1.46
1	B	891	ARG	NE-CZ	7.68	1.43	1.33
1	A	424	ARG	NE-CZ	7.36	1.42	1.33
1	B	420	MET	SD-CE	7.17	2.18	1.77
1	C	422	ARG	NE-CZ	6.34	1.41	1.33
1	B	421	GLU	CG-CD	-6.02	1.43	1.51
1	A	355	ARG	CD-NE	-5.05	1.37	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LEU	CA-CB-CG	11.87	142.61	115.30
1	B	324	ARG	NE-CZ-NH2	-8.87	115.87	120.30
1	C	109	ARG	NE-CZ-NH2	8.81	124.71	120.30
1	C	109	ARG	CD-NE-CZ	8.42	135.39	123.60
1	A	891	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	A	324	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	891	ARG	NE-CZ-NH2	7.61	124.10	120.30
1	B	891	ARG	NE-CZ-NH1	-7.47	116.57	120.30
1	A	147	MET	CG-SD-CE	-7.25	88.60	100.20
1	B	422	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	C	109	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	138	LEU	CA-CB-CG	6.76	130.85	115.30
1	B	892	ILE	CB-CG1-CD1	6.57	132.28	113.90
1	A	891	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	B	156	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	156	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	493	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	69	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	324	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	569	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	203	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	401	ARG	CG-CD-NE	5.77	123.92	111.80
1	A	401	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	569	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	422	ARG	CD-NE-CZ	5.63	131.49	123.60
1	C	279	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	247	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	493	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	493	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	786	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	B	401	ARG	CG-CD-NE	5.45	123.24	111.80
1	A	786	PHE	CB-CG-CD2	-5.44	116.99	120.80
1	B	156	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	264	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	156	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	69	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	703	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	380	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	55	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	69	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	C	424	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	740	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	264	ARG	NE-CZ-NH1	5.17	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	493	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	300	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	324	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	349	MET	CG-SD-CE	-5.04	92.14	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	891	ARG	Sidechain
1	B	891	ARG	Sidechain

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	6937	0	6755	7	0
1	B	6953	0	6771	11	0
1	C	6876	0	6701	11	0
2	A	168	0	0	0	0
2	B	72	0	0	0	0
2	C	72	0	0	1	0
3	A	25	0	45	0	0
3	B	15	0	27	0	0
3	C	30	0	54	0	0
4	A	162	0	0	0	1
4	B	141	0	0	0	0
4	C	170	0	0	2	0
All	All	21621	0	20353	29	1

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 1.

All (29) 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:C:524[A]:ARG:NH1	4:C:1001:HOH:O	1.80	1.12
1:A:763:MET:HE3	1:A:811:VAL:HG22	1.87	0.56
1:C:766:MET:HE1	1:C:811:VAL:HA	1.90	0.52
1:B:651:TYR:HB2	1:B:699:VAL:HB	1.93	0.51
1:B:151:GLU:HB3	1:B:216[A]:MET:SD	2.50	0.51
1:A:566:LEU:O	1:A:614:LYS:HD3	2.10	0.51
1:B:147[B]:MET:HA	1:B:147[B]:MET:CE	2.39	0.51
1:A:252:VAL:HG13	1:A:264:ARG:HB3	1.93	0.51
1:B:147[B]:MET:HA	1:B:147[B]:MET:HE3	1.95	0.49
1:B:566:LEU:O	1:B:614:LYS:HD3	2.13	0.49
1:A:78:LYS:HG3	1:A:163:THR:HG21	1.94	0.48
1:B:719:LYS:HE3	1:B:720:TYR:CZ	2.49	0.47
1:B:252:VAL:HG13	1:B:264:ARG:HB3	1.96	0.47
1:C:566:LEU:O	1:C:614:LYS:HD3	2.15	0.47
1:C:252:VAL:HG13	1:C:264:ARG:HB3	1.97	0.47
1:A:719:LYS:HE3	1:A:720:TYR:CZ	2.50	0.46
1:B:407:ILE:HG23	1:B:411:LEU:HD23	1.98	0.46
1:C:783:LEU:HD12	1:C:786:PHE:CE2	2.51	0.46
1:C:118:ILE:HD12	1:C:599:LEU:HD22	1.99	0.44
1:A:783:LEU:HD12	1:A:786:PHE:CE2	2.53	0.44
1:A:651:TYR:HB2	1:A:699:VAL:HB	2.00	0.44
1:C:99:ILE:HG12	1:C:118:ILE:HD11	2.01	0.43
1:C:651:TYR:HB2	1:C:699:VAL:HB	2.01	0.43
1:C:719:LYS:HE3	1:C:720:TYR:CZ	2.55	0.41
1:B:118:ILE:HD12	1:B:599:LEU:HD22	2.02	0.41
1:B:118:ILE:HD12	1:B:599:LEU:CD2	2.50	0.41
1:B:710:ARG:HB2	1:B:714:PHE:CD2	2.55	0.41
1:C:864:ARG:NH2	4:C:1008:HOH:O	2.54	0.41
1:C:688:ARG:HB2	2:C:902:D06:C16	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1088:HOH:O	4:A:1088:HOH:O[4_555]	1.70	0.50

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	851/898 (95%)	824 (97%)	27 (3%)	0	100	100
1	B	853/898 (95%)	825 (97%)	27 (3%)	1 (0%)	51	78
1	C	841/898 (94%)	817 (97%)	23 (3%)	1 (0%)	51	78
All	All	2545/2694 (94%)	2466 (97%)	77 (3%)	2 (0%)	51	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	445	ILE
1	C	445	ILE

5.3.2 Protein sidechains [i](#)

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	756/795 (95%)	752 (100%)	4 (0%)	88	96
1	B	758/795 (95%)	752 (99%)	6 (1%)	81	93
1	C	750/795 (94%)	743 (99%)	7 (1%)	78	92
All	All	2264/2385 (95%)	2247 (99%)	17 (1%)	81	93

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ASP

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Mol	Chain	Res	Type
1	A	216	MET
1	A	294	SER
1	A	718	PHE
1	B	80	PRO
1	B	435	PRO
1	B	473	LYS
1	B	718	PHE
1	B	763	MET
1	B	843	ILE
1	C	80	PRO
1	C	161	ILE
1	C	294	SER
1	C	704	ASN
1	C	708	CYS
1	C	718	PHE
1	C	829	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	801	GLN
1	C	403	GLN
1	C	882	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 monosaccharides in this entry.

5.6 Ligand geometry

27 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	D06	A	907	-	27,27,27	0.84	0	33,38,38	3.35	7 (21%)
3	TMO	C	905	-	4,4,4	6.32	1 (25%)	6,6,6	0.21	0
2	D06	C	903	-	27,27,27	0.67	0	33,38,38	3.60	5 (15%)
3	TMO	A	912	-	4,4,4	6.08	1 (25%)	6,6,6	0.27	0
3	TMO	C	904	-	4,4,4	6.23	1 (25%)	6,6,6	0.26	0
2	D06	C	902	-	27,27,27	0.57	0	33,38,38	3.07	8 (24%)
2	D06	B	903	-	27,27,27	0.73	0	33,38,38	3.59	8 (24%)
3	TMO	C	908	-	4,4,4	6.36	1 (25%)	6,6,6	0.20	0
3	TMO	C	907	-	4,4,4	6.40	1 (25%)	6,6,6	0.18	0
3	TMO	A	909	-	4,4,4	6.02	1 (25%)	6,6,6	0.27	0
2	D06	A	905	-	27,27,27	0.78	0	33,38,38	3.33	8 (24%)
3	TMO	B	905	-	4,4,4	6.26	1 (25%)	6,6,6	0.22	0
3	TMO	C	906	-	4,4,4	6.23	1 (25%)	6,6,6	0.20	0
3	TMO	B	904	-	4,4,4	6.22	1 (25%)	6,6,6	0.23	0
2	D06	A	906	-	27,27,27	0.71	0	33,38,38	3.65	7 (21%)
2	D06	B	901	-	27,27,27	0.68	1 (3%)	33,38,38	2.81	7 (21%)
3	TMO	A	910	-	4,4,4	6.27	1 (25%)	6,6,6	0.17	0
3	TMO	B	906	-	4,4,4	6.23	1 (25%)	6,6,6	0.18	0
2	D06	B	902	-	27,27,27	0.73	0	33,38,38	3.57	10 (30%)
3	TMO	C	909	-	4,4,4	6.21	1 (25%)	6,6,6	0.21	0
2	D06	A	903	-	27,27,27	0.86	0	33,38,38	3.34	8 (24%)
3	TMO	A	911	-	4,4,4	6.37	1 (25%)	6,6,6	0.20	0
2	D06	C	901	-	27,27,27	0.80	1 (3%)	33,38,38	2.69	6 (18%)
2	D06	A	904	-	27,27,27	0.75	0	33,38,38	2.97	9 (27%)
3	TMO	A	908	-	4,4,4	6.23	1 (25%)	6,6,6	0.21	0
2	D06	A	902	-	27,27,27	0.68	0	33,38,38	3.68	11 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	D06	A	901	-	27,27,27	0.62	0	33,38,38	2.97	7 (21%)

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	D06	A	907	-	-	1/16/41/41	0/4/4/4
2	D06	A	906	-	-	0/16/41/41	0/4/4/4
2	D06	B	901	-	-	0/16/41/41	0/4/4/4
2	D06	A	903	-	-	1/16/41/41	0/4/4/4
2	D06	C	902	-	-	0/16/41/41	0/4/4/4
2	D06	B	903	-	-	0/16/41/41	0/4/4/4
2	D06	C	903	-	-	0/16/41/41	0/4/4/4
2	D06	C	901	-	-	0/16/41/41	0/4/4/4
2	D06	A	904	-	-	1/16/41/41	0/4/4/4
2	D06	B	902	-	-	4/16/41/41	0/4/4/4
2	D06	A	902	-	-	2/16/41/41	0/4/4/4
2	D06	A	905	-	-	1/16/41/41	0/4/4/4
2	D06	A	901	-	-	0/16/41/41	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	907	TMO	OAE-NAC	-12.75	1.25	1.42
3	A	911	TMO	OAE-NAC	-12.72	1.25	1.42
3	C	908	TMO	OAE-NAC	-12.67	1.25	1.42
3	C	905	TMO	OAE-NAC	-12.61	1.25	1.42
3	A	910	TMO	OAE-NAC	-12.52	1.25	1.42
3	B	905	TMO	OAE-NAC	-12.49	1.25	1.42
3	B	906	TMO	OAE-NAC	-12.45	1.25	1.42
3	C	906	TMO	OAE-NAC	-12.44	1.25	1.42
3	A	908	TMO	OAE-NAC	-12.43	1.25	1.42
3	C	904	TMO	OAE-NAC	-12.40	1.25	1.42
3	B	904	TMO	OAE-NAC	-12.40	1.25	1.42
3	C	909	TMO	OAE-NAC	-12.40	1.25	1.42
3	A	912	TMO	OAE-NAC	-12.13	1.26	1.42
3	A	909	TMO	OAE-NAC	-12.00	1.26	1.42
2	C	901	D06	C2-C17	-2.44	1.50	1.53
2	B	901	D06	C2-C17	-2.21	1.50	1.53

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	906	D06	C21-C20-N19	15.89	109.97	102.46
2	C	903	D06	C21-C20-N19	14.99	109.55	102.46
2	B	903	D06	C21-C20-N19	14.56	109.35	102.46
2	A	907	D06	C26-C27-N19	14.53	109.33	102.46
2	B	902	D06	C26-C27-N19	13.71	108.94	102.46
2	A	902	D06	C26-C27-N19	13.42	108.81	102.46
2	A	903	D06	C26-C27-N19	13.07	108.64	102.46
2	A	902	D06	C21-C20-N19	12.32	108.29	102.46
2	A	905	D06	C21-C20-N19	12.20	108.23	102.46
2	A	905	D06	C26-C27-N19	12.19	108.22	102.46
2	B	903	D06	C26-C27-N19	12.04	108.15	102.46
2	C	902	D06	C26-C27-N19	11.81	108.05	102.46
2	C	903	D06	C26-C27-N19	11.77	108.02	102.46
2	A	903	D06	C21-C20-N19	11.68	107.98	102.46
2	B	902	D06	C21-C20-N19	11.67	107.98	102.46
2	A	904	D06	C26-C27-N19	11.58	107.94	102.46
2	A	906	D06	C26-C27-N19	11.14	107.73	102.46
2	C	901	D06	C26-C27-N19	10.79	107.56	102.46
2	B	901	D06	C26-C27-N19	10.70	107.52	102.46
2	A	901	D06	C26-C27-N19	10.65	107.50	102.46
2	A	901	D06	C21-C20-N19	10.12	107.25	102.46
2	C	902	D06	C21-C20-N19	9.71	107.05	102.46
2	A	907	D06	C21-C20-N19	9.35	106.88	102.46
2	A	904	D06	C21-C20-N19	9.01	106.72	102.46
2	B	901	D06	C21-C20-N19	8.61	106.53	102.46
2	C	901	D06	C21-C20-N19	8.00	106.25	102.46
2	A	902	D06	C16-N12-C8	4.93	118.89	114.12
2	C	902	D06	C16-N12-C8	4.55	118.52	114.12
2	B	901	D06	C17-C2-N1	-4.22	103.79	110.22
2	A	907	D06	C27-C26-C21	-3.89	107.45	110.53
2	C	903	D06	C20-C21-C26	-3.78	107.53	110.53
2	A	906	D06	C20-C21-C26	-3.75	107.56	110.53
2	A	901	D06	C17-C2-N1	-3.63	104.69	110.22
2	A	904	D06	C27-C26-C21	-3.61	107.67	110.53
2	B	902	D06	C15-C16-N12	3.57	109.97	104.15
2	B	902	D06	C16-N12-C8	3.54	117.54	114.12
2	C	901	D06	C27-C26-C21	-3.36	107.87	110.53
2	B	901	D06	C27-C26-C21	-3.33	107.89	110.53
2	B	902	D06	C27-C26-C21	-3.33	107.89	110.53
2	A	904	D06	C15-C16-N12	3.32	109.56	104.15
2	B	903	D06	C20-C21-C26	-3.28	107.93	110.53
2	A	902	D06	C15-C16-N12	3.27	109.48	104.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	D06	C27-C26-C21	-3.25	107.95	110.53
2	A	902	D06	C6-C7-C8	3.15	116.34	109.81
2	A	901	D06	C11-C4-C2	-3.08	107.76	111.86
2	A	904	D06	C10-C8-C7	-3.07	104.12	111.19
2	B	903	D06	O18-C17-N19	-3.07	118.08	121.67
2	B	902	D06	C6-C7-C8	3.06	116.15	109.81
2	A	905	D06	C6-C4-C2	-3.04	107.81	111.86
2	A	902	D06	C6-C4-C2	2.94	115.79	111.86
2	A	902	D06	C27-C26-C21	-2.94	108.20	110.53
2	A	903	D06	C27-C26-C21	-2.93	108.21	110.53
2	C	902	D06	C27-C26-C21	-2.93	108.21	110.53
2	B	902	D06	C10-C11-C4	-2.86	105.81	112.24
2	A	905	D06	C27-C26-C21	-2.85	108.27	110.53
2	A	903	D06	O18-C17-N19	-2.80	118.39	121.67
2	A	907	D06	C10-C8-C7	-2.75	104.85	111.19
2	B	902	D06	C11-C4-C6	-2.73	104.62	109.44
2	A	904	D06	C13-N12-C8	2.73	116.76	114.12
2	A	902	D06	C10-C11-C4	-2.68	106.21	112.24
2	A	904	D06	C6-C4-C2	-2.67	108.30	111.86
2	A	903	D06	C15-C16-N12	2.65	108.46	104.15
2	A	905	D06	C20-C21-C26	-2.65	108.43	110.53
2	C	901	D06	C17-C2-N1	-2.64	106.20	110.22
2	A	902	D06	C11-C4-C6	-2.60	104.85	109.44
2	A	905	D06	O18-C17-N19	-2.59	118.63	121.67
2	C	902	D06	C13-N12-C8	2.57	116.60	114.12
2	C	902	D06	C15-C16-N12	2.56	108.32	104.15
2	B	903	D06	C6-C7-C8	2.50	114.99	109.81
2	A	906	D06	C15-C16-N12	2.48	108.20	104.15
2	A	906	D06	C27-C26-C21	-2.48	108.56	110.53
2	A	902	D06	C20-C21-C26	-2.47	108.57	110.53
2	A	902	D06	C14-C15-C16	-2.47	98.21	105.19
2	C	903	D06	C15-C16-N12	2.47	108.17	104.15
2	A	901	D06	C15-C16-N12	2.47	108.17	104.15
2	C	901	D06	C11-C4-C2	-2.46	108.58	111.86
2	A	906	D06	O18-C17-N19	-2.46	118.79	121.67
2	B	902	D06	C6-C4-C2	2.45	115.13	111.86
2	B	903	D06	C15-C16-N12	2.44	108.13	104.15
2	A	907	D06	C6-C4-C2	-2.43	108.62	111.86
2	B	903	D06	C11-C4-C6	-2.40	105.20	109.44
2	A	901	D06	O18-C17-N19	-2.39	118.87	121.67
2	A	904	D06	C20-C21-C26	-2.38	108.64	110.53
2	A	903	D06	C17-C2-N1	-2.34	106.64	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	907	D06	C15-C16-N12	2.34	107.96	104.15
2	C	903	D06	O18-C17-N19	-2.33	118.94	121.67
2	A	903	D06	C10-C8-C7	-2.30	105.88	111.19
2	A	903	D06	C20-C21-C26	-2.27	108.73	110.53
2	B	901	D06	C11-C4-C2	-2.25	108.86	111.86
2	B	903	D06	C27-C26-C21	-2.22	108.77	110.53
2	C	902	D06	C14-C13-N12	2.19	107.72	104.15
2	C	902	D06	C7-C6-C4	-2.16	107.39	112.24
2	C	901	D06	O18-C17-N19	-2.14	119.17	121.67
2	A	904	D06	C11-C4-C6	2.08	113.11	109.44
2	A	906	D06	C27-C26-C25	2.06	132.92	128.85
2	B	901	D06	C13-N12-C8	2.06	116.11	114.12
2	A	907	D06	C14-C13-N12	2.03	107.46	104.15
2	B	901	D06	O18-C17-N19	-2.03	119.29	121.67
2	B	902	D06	C20-C21-C26	-2.03	108.92	110.53
2	A	905	D06	C14-C13-N12	2.02	107.45	104.15
2	A	905	D06	C10-C8-C7	-2.00	106.58	111.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	902	D06	C10-C8-N12-C16
2	A	903	D06	C17-C2-C4-C6
2	A	905	D06	C17-C2-C4-C6
2	A	907	D06	C17-C2-C4-C6
2	B	902	D06	C7-C8-N12-C16
2	B	902	D06	C7-C8-N12-C13
2	B	902	D06	C10-C8-N12-C16
2	B	902	D06	C10-C8-N12-C13
2	A	904	D06	C17-C2-C4-C6
2	A	902	D06	C7-C8-N12-C16

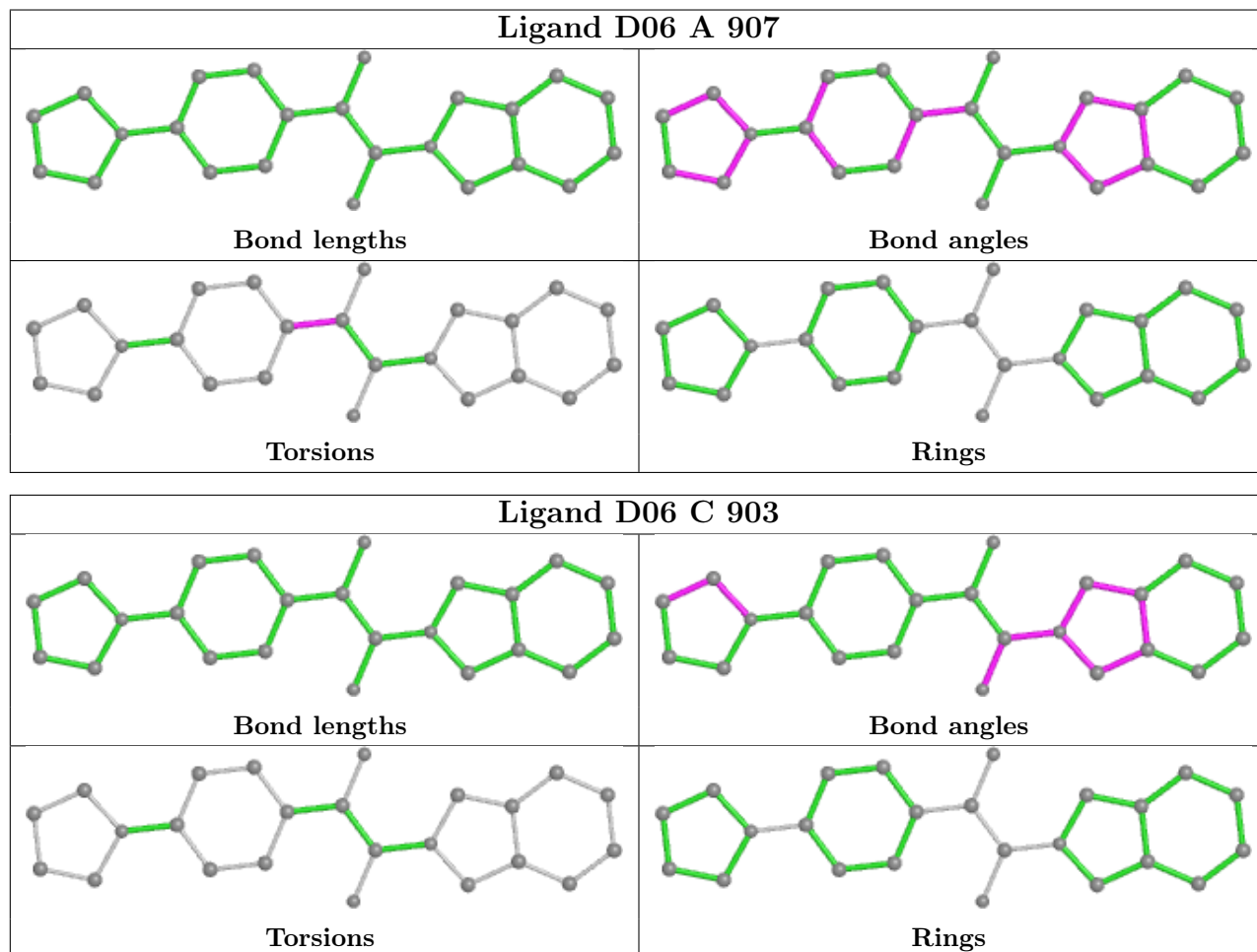
There are no ring outliers.

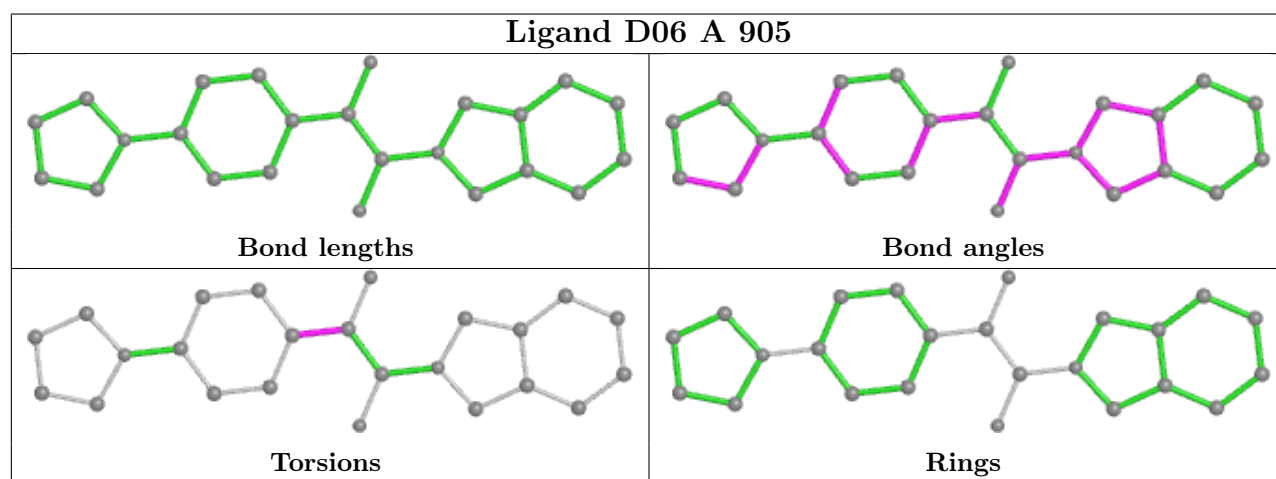
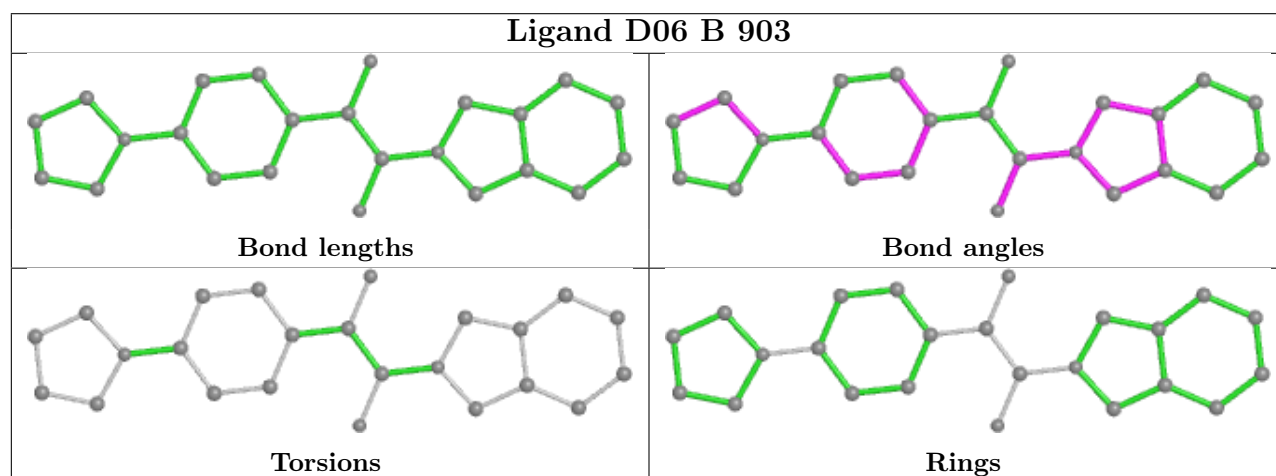
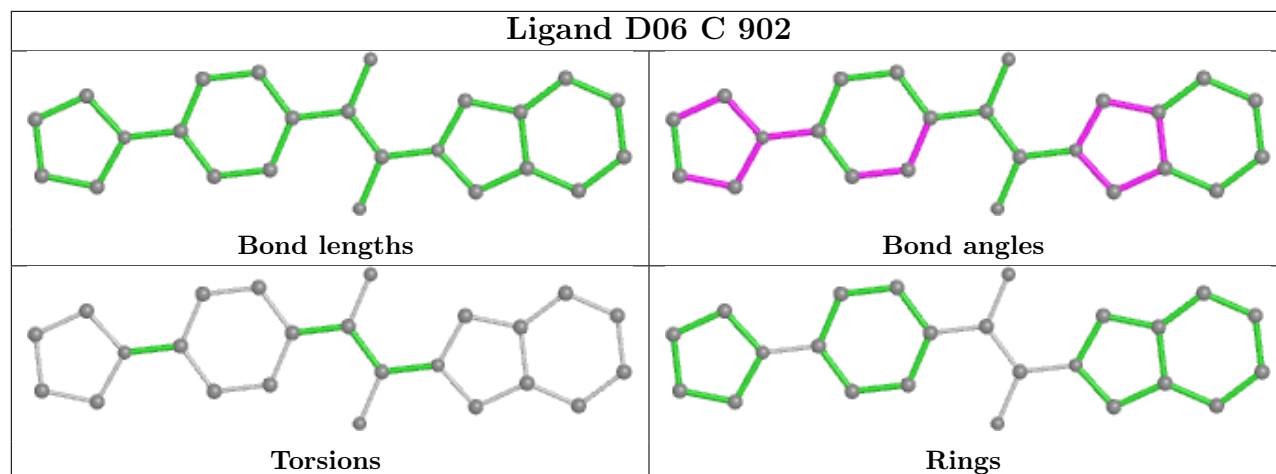
1 monomer is involved in 1 short contact:

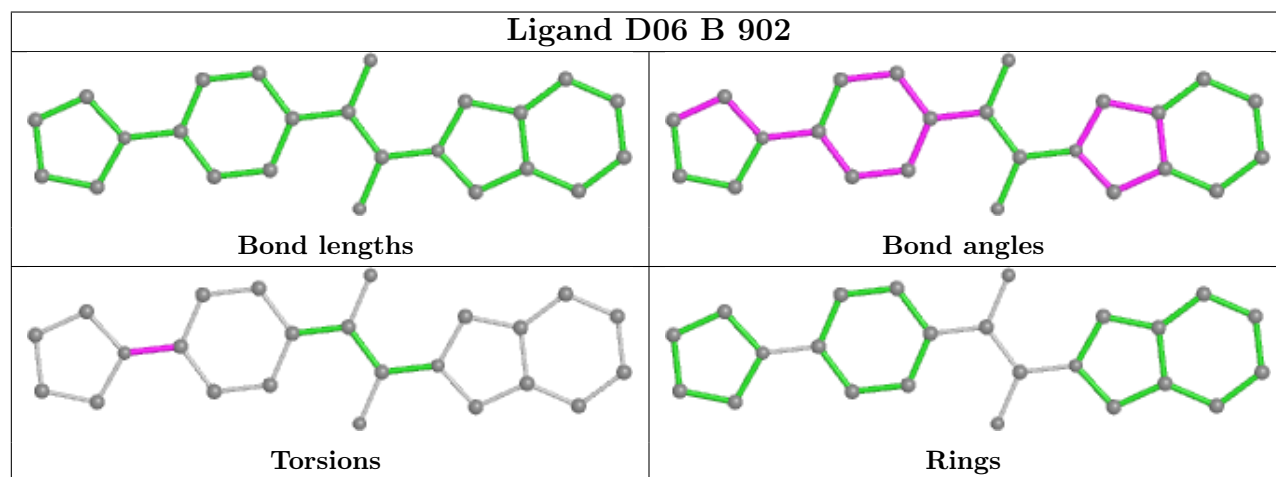
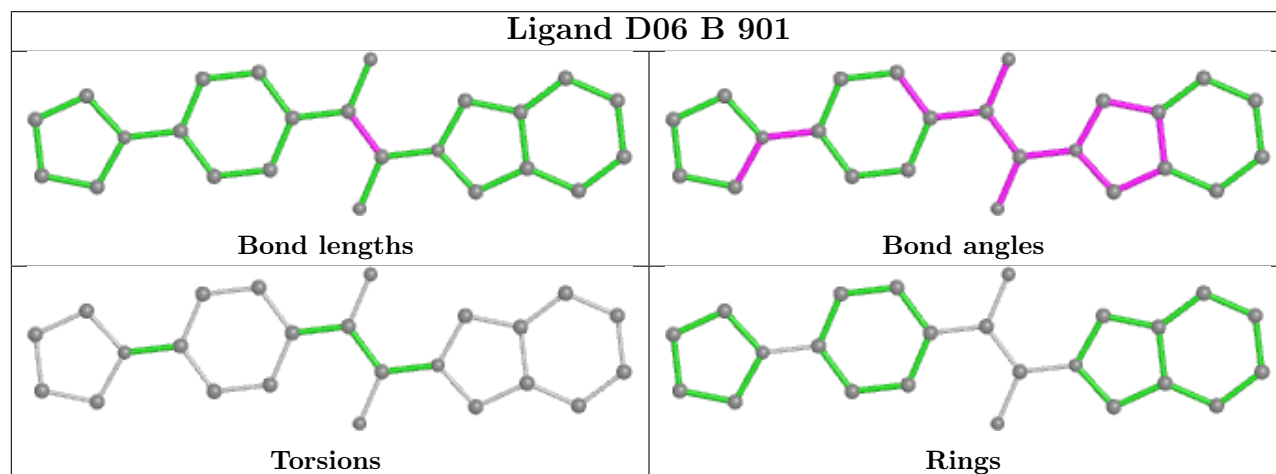
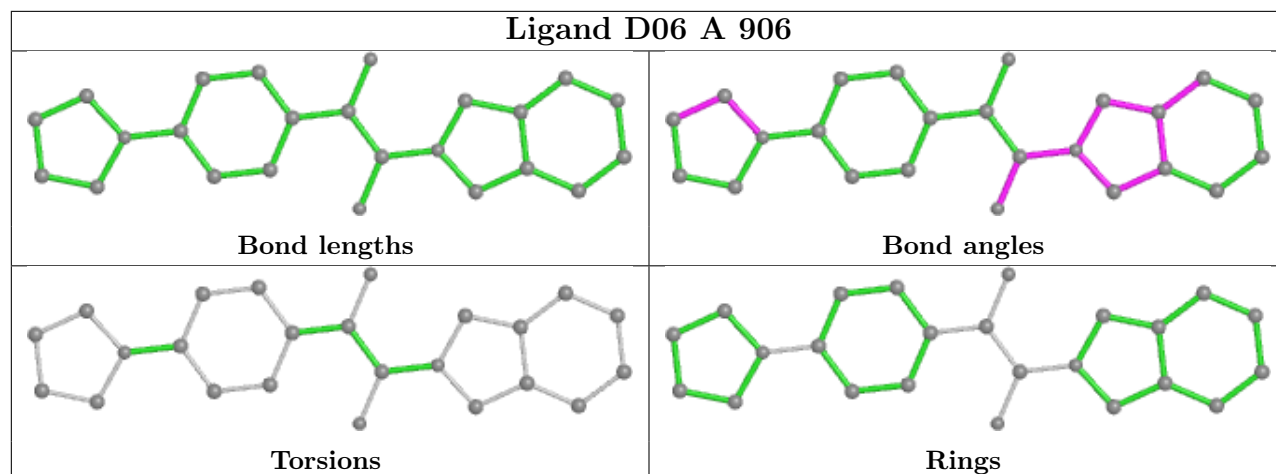
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	902	D06	1	0

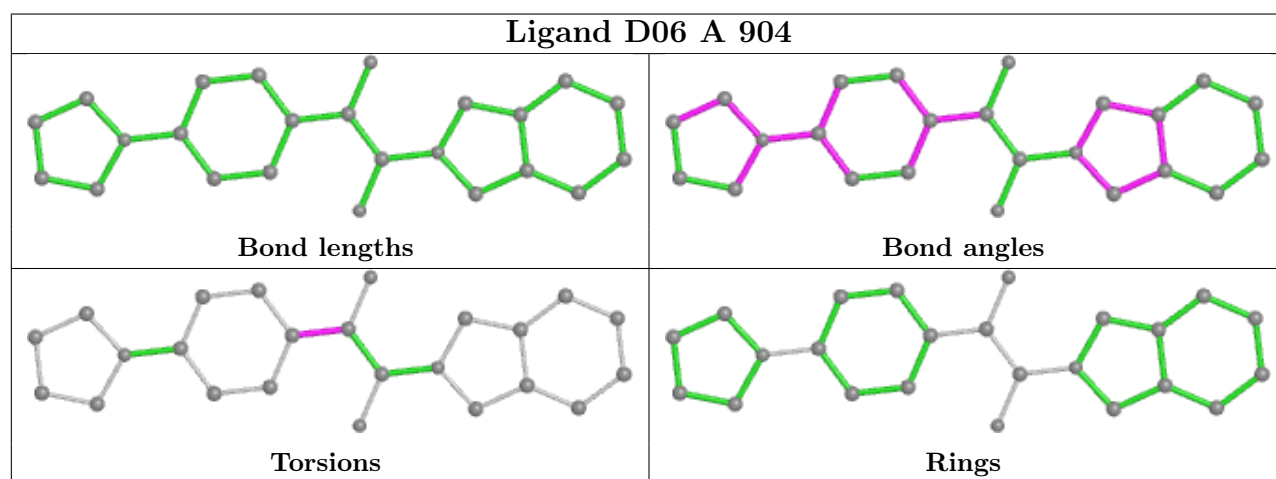
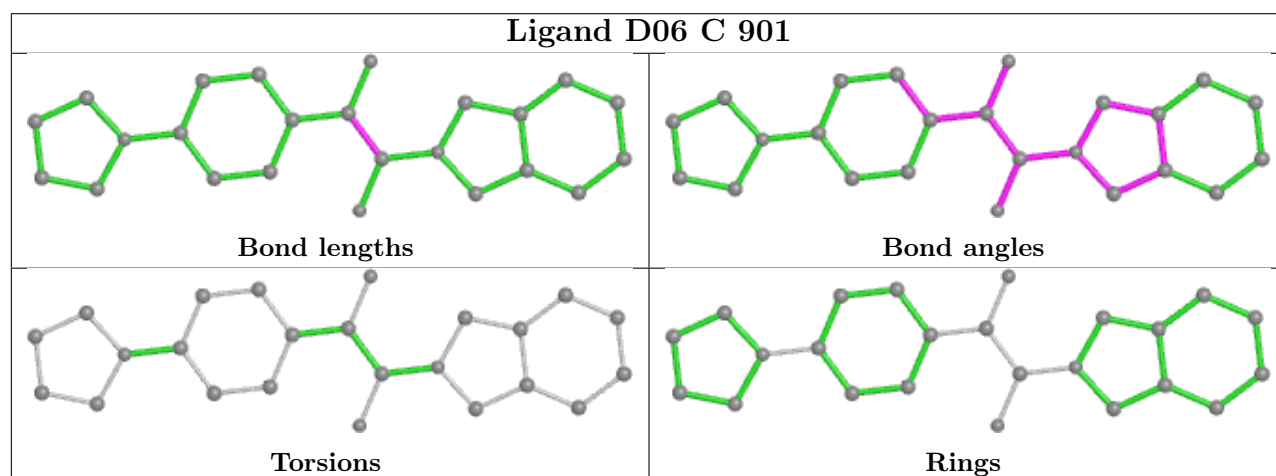
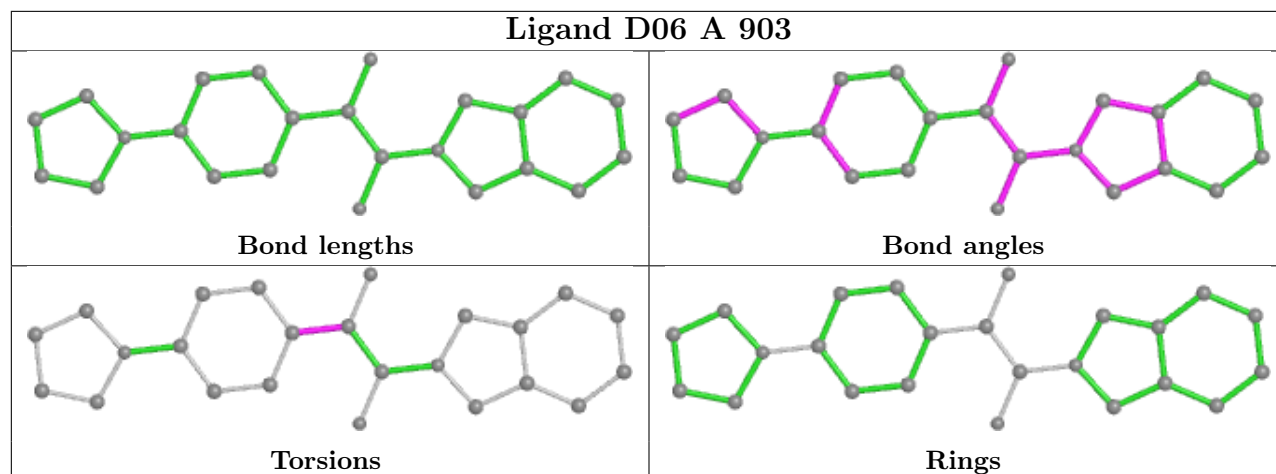
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

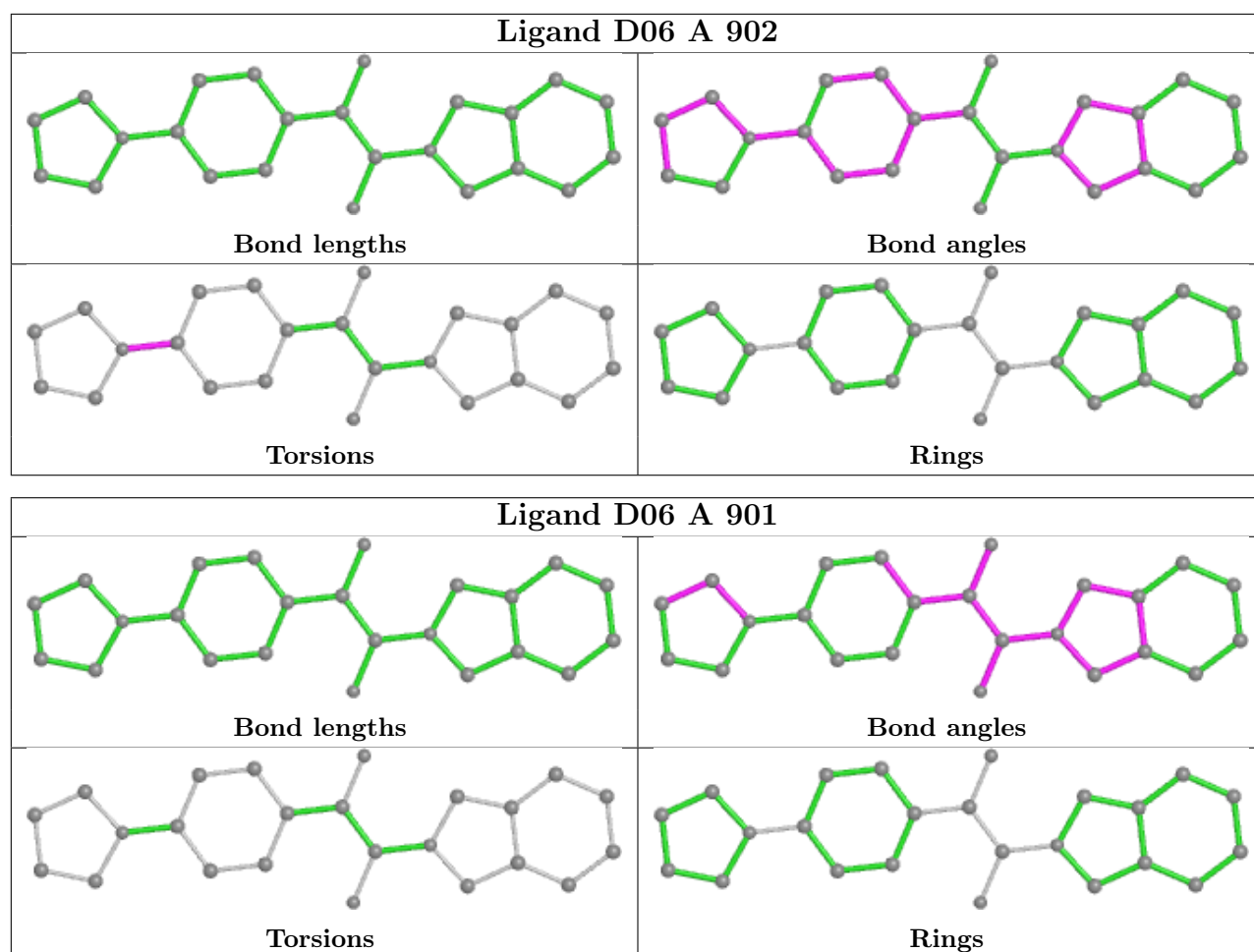
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.











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	852/898 (94%)	-0.10	21 (2%) 57 59	39, 59, 104, 162	46 (5%)
1	B	852/898 (94%)	-0.10	22 (2%) 56 57	39, 61, 107, 167	44 (5%)
1	C	843/898 (93%)	-0.13	18 (2%) 63 65	37, 56, 98, 152	37 (4%)
All	All	2547/2694 (94%)	-0.11	61 (2%) 59 60	37, 59, 104, 167	127 (4%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	71	TYR	5.5
1	A	141	ALA	5.5
1	A	139	PHE	5.0
1	C	624	ALA	4.8
1	B	141	ALA	4.4
1	B	74	TYR	4.3
1	C	524[A]	ARG	4.1
1	A	624	ALA	4.1
1	B	47	LYS	3.6
1	B	71	TYR	3.6
1	B	624	ALA	3.6
1	A	140	GLN	3.5
1	B	139	PHE	3.2
1	C	48	LEU	3.0
1	B	524	ARG	3.0
1	C	75	MET	2.9
1	C	625	GLY	2.9
1	A	417	ASP	2.8
1	A	146	GLY	2.8
1	B	106	GLY	2.8
1	A	71	TYR	2.7
1	A	525	HIS	2.7
1	B	49	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	417	ASP	2.6
1	C	105	SER	2.6
1	B	48	LEU	2.6
1	A	105	SER	2.5
1	C	262	ASP	2.4
1	A	142	THR	2.4
1	B	140	GLN	2.4
1	C	420	MET	2.4
1	B	420	MET	2.3
1	C	126	ALA	2.3
1	B	72	HIS	2.3
1	C	293	PRO	2.3
1	A	625	GLY	2.3
1	B	278	ASP	2.3
1	A	742	ASP	2.3
1	A	658	PRO	2.3
1	A	145	TYR	2.3
1	A	147	MET	2.3
1	A	293	PRO	2.3
1	C	76	MET	2.2
1	A	524	ARG	2.2
1	B	145	TYR	2.2
1	C	626	PRO	2.2
1	A	420	MET	2.2
1	C	659	GLY	2.2
1	B	70	LYS	2.2
1	C	898	ILE	2.2
1	C	525	HIS	2.2
1	A	419	VAL	2.2
1	C	74	TYR	2.1
1	A	510	GLU	2.1
1	B	147[A]	MET	2.1
1	B	525	HIS	2.1
1	C	108	ASN	2.1
1	B	293	PRO	2.1
1	B	296	GLY	2.1
1	B	256	LEU	2.1
1	A	495	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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

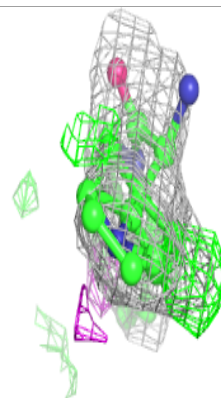
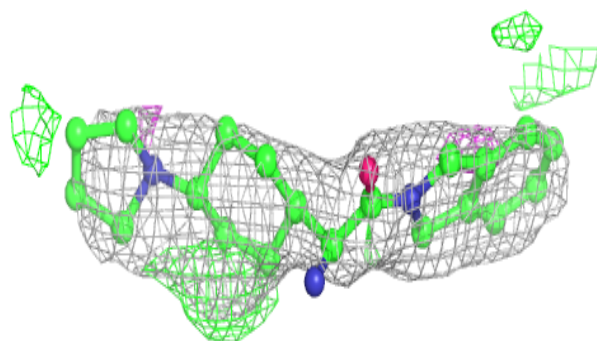
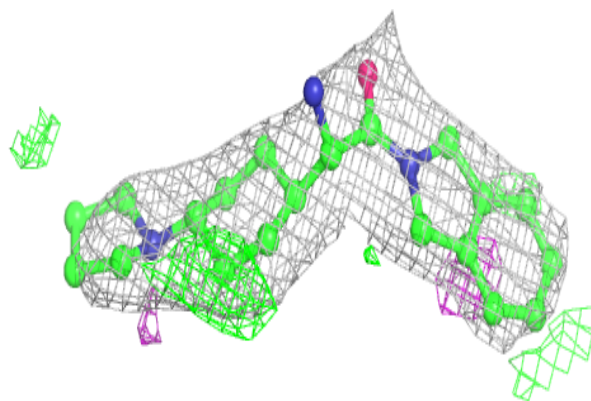
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	D06	A	903	24/24	0.86	0.35	80,111,125,143	0
2	D06	A	905	24/24	0.89	0.44	85,105,145,163	0
3	TMO	A	908	5/5	0.89	0.41	80,114,128,130	0
3	TMO	C	906	5/5	0.89	0.53	75,104,112,116	0
2	D06	A	907	24/24	0.90	0.45	65,141,172,180	0
2	D06	B	902	24/24	0.90	0.29	55,102,125,148	0
3	TMO	C	908	5/5	0.90	0.31	95,110,126,138	0
3	TMO	A	912	5/5	0.91	0.34	100,105,114,121	0
3	TMO	B	906	5/5	0.91	0.77	109,116,127,142	0
2	D06	B	903	24/24	0.92	0.23	83,102,149,161	0
2	D06	C	902	24/24	0.92	0.30	61,111,134,186	0
3	TMO	C	904	5/5	0.92	0.23	75,82,103,115	0
2	D06	A	904	24/24	0.92	0.37	67,142,173,176	0
3	TMO	A	910	5/5	0.92	0.44	94,97,119,125	0
3	TMO	C	909	5/5	0.92	0.35	106,114,135,137	0
3	TMO	C	905	5/5	0.93	0.74	110,115,126,135	0
3	TMO	B	905	5/5	0.93	0.29	97,97,119,123	0
2	D06	C	903	24/24	0.93	0.28	80,98,134,149	0
2	D06	A	902	24/24	0.93	0.35	63,108,138,141	0
3	TMO	A	909	5/5	0.95	0.32	90,98,107,117	0
3	TMO	B	904	5/5	0.95	0.31	97,100,119,139	0
2	D06	A	906	24/24	0.95	0.31	87,101,151,158	0
3	TMO	A	911	5/5	0.96	0.15	93,99,117,120	0
2	D06	A	901	24/24	0.97	0.30	32,42,52,56	0
3	TMO	C	907	5/5	0.97	0.46	97,111,118,123	0
2	D06	B	901	24/24	0.98	0.23	30,41,56,58	0
2	D06	C	901	24/24	0.98	0.29	34,41,47,51	0

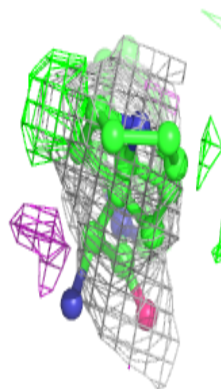
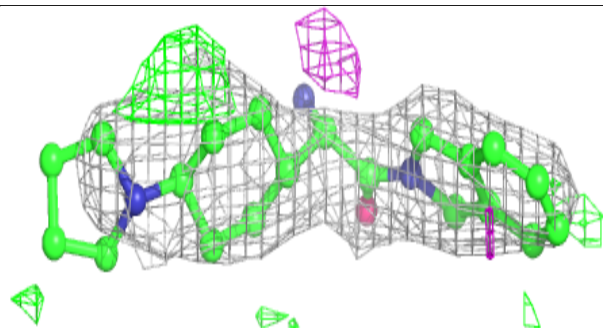
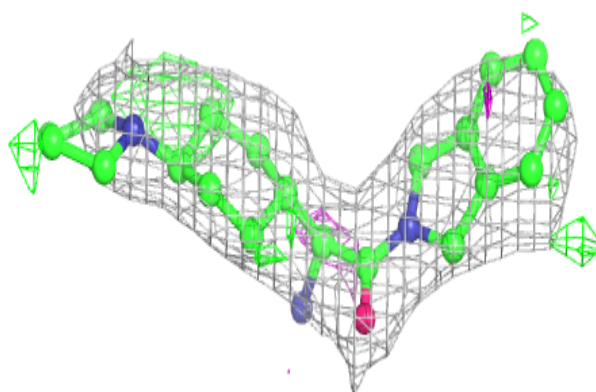
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around D06 A 903:

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

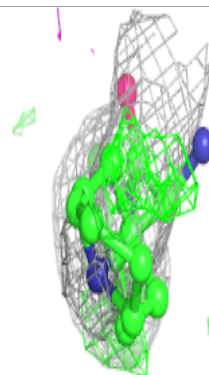
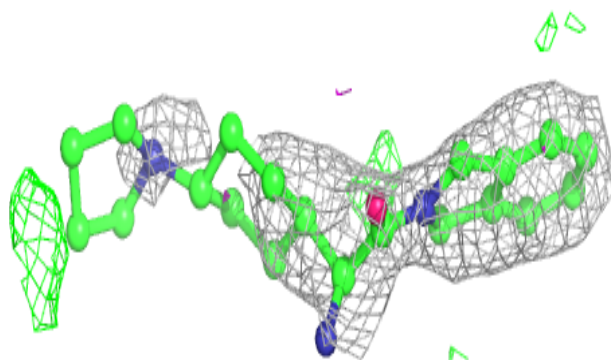
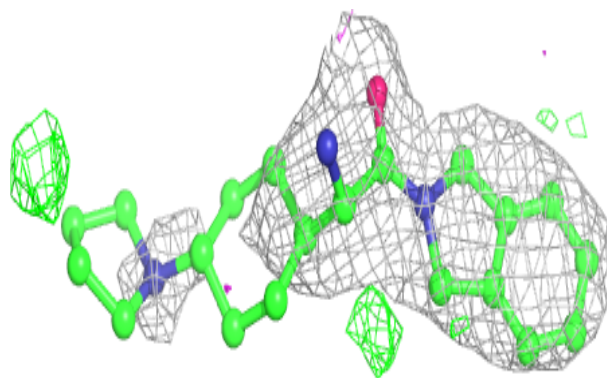
**Electron density around D06 A 905:**

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

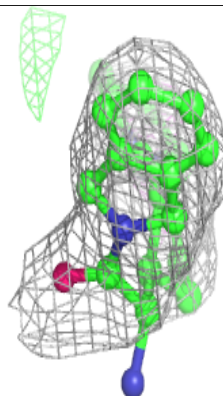
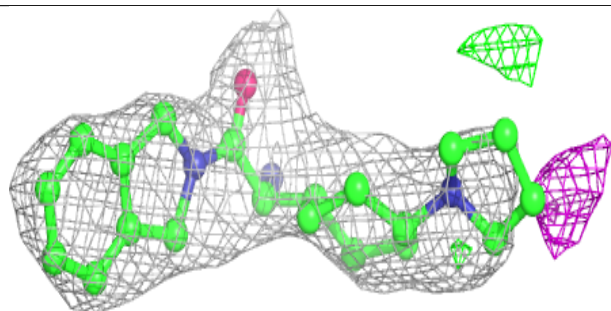
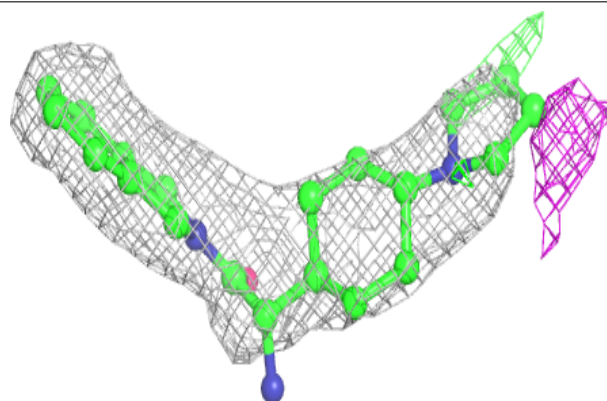


Electron density around D06 A 907:

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

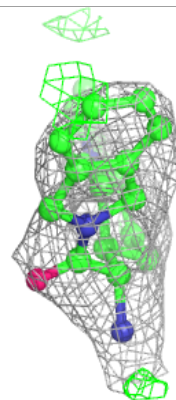
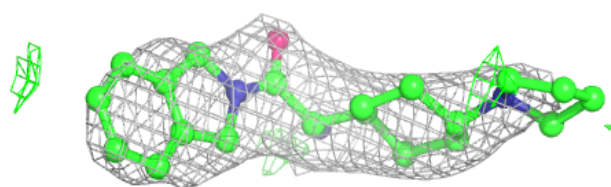
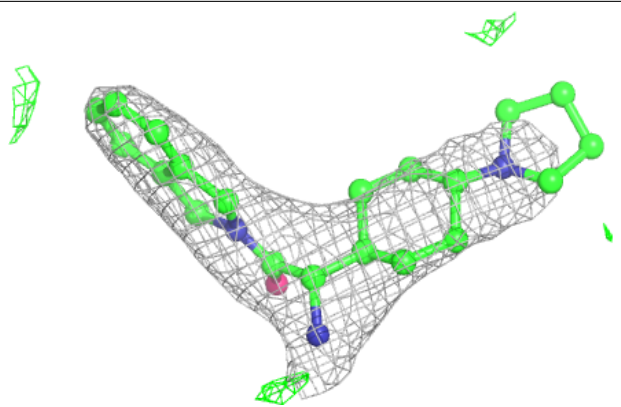
**Electron density around D06 B 902:**

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

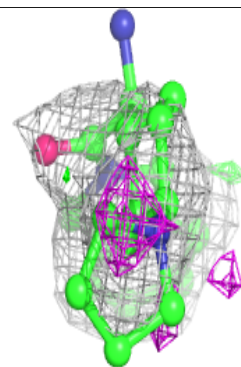
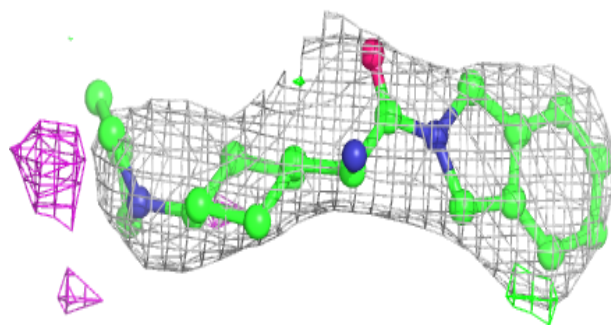
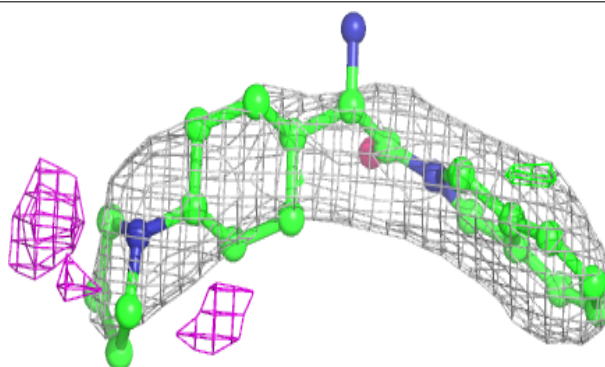


Electron density around D06 B 903:

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

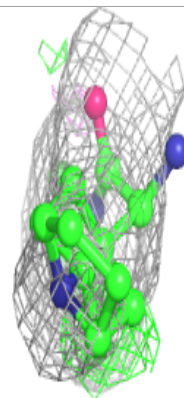
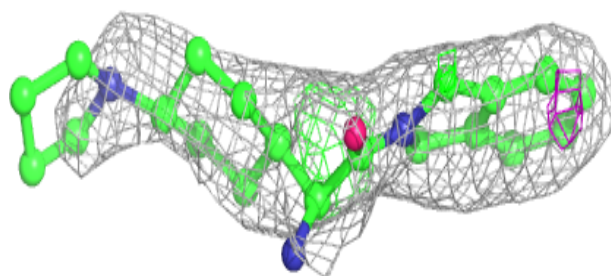
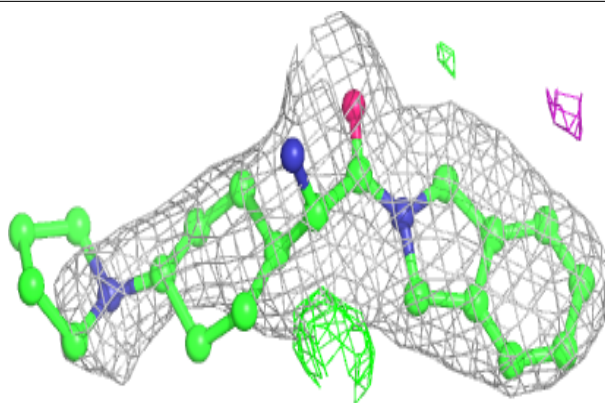
**Electron density around D06 C 902:**

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

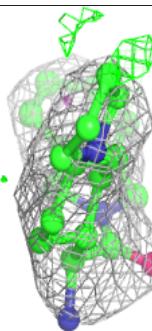
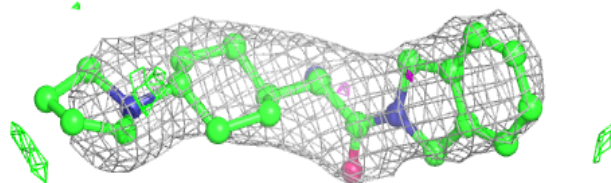
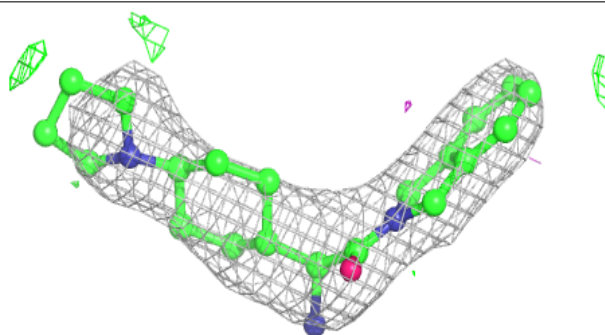


Electron density around D06 A 904:

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

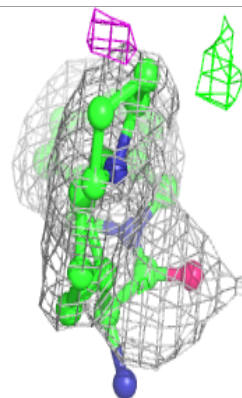
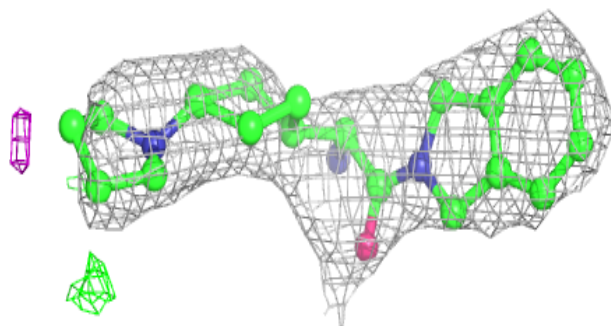
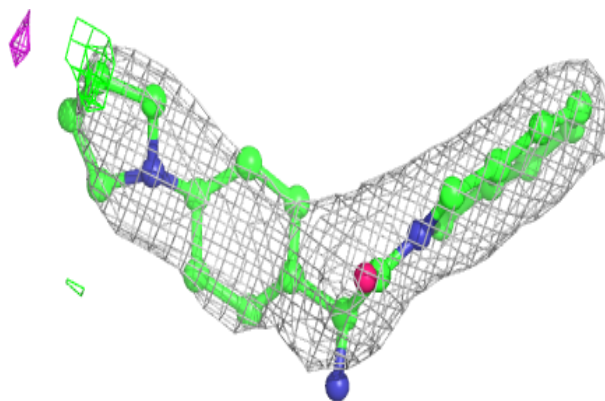
**Electron density around D06 C 903:**

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

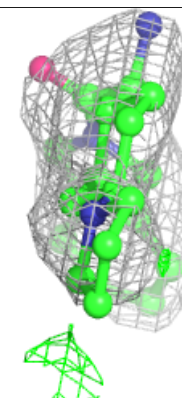
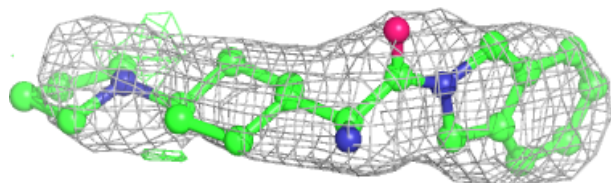
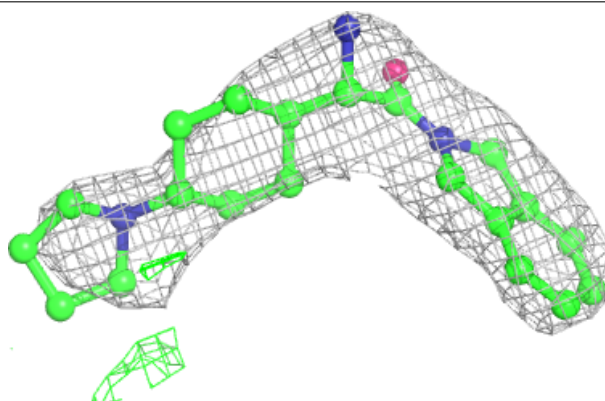


Electron density around D06 A 902:

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

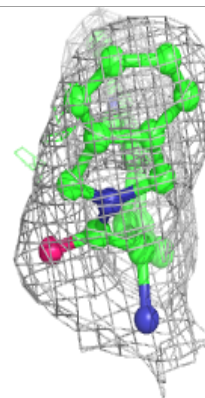
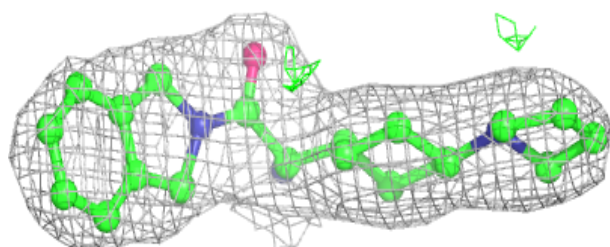
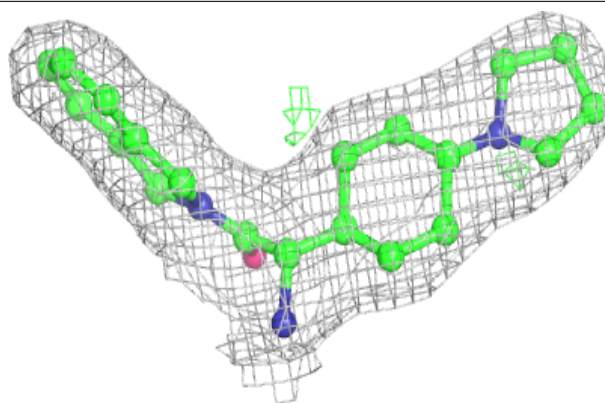
**Electron density around D06 A 906:**

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

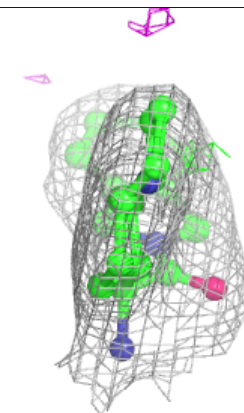
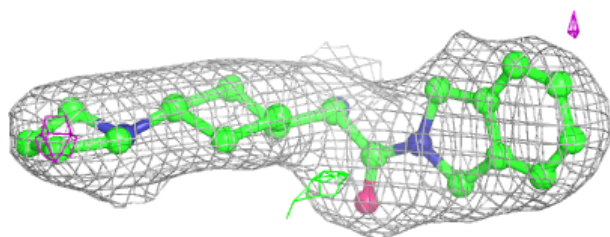
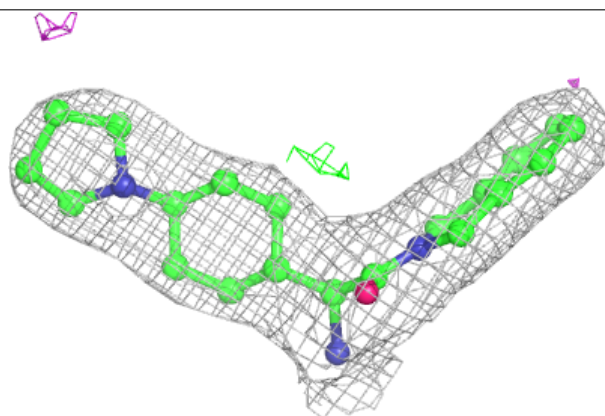


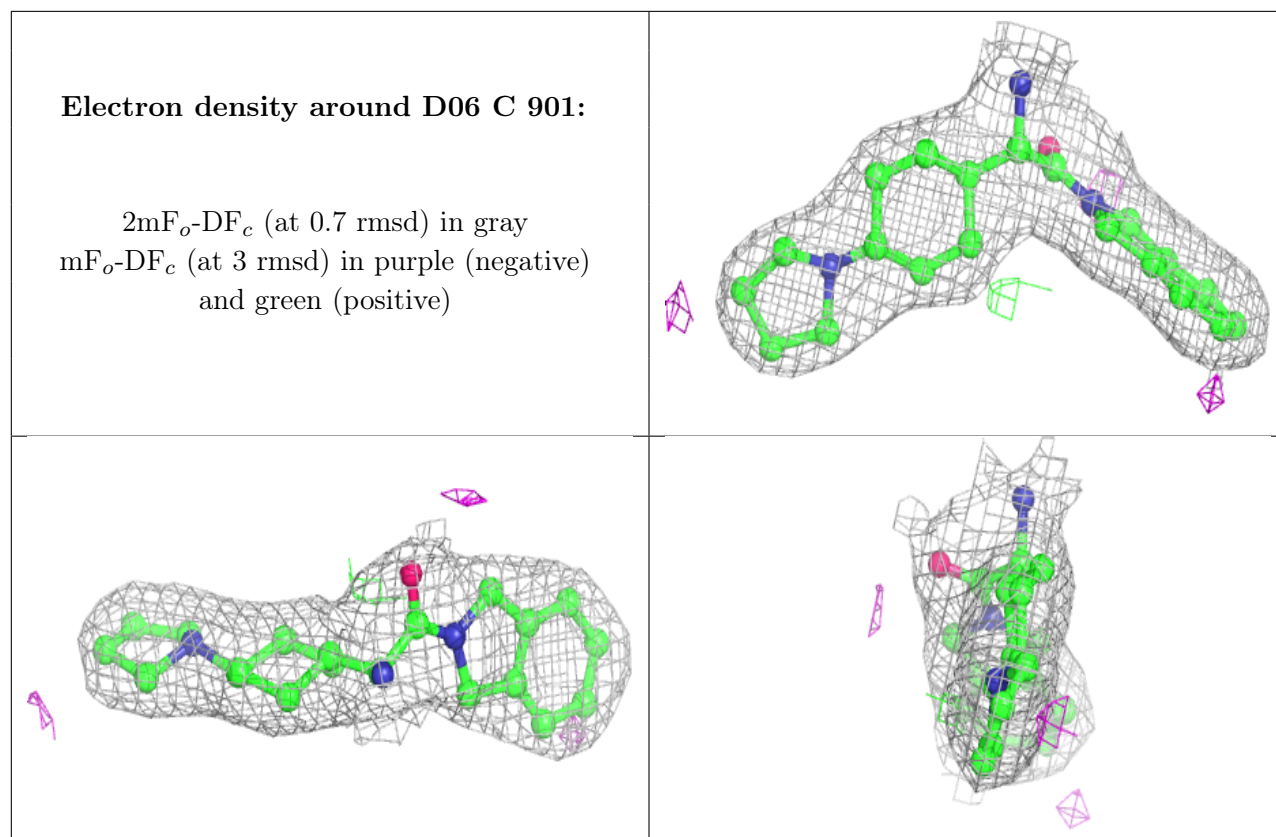
Electron density around D06 A 901:

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

**Electron density around D06 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.