



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:41 PM BST

PDB ID : 5TIO
Title : Crystal Structure of Human Glycine Receptor alpha-3 Bound to AM-3607
Authors : Shaffer, P.L.; Huang, X.; Chen, H.
Deposited on : 2016-10-03
Resolution : 3.25 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 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 : 2.13.1
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) : 2.13.1

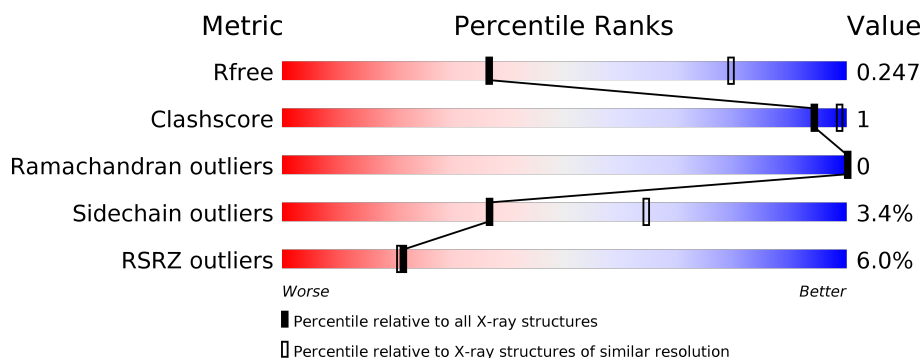
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 on 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	362	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>7%</div> </div> </div>
1	B	362	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
1	C	362	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>7%</div> </div> </div>
1	D	362	<div> <div>7%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	E	362	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13727 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 Glycine receptor subunit alpha-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	338	Total	C	N	O	S	0	0	0
			2692	1757	428	487	20			
1	A	338	Total	C	N	O	S	0	0	0
			2702	1762	431	489	20			
1	B	343	Total	C	N	O	S	0	0	0
			2719	1774	433	492	20			
1	D	343	Total	C	N	O	S	0	0	0
			2724	1775	436	494	19			
1	E	338	Total	C	N	O	S	0	0	0
			2706	1765	432	489	20			

There are 55 discrepancies between the modelled and reference sequences:

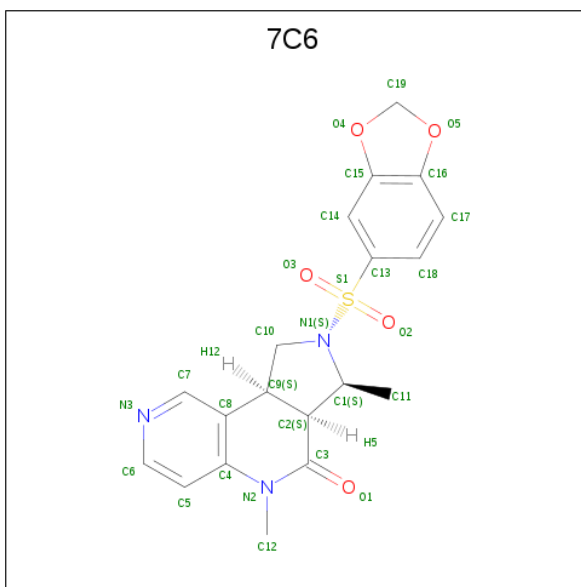
Chain	Residue	Modelled	Actual	Comment	Reference
C	310	ALA	-	linker	UNP O75311
C	311	GLY	-	linker	UNP O75311
C	312	THR	-	linker	UNP O75311
C	355	TRP	-	expression tag	UNP O75311
C	356	SER	-	expression tag	UNP O75311
C	357	HIS	-	expression tag	UNP O75311
C	358	PRO	-	expression tag	UNP O75311
C	359	GLN	-	expression tag	UNP O75311
C	360	PHE	-	expression tag	UNP O75311
C	361	GLU	-	expression tag	UNP O75311
C	362	LYS	-	expression tag	UNP O75311
A	310	ALA	-	linker	UNP O75311
A	311	GLY	-	linker	UNP O75311
A	312	THR	-	linker	UNP O75311
A	355	TRP	-	expression tag	UNP O75311
A	356	SER	-	expression tag	UNP O75311
A	357	HIS	-	expression tag	UNP O75311
A	358	PRO	-	expression tag	UNP O75311
A	359	GLN	-	expression tag	UNP O75311

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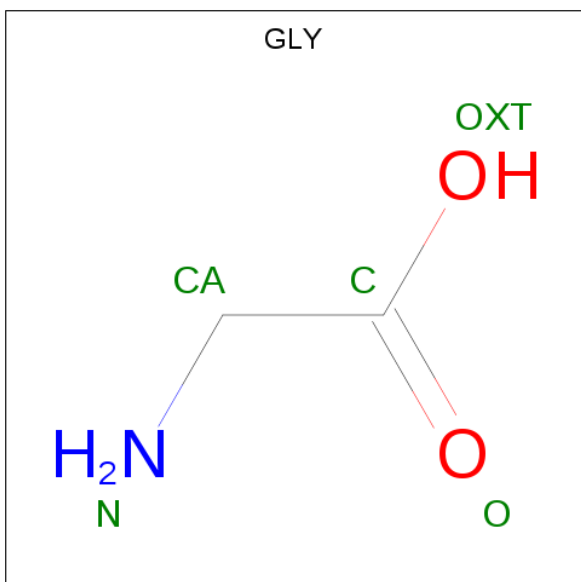
Chain	Residue	Modelled	Actual	Comment	Reference
A	360	PHE	-	expression tag	UNP O75311
A	361	GLU	-	expression tag	UNP O75311
A	362	LYS	-	expression tag	UNP O75311
B	310	ALA	-	linker	UNP O75311
B	311	GLY	-	linker	UNP O75311
B	312	THR	-	linker	UNP O75311
B	355	TRP	-	expression tag	UNP O75311
B	356	SER	-	expression tag	UNP O75311
B	357	HIS	-	expression tag	UNP O75311
B	358	PRO	-	expression tag	UNP O75311
B	359	GLN	-	expression tag	UNP O75311
B	360	PHE	-	expression tag	UNP O75311
B	361	GLU	-	expression tag	UNP O75311
B	362	LYS	-	expression tag	UNP O75311
D	310	ALA	-	linker	UNP O75311
D	311	GLY	-	linker	UNP O75311
D	312	THR	-	linker	UNP O75311
D	355	TRP	-	expression tag	UNP O75311
D	356	SER	-	expression tag	UNP O75311
D	357	HIS	-	expression tag	UNP O75311
D	358	PRO	-	expression tag	UNP O75311
D	359	GLN	-	expression tag	UNP O75311
D	360	PHE	-	expression tag	UNP O75311
D	361	GLU	-	expression tag	UNP O75311
D	362	LYS	-	expression tag	UNP O75311
E	310	ALA	-	linker	UNP O75311
E	311	GLY	-	linker	UNP O75311
E	312	THR	-	linker	UNP O75311
E	355	TRP	-	expression tag	UNP O75311
E	356	SER	-	expression tag	UNP O75311
E	357	HIS	-	expression tag	UNP O75311
E	358	PRO	-	expression tag	UNP O75311
E	359	GLN	-	expression tag	UNP O75311
E	360	PHE	-	expression tag	UNP O75311
E	361	GLU	-	expression tag	UNP O75311
E	362	LYS	-	expression tag	UNP O75311

- Molecule 2 is (3S,3aS,9bS)-2-[(2H-1,3-benzodioxol-5-yl)sulfonyl]-3,5-dimethyl-1,2,3,3a,5,9b-hexahydro-4H-pyrrolo[3,4-c][1,6]naphthyridin-4-one (three-letter code: 7C6) (formula: C₁₉H₁₉N₃O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	B	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	D	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	E	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).

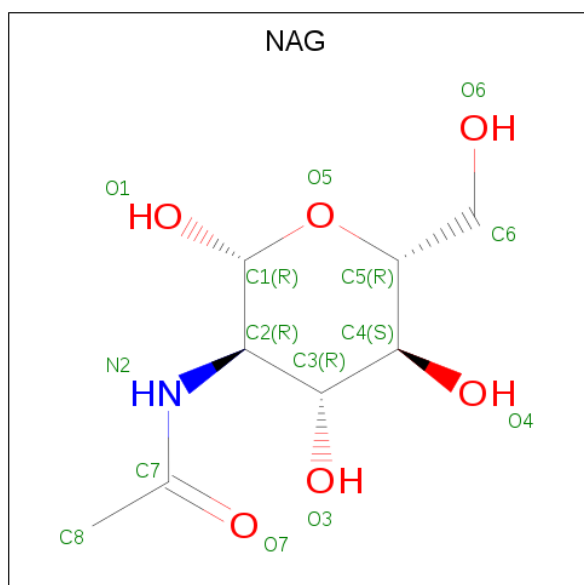


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O 5 2 1 2	0	0
3	A	1	Total C N O 5 2 1 2	0	0
3	B	1	Total C N O 5 2 1 2	0	0
3	D	1	Total C N O 5 2 1 2	0	0
3	E	1	Total C N O 5 2 1 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	A	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	E	1	Total Zn 1 1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

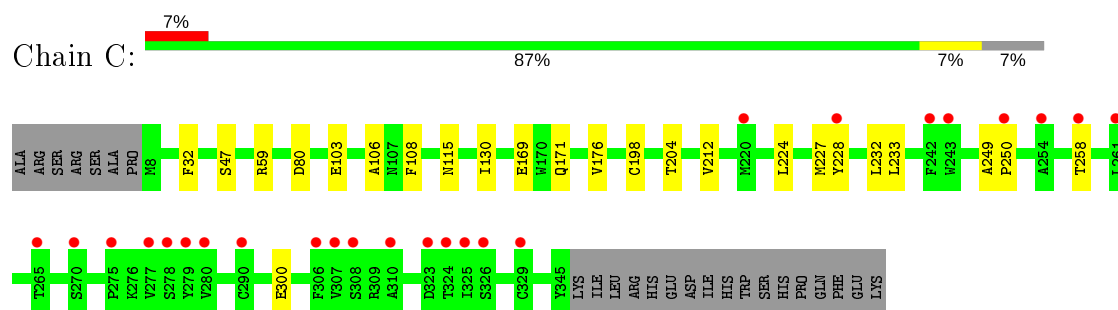


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

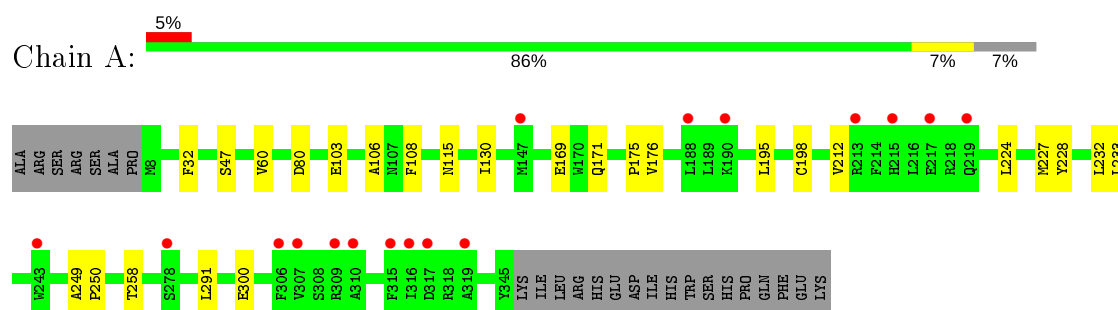
3 Residue-property plots [i](#)

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.

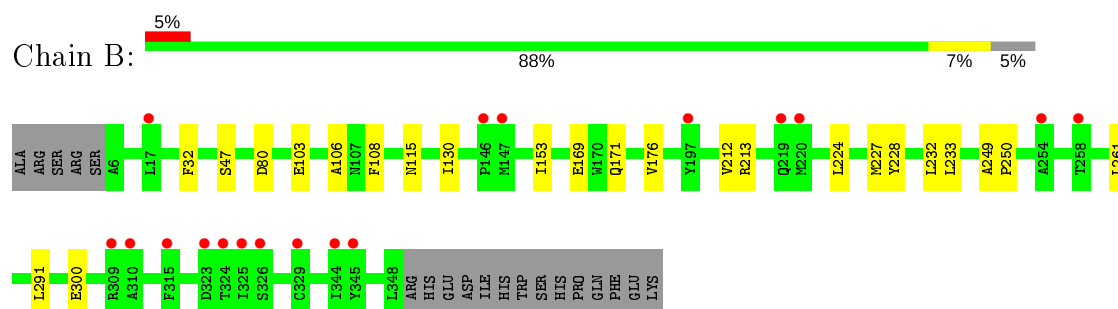
- Molecule 1: Glycine receptor subunit alpha-3



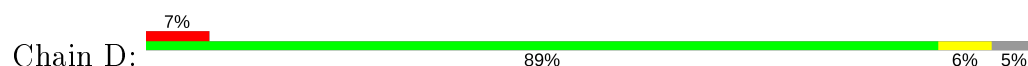
- Molecule 1: Glycine receptor subunit alpha-3

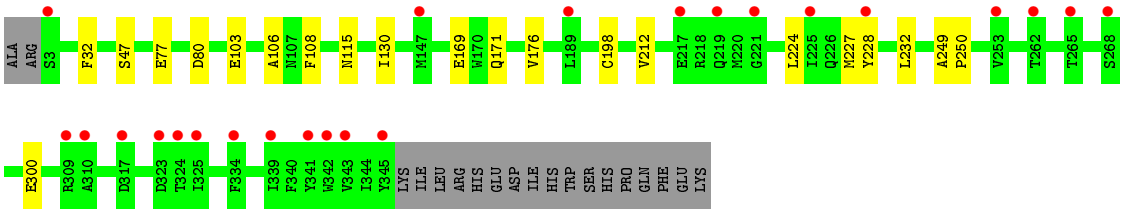


- Molecule 1: Glycine receptor subunit alpha-3

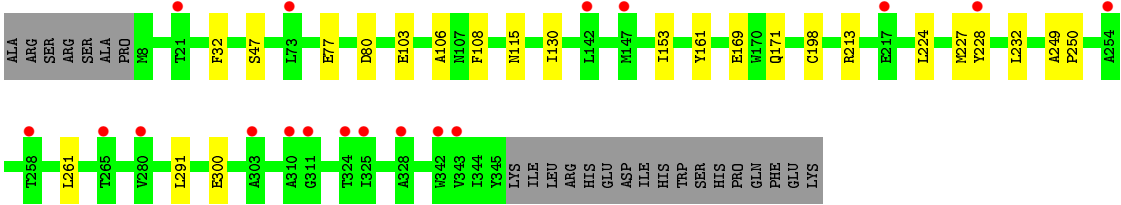
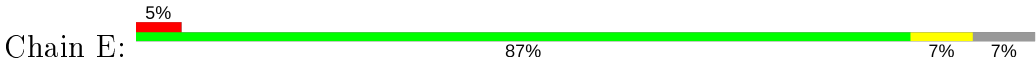


- Molecule 1: Glycine receptor subunit alpha-3





• Molecule 1: Glycine receptor subunit alpha-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.12Å 119.12Å 429.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 42.12 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.25) 99.8 (42.12-3.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.233 , 0.254 0.228 , 0.247	Depositor DCC
R_{free} test set	2490 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	92.8	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13727	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: ZN, NAG, 7C6

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	0.34	0/2773	0.53	0/3776
1	B	0.34	0/2791	0.52	0/3804
1	C	0.33	0/2763	0.53	0/3764
1	D	0.33	0/2796	0.52	0/3810
1	E	0.33	0/2777	0.52	0/3780
All	All	0.34	0/13900	0.53	0/18934

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2702	0	2651	9	0
1	B	2719	0	2654	9	0
1	C	2692	0	2635	8	0
1	D	2724	0	2664	6	0
1	E	2706	0	2662	9	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
2	C	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	0	0	0
2	E	28	0	0	1	0
3	A	5	0	2	0	0
3	B	5	0	2	0	0
3	C	5	0	2	1	0
3	D	5	0	2	0	0
3	E	5	0	2	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	C	14	0	13	0	0
All	All	13727	0	13289	36	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 1.

All (36) 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:291:LEU:HD21	1:B:233:LEU:CD2	2.37	0.53
1:A:108:PHE:CD1	1:A:130:ILE:HD11	2.45	0.52
1:D:108:PHE:CD1	1:D:130:ILE:HD11	2.46	0.51
1:C:108:PHE:CD1	1:C:130:ILE:HD11	2.45	0.51
1:E:108:PHE:CD1	1:E:130:ILE:HD11	2.46	0.50
1:B:108:PHE:CD1	1:B:130:ILE:HD11	2.47	0.50
1:A:258:THR:HB	1:E:261:LEU:HD11	1.94	0.49
1:E:103:GLU:HG3	1:E:106:ALA:HB2	1.95	0.48
1:C:103:GLU:HG3	1:C:106:ALA:HB2	1.95	0.48
1:A:103:GLU:HG3	1:A:106:ALA:HB2	1.95	0.48
1:D:103:GLU:HG3	1:D:106:ALA:HB2	1.95	0.47
1:B:103:GLU:HG3	1:B:106:ALA:HB2	1.95	0.46
1:A:233:LEU:CD2	1:E:291:LEU:HD21	2.45	0.46
1:C:233:LEU:CD2	1:B:291:LEU:HD21	2.47	0.44
1:D:224:LEU:HA	1:D:228:TYR:HB2	2.00	0.43
1:C:249:ALA:N	1:C:250:PRO:HD2	2.34	0.43
1:C:224:LEU:HA	1:C:228:TYR:HB2	2.00	0.43
1:E:224:LEU:HA	1:E:228:TYR:HB2	2.00	0.43
1:D:249:ALA:N	1:D:250:PRO:HD2	2.34	0.43
1:E:249:ALA:N	1:E:250:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ALA:N	1:A:250:PRO:HD2	2.34	0.43
1:B:224:LEU:HA	1:B:228:TYR:HB2	2.01	0.43
1:B:249:ALA:N	1:B:250:PRO:HD2	2.33	0.42
1:A:224:LEU:HA	1:A:228:TYR:HB2	2.00	0.42
1:C:258:THR:HB	1:B:261:LEU:HD11	2.01	0.42
1:D:77:GLU:OE1	1:D:77:GLU:N	2.53	0.42
1:C:176:VAL:HG21	1:C:212:VAL:HG21	2.02	0.41
1:E:161:TYR:CE1	2:E:401:7C6:C15	3.03	0.41
1:A:175:PRO:HG2	1:A:195:LEU:HD11	2.03	0.41
1:B:176:VAL:HG21	1:B:212:VAL:HG21	2.03	0.41
1:E:77:GLU:N	1:E:77:GLU:OE1	2.53	0.41
1:D:176:VAL:HG21	1:D:212:VAL:HG21	2.03	0.41
1:B:153:ILE:HG22	1:B:213:ARG:HG2	2.03	0.40
1:A:176:VAL:HG21	1:A:212:VAL:HG21	2.03	0.40
1:E:153:ILE:HG22	1:E:213:ARG:HG2	2.04	0.40
1:C:204:THR:OG1	3:C:402:GLY:OXT	2.32	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	336/362 (93%)	329 (98%)	7 (2%)	0	100	100
1	B	341/362 (94%)	332 (97%)	9 (3%)	0	100	100
1	C	336/362 (93%)	329 (98%)	7 (2%)	0	100	100
1	D	341/362 (94%)	334 (98%)	7 (2%)	0	100	100
1	E	336/362 (93%)	329 (98%)	7 (2%)	0	100	100
All	All	1690/1810 (93%)	1653 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/326 (91%)	285 (96%)	11 (4%)	34	62
1	B	295/326 (90%)	286 (97%)	9 (3%)	40	67
1	C	294/326 (90%)	283 (96%)	11 (4%)	34	62
1	D	297/326 (91%)	287 (97%)	10 (3%)	37	64
1	E	297/326 (91%)	287 (97%)	10 (3%)	37	64
All	All	1479/1630 (91%)	1428 (97%)	51 (3%)	37	64

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	32	PHE
1	C	47	SER
1	C	59	ARG
1	C	80	ASP
1	C	115	ASN
1	C	169	GLU
1	C	171	GLN
1	C	198	CYS
1	C	227	MET
1	C	232	LEU
1	C	300	GLU
1	A	32	PHE
1	A	47	SER
1	A	60	VAL
1	A	80	ASP
1	A	115	ASN
1	A	169	GLU
1	A	171	GLN
1	A	198	CYS
1	A	227	MET
1	A	232	LEU
1	A	300	GLU
1	B	32	PHE

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Mol	Chain	Res	Type
1	B	47	SER
1	B	80	ASP
1	B	115	ASN
1	B	169	GLU
1	B	171	GLN
1	B	227	MET
1	B	232	LEU
1	B	300	GLU
1	D	32	PHE
1	D	47	SER
1	D	80	ASP
1	D	115	ASN
1	D	169	GLU
1	D	171	GLN
1	D	198	CYS
1	D	227	MET
1	D	232	LEU
1	D	300	GLU
1	E	32	PHE
1	E	47	SER
1	E	80	ASP
1	E	115	ASN
1	E	169	GLU
1	E	171	GLN
1	E	198	CYS
1	E	227	MET
1	E	232	LEU
1	E	300	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	203	ASN

5.3.3 RNA ⓘ

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 [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

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	7C6	D	401	-	31,32,32	2.36	6 (19%)	41,50,50	1.95	10 (24%)
2	7C6	E	401	-	31,32,32	2.04	5 (16%)	41,50,50	1.85	9 (21%)
2	7C6	B	401	-	31,32,32	2.06	6 (19%)	41,50,50	2.09	11 (26%)
2	7C6	C	401	-	31,32,32	1.92	6 (19%)	41,50,50	1.87	8 (19%)
5	NAG	C	404	1	14,14,15	0.50	0	17,19,21	1.56	2 (11%)
2	7C6	A	401	-	31,32,32	2.20	5 (16%)	41,50,50	2.02	11 (26%)

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	7C6	D	401	-	-	0/12/50/50	0/5/5/5
2	7C6	E	401	-	-	0/12/50/50	0/5/5/5
2	7C6	B	401	-	-	0/12/50/50	0/5/5/5
2	7C6	C	401	-	-	0/12/50/50	0/5/5/5
5	NAG	C	404	1	-	1/6/23/26	0/1/1/1
2	7C6	A	401	-	-	0/12/50/50	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	7C6	O3-S1	7.00	1.51	1.43
2	B	401	7C6	O3-S1	6.93	1.51	1.43
2	E	401	7C6	O3-S1	6.86	1.51	1.43
2	D	401	7C6	O2-S1	6.63	1.50	1.43
2	E	401	7C6	O2-S1	6.36	1.50	1.43
2	D	401	7C6	C13-S1	-6.22	1.67	1.76
2	B	401	7C6	O2-S1	6.20	1.50	1.43
2	A	401	7C6	O3-S1	6.12	1.50	1.43
2	C	401	7C6	O3-S1	6.02	1.50	1.43
2	A	401	7C6	C13-S1	-5.82	1.68	1.76
2	A	401	7C6	O2-S1	5.79	1.50	1.43
2	C	401	7C6	O2-S1	5.75	1.49	1.43
2	C	401	7C6	C13-S1	-4.34	1.70	1.76
2	A	401	7C6	C1-N1	-4.04	1.47	1.50
2	D	401	7C6	S1-N1	3.24	1.68	1.63
2	E	401	7C6	C3-N2	3.23	1.42	1.36
2	B	401	7C6	C1-N1	-3.16	1.47	1.50
2	A	401	7C6	O5-C16	-3.09	1.33	1.38
2	B	401	7C6	C2-C3	2.94	1.55	1.51
2	B	401	7C6	C13-S1	-2.87	1.72	1.76
2	D	401	7C6	O5-C16	-2.66	1.34	1.38
2	E	401	7C6	O5-C16	-2.52	1.34	1.38
2	E	401	7C6	C2-C3	2.50	1.54	1.51
2	D	401	7C6	C2-C3	2.39	1.54	1.51
2	B	401	7C6	C3-N2	2.24	1.40	1.36
2	C	401	7C6	O5-C16	-2.16	1.34	1.38
2	C	401	7C6	C3-N2	2.06	1.40	1.36
2	C	401	7C6	C1-N1	-2.05	1.48	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	7C6	C1-N1-S1	-6.32	109.05	120.06
2	C	401	7C6	C1-N1-S1	-5.80	109.94	120.06
2	D	401	7C6	O3-S1-O2	-5.48	110.64	119.52
2	E	401	7C6	O3-S1-O2	-5.19	111.11	119.52
2	B	401	7C6	O3-S1-O2	-5.00	111.42	119.52
2	A	401	7C6	O3-S1-O2	-4.96	111.49	119.52
5	C	404	NAG	C1-O5-C5	4.87	118.80	112.19
2	B	401	7C6	C7-C8-C9	-4.82	120.08	125.03
2	A	401	7C6	C7-C8-C9	-4.76	120.14	125.03
2	E	401	7C6	C1-N1-S1	-4.51	112.19	120.06
2	C	401	7C6	C7-C8-C9	-4.50	120.41	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	7C6	O3-S1-O2	-4.42	112.36	119.52
2	D	401	7C6	C7-C8-C9	-4.38	120.53	125.03
2	C	401	7C6	C10-N1-S1	-4.12	110.79	118.80
2	D	401	7C6	O1-C3-N2	-4.08	118.33	122.44
2	E	401	7C6	C10-N1-S1	-4.04	110.94	118.80
2	A	401	7C6	C1-N1-S1	-3.79	113.45	120.06
2	E	401	7C6	C7-C8-C9	-3.75	121.18	125.03
2	D	401	7C6	C1-N1-S1	-3.75	113.53	120.06
2	A	401	7C6	O1-C3-N2	-3.24	119.17	122.44
2	B	401	7C6	C13-S1-N1	3.23	113.11	107.36
2	A	401	7C6	C13-S1-N1	3.18	113.03	107.36
2	A	401	7C6	O5-C19-O4	-3.02	103.25	108.08
2	B	401	7C6	O4-C15-C14	3.01	131.88	127.85
2	A	401	7C6	C19-O4-C15	-2.97	101.49	105.34
2	D	401	7C6	O5-C19-O4	-2.96	103.35	108.08
2	B	401	7C6	C10-N1-S1	-2.92	113.12	118.80
2	B	401	7C6	O5-C19-O4	-2.89	103.47	108.08
2	D	401	7C6	C13-S1-N1	2.85	112.43	107.36
2	C	401	7C6	C13-S1-N1	2.73	112.23	107.36
2	D	401	7C6	C10-N1-S1	-2.70	113.55	118.80
2	B	401	7C6	C6-N3-C7	2.69	121.51	116.85
2	A	401	7C6	C10-N1-S1	-2.69	113.56	118.80
2	A	401	7C6	O4-C15-C14	2.59	131.31	127.85
2	E	401	7C6	C13-S1-N1	2.54	111.88	107.36
2	E	401	7C6	O4-C15-C14	2.50	131.19	127.85
2	C	401	7C6	O4-C15-C14	2.47	131.16	127.85
2	D	401	7C6	O4-C15-C14	2.34	130.97	127.85
2	A	401	7C6	O2-S1-C13	-2.30	105.14	108.05
2	B	401	7C6	O1-C3-N2	-2.26	120.16	122.44
2	D	401	7C6	C6-N3-C7	2.26	120.76	116.85
2	A	401	7C6	C19-O5-C16	-2.26	102.41	105.34
5	C	404	NAG	O5-C1-C2	-2.25	107.73	111.29
2	C	401	7C6	C6-N3-C7	2.22	120.69	116.85
2	D	401	7C6	O3-S1-N1	2.19	110.96	106.97
2	B	401	7C6	O3-S1-N1	2.15	110.89	106.97
2	C	401	7C6	O1-C3-N2	-2.15	120.28	122.44
2	E	401	7C6	C12-N2-C3	2.13	120.17	117.89
2	E	401	7C6	C6-N3-C7	2.11	120.50	116.85
2	E	401	7C6	O5-C19-O4	-2.06	104.79	108.08
2	B	401	7C6	C11-C1-N1	-2.04	108.47	111.57

There are no chirality outliers.

All (1) torsion outliers are listed below:

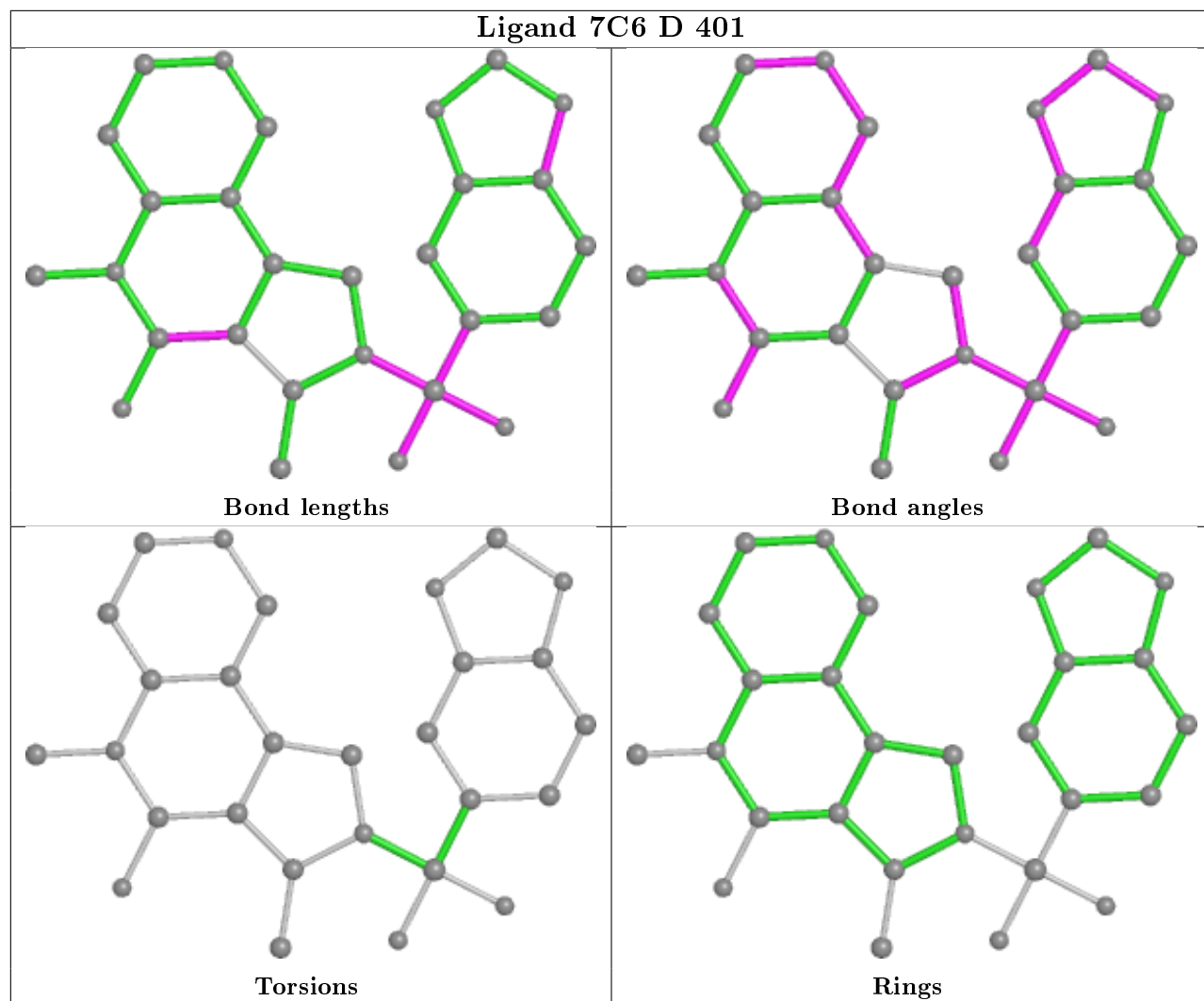
Mol	Chain	Res	Type	Atoms
5	C	404	NAG	O5-C5-C6-O6

There are no ring outliers.

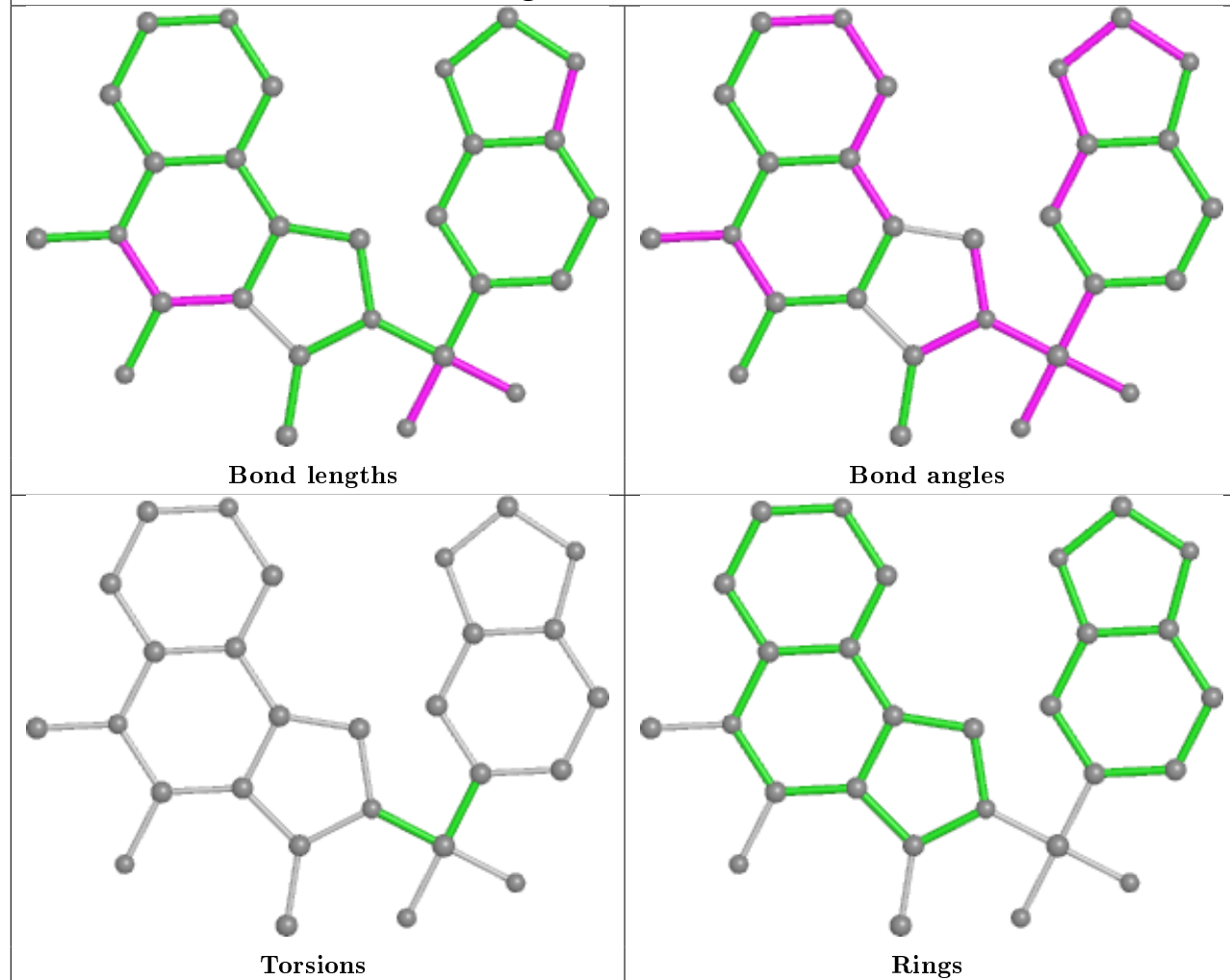
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	7C6	1	0

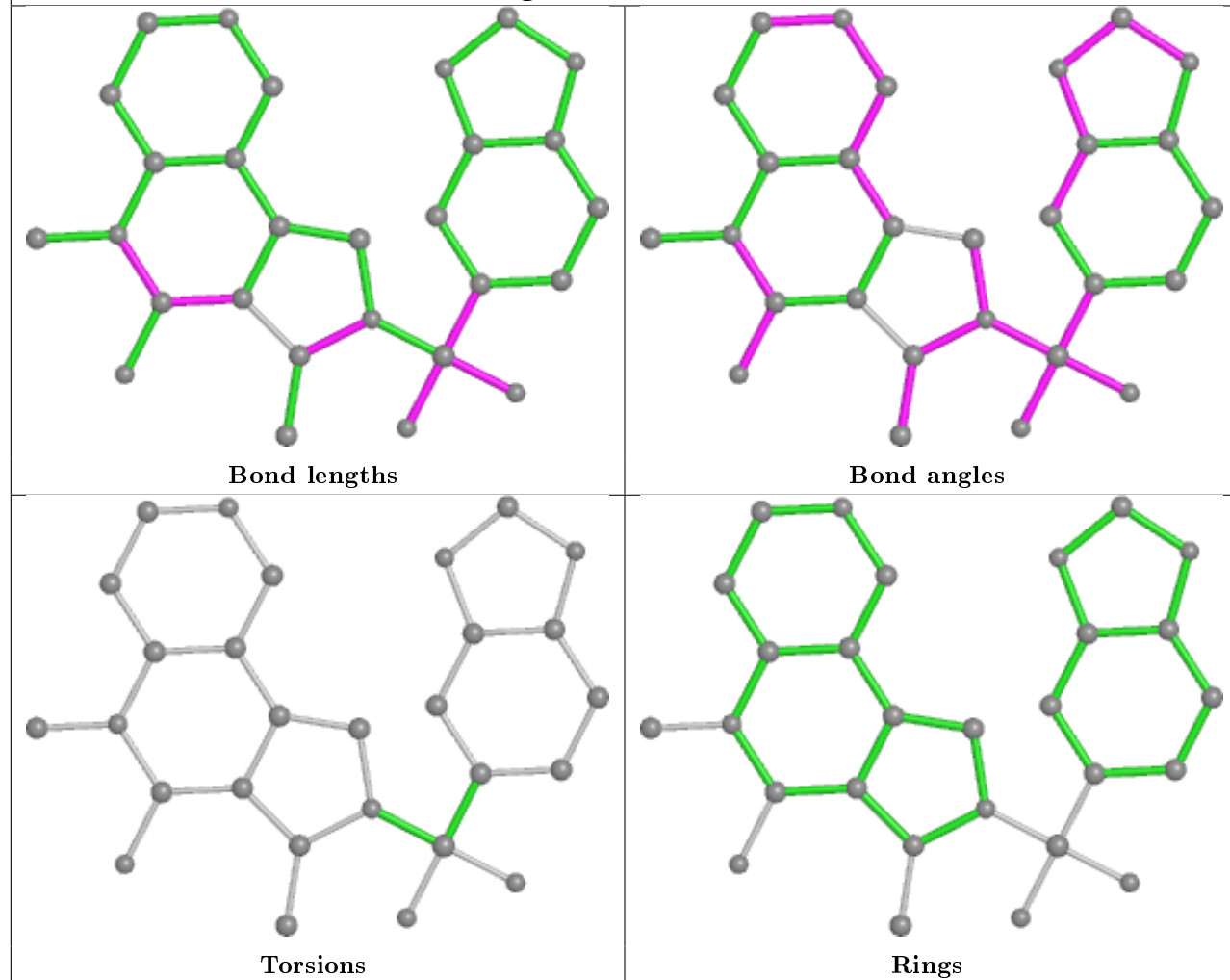
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



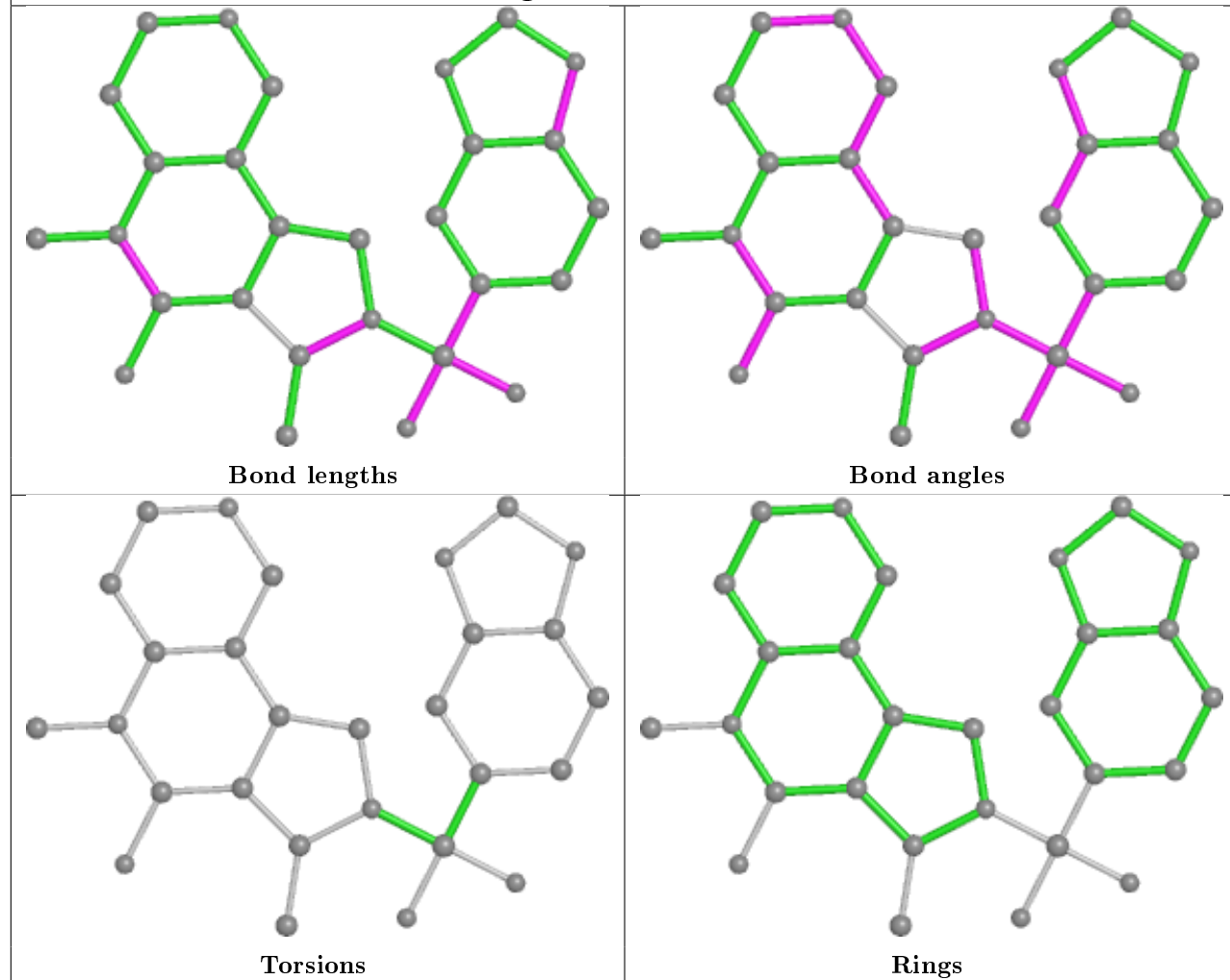
Ligand 7C6 E 401

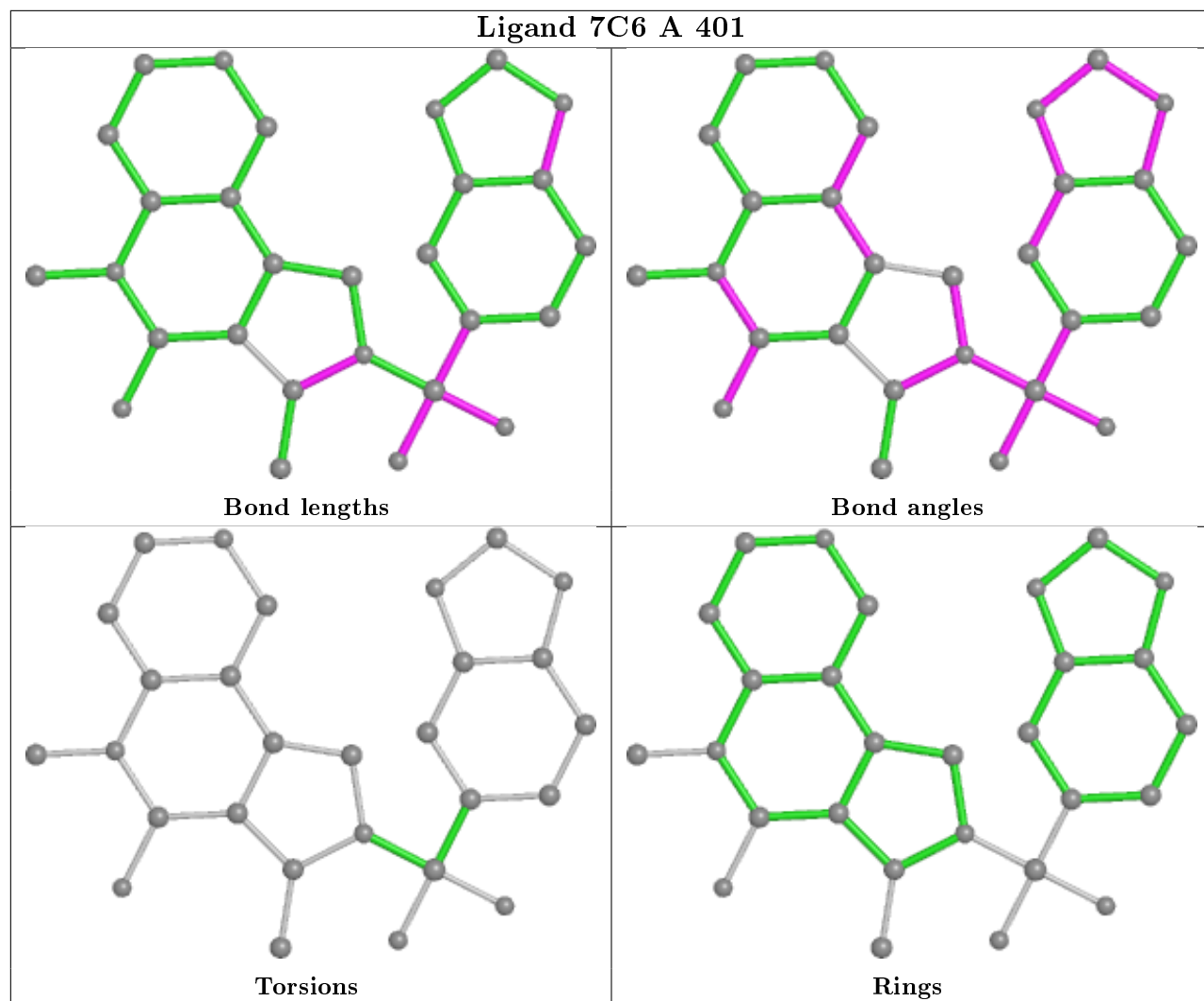


Ligand 7C6 B 401



Ligand 7C6 C 401





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	338/362 (93%)	0.10	17 (5%)	28	26	57, 97, 193, 238	0
1	B	343/362 (94%)	0.15	18 (5%)	27	25	57, 99, 193, 250	0
1	C	338/362 (93%)	0.22	25 (7%)	14	14	59, 110, 241, 299	0
1	D	343/362 (94%)	0.23	24 (6%)	16	15	70, 116, 232, 285	0
1	E	338/362 (93%)	0.16	18 (5%)	26	24	64, 110, 205, 256	0
All	All	1700/1810 (93%)	0.17	102 (6%)	21	21	57, 107, 219, 299	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	324	THR	7.6
1	A	319	ALA	5.7
1	B	219	GLN	5.3
1	A	310	ALA	5.2
1	D	147	MET	4.9
1	C	242	PHE	4.9
1	A	306	PHE	4.7
1	C	278	SER	4.7
1	C	324	THR	4.5
1	E	254	ALA	4.3
1	A	278	SER	4.3
1	C	323	ASP	4.0
1	C	325	ILE	4.0
1	C	307	VAL	3.9
1	C	308	SER	3.9
1	B	220	MET	3.8
1	D	3	SER	3.8
1	E	310	ALA	3.7
1	E	324	THR	3.7
1	D	310	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	307	VAL	3.6
1	E	311	GLY	3.5
1	C	306	PHE	3.5
1	D	345	TYR	3.3
1	B	310	ALA	3.3
1	E	258	THR	3.3
1	C	277	VAL	3.3
1	B	345	TYR	3.2
1	B	258	THR	3.1
1	D	317	ASP	3.1
1	C	261	LEU	3.1
1	D	265	THR	3.1
1	D	341	TYR	3.0
1	D	219	GLN	3.0
1	A	243	TRP	2.9
1	B	324	THR	2.9
1	E	142	LEU	2.8
1	B	323	ASP	2.8
1	B	197	TYR	2.8
1	B	147	MET	2.8
1	C	310	ALA	2.8
1	C	250	PRO	2.8
1	A	317	ASP	2.8
1	D	325	ILE	2.8
1	D	342	TRP	2.7
1	B	309	ARG	2.7
1	C	258	THR	2.7
1	D	323	ASP	2.7
1	C	329	CYS	2.7
1	E	328	ALA	2.7
1	A	215	HIS	2.7
1	E	265	THR	2.7
1	D	343	VAL	2.6
1	C	279	TYR	2.6
1	D	217	GLU	2.6
1	C	243	TRP	2.6
1	A	309	ARG	2.6
1	D	262	THR	2.6
1	A	217	GLU	2.5
1	E	280	VAL	2.5
1	C	265	THR	2.5
1	B	254	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	315	PHE	2.5
1	B	146	PRO	2.5
1	E	73	LEU	2.5
1	D	253	VAL	2.4
1	E	21	THR	2.4
1	D	334	PHE	2.4
1	B	329	CYS	2.4
1	B	326	SER	2.4
1	D	339	ILE	2.4
1	E	343	VAL	2.4
1	A	188	LEU	2.4
1	E	342	TRP	2.3
1	A	190	LYS	2.3
1	A	316	ILE	2.3
1	C	280	VAL	2.3
1	E	217	GLU	2.3
1	B	325	ILE	2.3
1	B	344	ILE	2.3
1	A	315	PHE	2.3
1	C	270	SER	2.3
1	A	219	GLN	2.3
1	D	221	GLY	2.2
1	C	228	TYR	2.2
1	C	254	ALA	2.2
1	D	309	ARG	2.2
1	D	189	LEU	2.2
1	E	303	ALA	2.2
1	A	147	MET	2.1
1	D	225	ILE	2.1
1	C	275	PRO	2.1
1	B	17	LEU	2.1
1	C	326	SER	2.1
1	D	268	SER	2.0
1	C	220	MET	2.0
1	E	228	TYR	2.0
1	A	213	ARG	2.0
1	E	325	ILE	2.0
1	C	290	CYS	2.0
1	E	147	MET	2.0
1	D	228	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 monosaccharides in this entry.

6.4 Ligands [i](#)

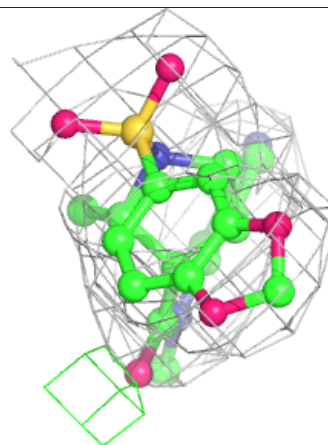
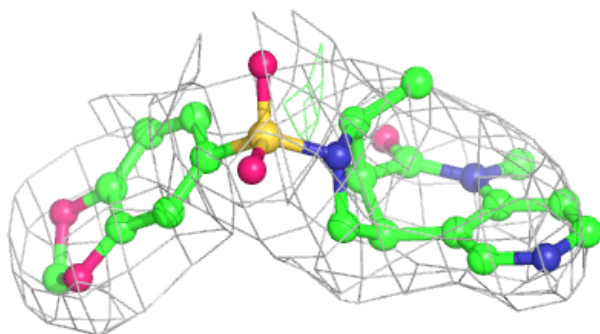
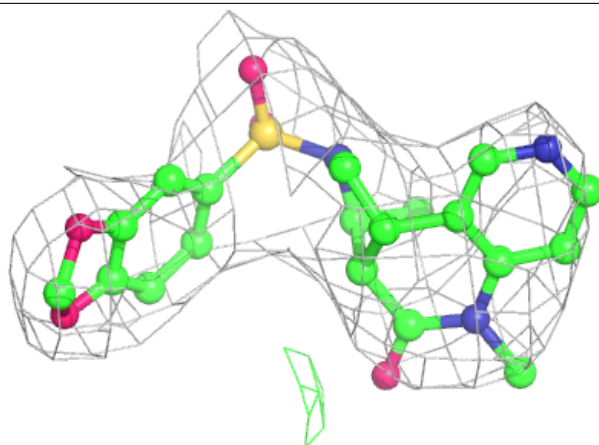
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ZN	E	403	1/1	0.71	0.28	105,105,105,105	1
5	NAG	C	404	14/15	0.78	0.28	139,146,151,152	0
4	ZN	C	403	1/1	0.86	0.17	133,133,133,133	1
4	ZN	D	403	1/1	0.87	0.28	150,150,150,150	1
4	ZN	A	403	1/1	0.88	0.07	107,107,107,107	1
3	GLY	A	402	5/5	0.91	0.32	71,72,73,76	0
4	ZN	B	403	1/1	0.93	0.45	117,117,117,117	1
3	GLY	C	402	5/5	0.93	0.26	85,85,86,87	0
3	GLY	B	402	5/5	0.93	0.32	82,83,88,90	0
3	GLY	D	402	5/5	0.94	0.32	83,83,84,85	0
3	GLY	E	402	5/5	0.94	0.23	74,77,77,80	0
2	7C6	E	401	28/28	0.96	0.23	78,93,100,100	0
2	7C6	B	401	28/28	0.96	0.27	78,84,89,91	0
2	7C6	D	401	28/28	0.97	0.22	90,93,100,100	0
2	7C6	A	401	28/28	0.97	0.24	70,82,88,89	0
2	7C6	C	401	28/28	0.97	0.24	74,94,103,104	0

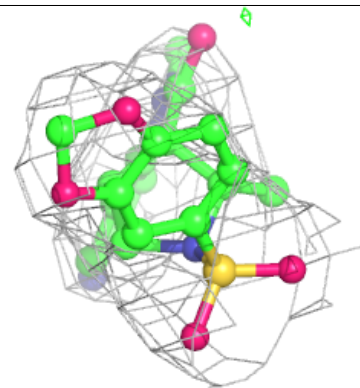
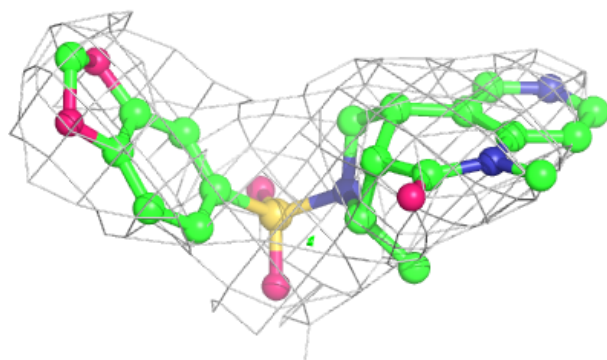
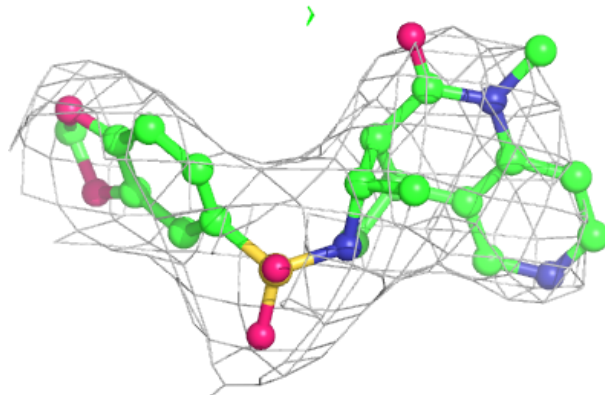
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7C6 E 401:

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

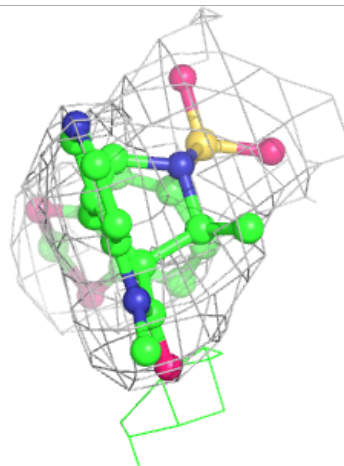
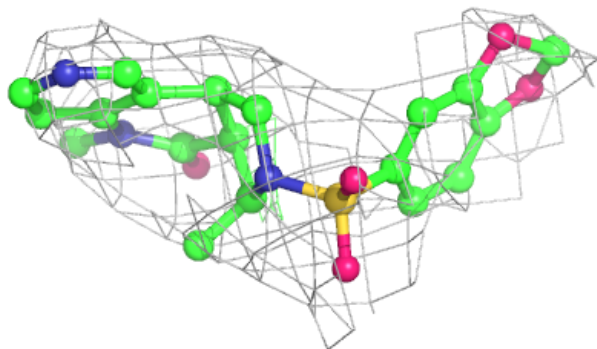
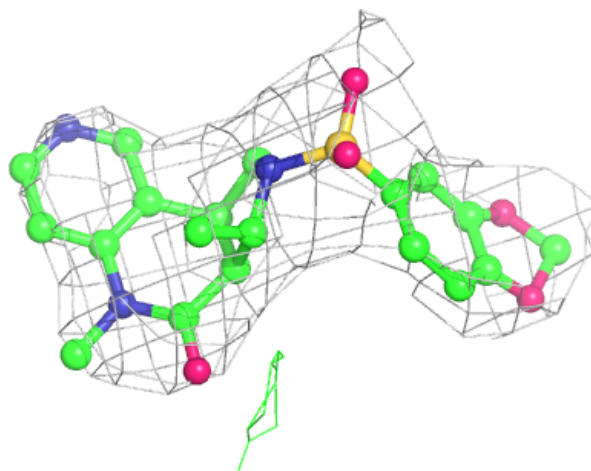
**Electron density around 7C6 B 401:**

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



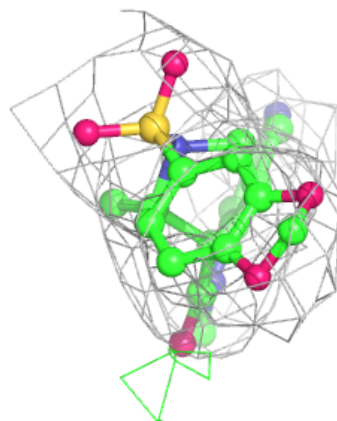
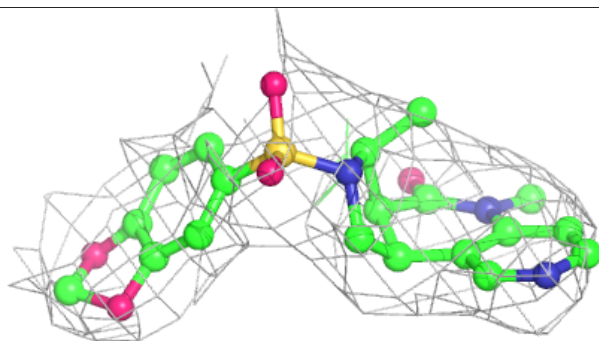
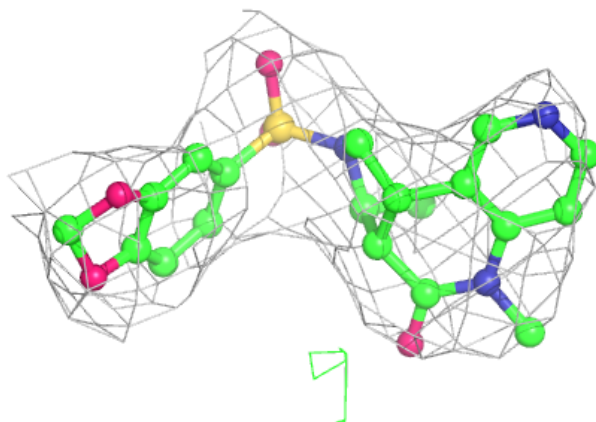
Electron density around 7C6 D 401:

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



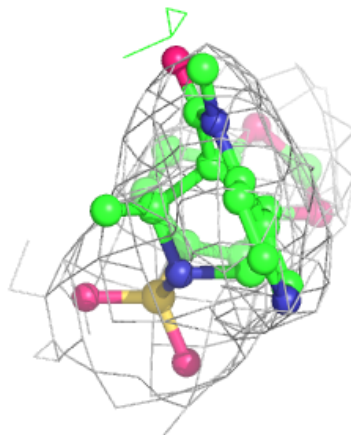
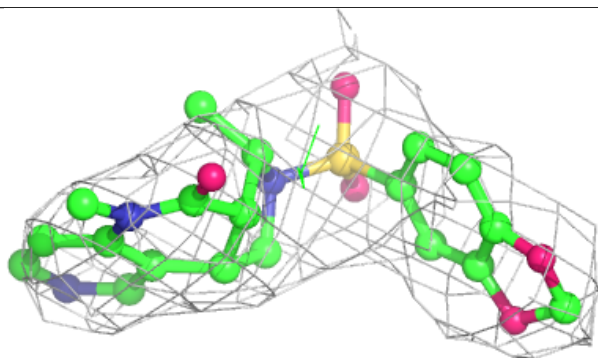
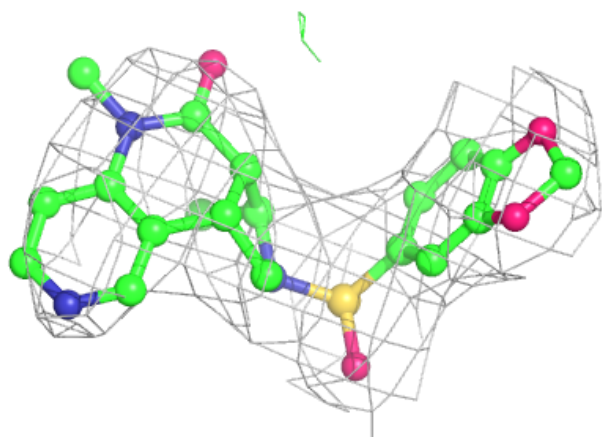
Electron density around 7C6 A 401:

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



Electron density around 7C6 C 401:

$2mF_o-DF_c$ (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.