



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:33 AM UTC

PDB ID : 5TIO / pdb_00005tio
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

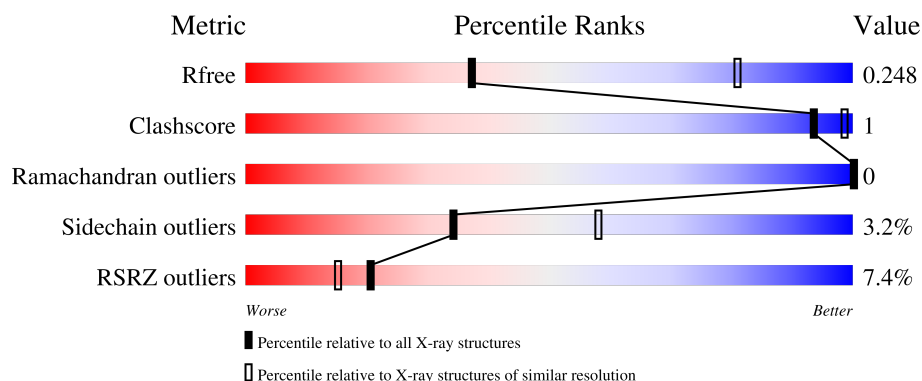
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (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 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	362	4% 87% 6% 7%
1	B	362	5% 88% 7% 5%
1	C	362	8% 88% 6% 7%
1	D	362	10% 89% 6% 5%
1	E	362	8% 87% 6% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLY	B	402	-	X	-	-
3	GLY	D	402	-	X	-	-

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:

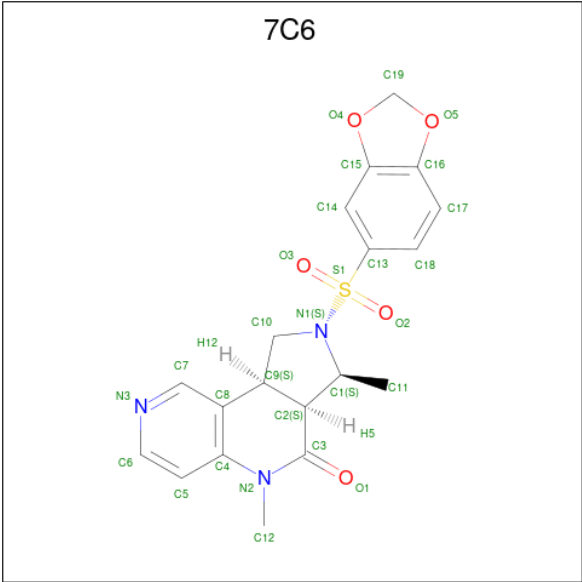
Chain	Residue	Modelled	Actual	Comment	Reference
C	310	ALA	-	linker	UNP O75311
C	311	GLY	-	linker	UNP O75311
C	312	THR	-	linker	UNP O75311
C	355	TRP	-	expression tag	UNP O75311
C	356	SER	-	expression tag	UNP O75311
C	357	HIS	-	expression tag	UNP O75311
C	358	PRO	-	expression tag	UNP O75311
C	359	GLN	-	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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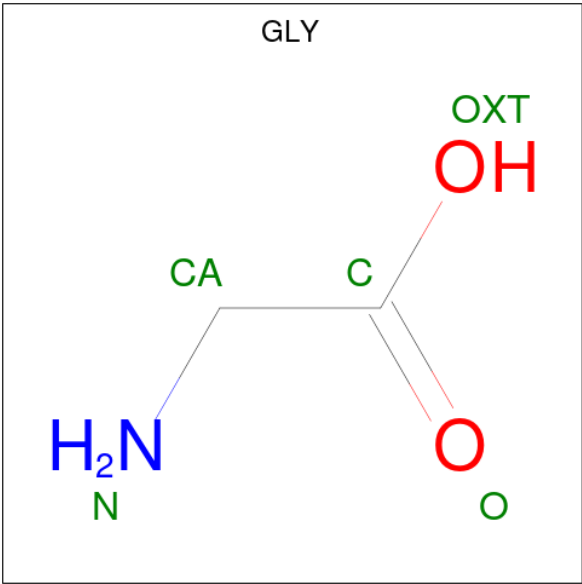
Chain	Residue	Modelled	Actual	Comment	Reference
A	360	PHE	-	expression tag	UNP O75311
A	361	GLU	-	expression tag	UNP O75311
A	362	LYS	-	expression tag	UNP O75311
B	310	ALA	-	linker	UNP O75311
B	311	GLY	-	linker	UNP O75311
B	312	THR	-	linker	UNP O75311
B	355	TRP	-	expression tag	UNP O75311
B	356	SER	-	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-h exahydro-4H-pyrrolo[3,4-c][1,6]naphthyridin-4-one (CCD ID: 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 (CCD ID: GLY) (formula: C₂H₅NO₂).

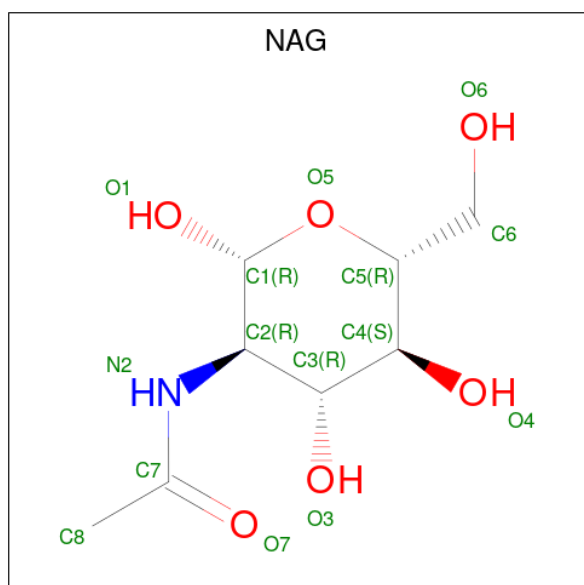


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			5	2	1	2		
3	A	1	Total	C	N	O	0	0
			5	2	1	2		
3	B	1	Total	C	N	O	0	0
			5	2	1	2		
3	D	1	Total	C	N	O	0	0
			5	2	1	2		
3	E	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

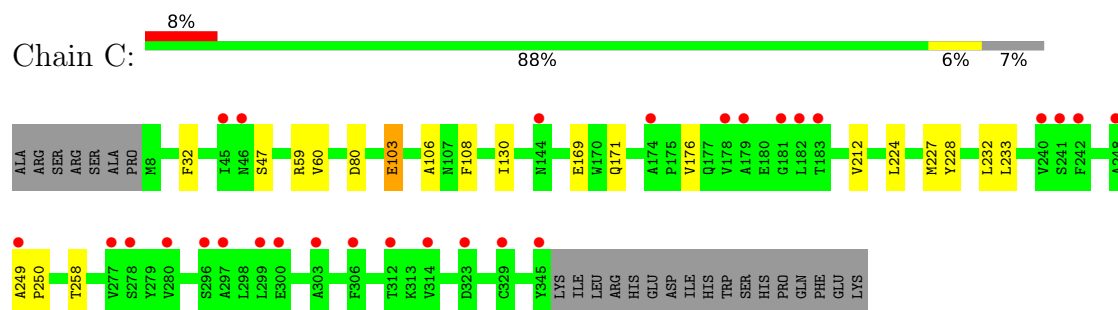


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

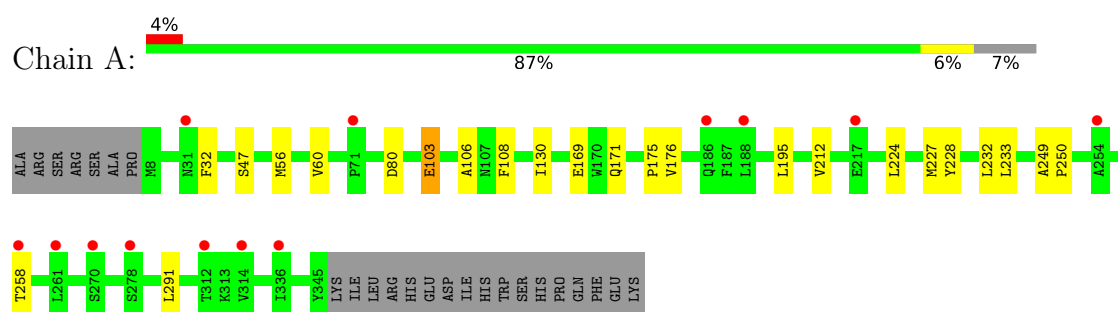
3 Residue-property plots [i](#)

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.

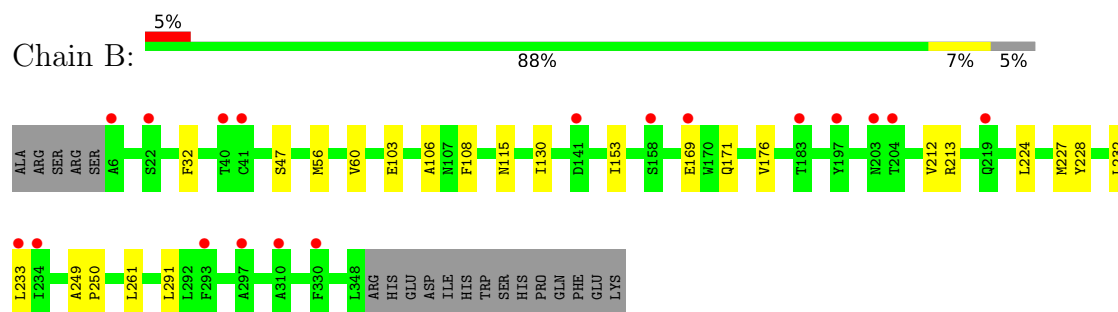
- Molecule 1: Glycine receptor subunit alpha-3



- Molecule 1: Glycine receptor subunit alpha-3

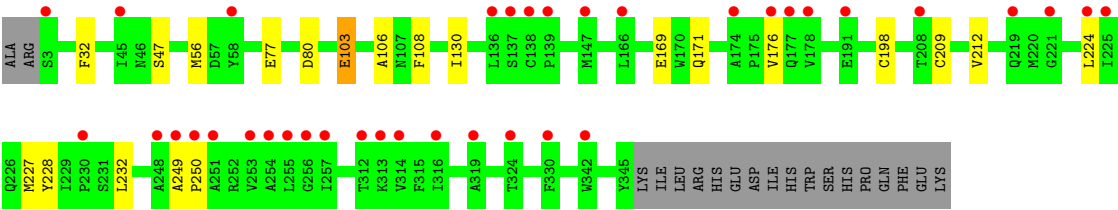


- Molecule 1: Glycine receptor subunit alpha-3

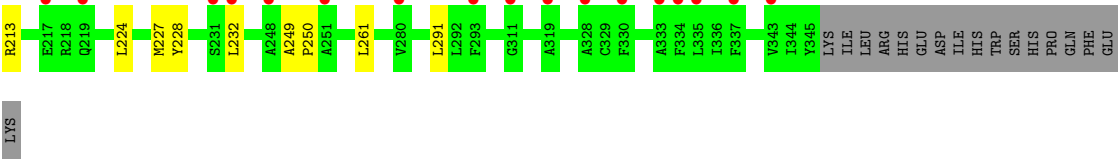
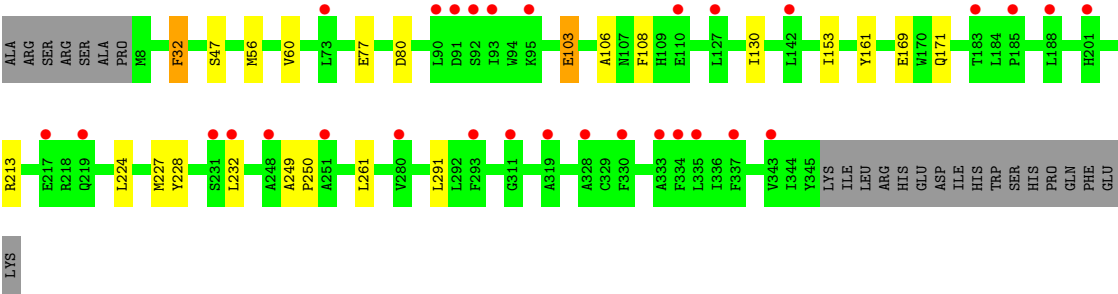
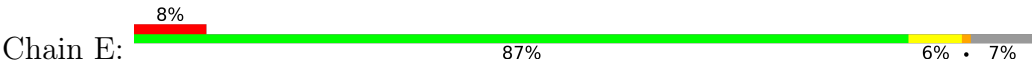


- Molecule 1: Glycine receptor subunit alpha-3





● Molecule 1: Glycine receptor subunit alpha-3



LYS

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 50.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.25) 99.7 (50.00-3.25)	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 0.229 , 0.248	Depositor DCC
R_{free} test set	2490 reflections (3.39%)	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)	0.29 , 70.4	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	0.88	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: NAG, 7C6, ZN

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	0.47	0/2773	0.72	0/3776
1	B	0.48	0/2791	0.72	0/3804
1	C	0.47	0/2763	0.72	0/3764
1	D	0.47	0/2796	0.71	0/3810
1	E	0.46	0/2777	0.72	0/3780
All	All	0.47	0/13900	0.72	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	7	0
1	D	2724	0	2664	7	0
1	E	2706	0	2662	10	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	0	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	37	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 (37) 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:N	1:D:77:GLU:OE1	2.53	0.42
1:C:176:VAL:HG21	1:C:212:VAL:HG21	2.02	0.41
1:D:198:CYS:SG	1:D:209:CYS:C	3.04	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:D:176:VAL:HG21	1:D:212:VAL:HG21	2.03	0.41
1:E:77:GLU:OE1	1:E:77:GLU:N	2.53	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:E:32:PHE:CD1	1:E:32:PHE:C	2.99	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	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%)	286 (97%)	10 (3%)	32	57
1	B	295/326 (90%)	286 (97%)	9 (3%)	35	59
1	C	294/326 (90%)	284 (97%)	10 (3%)	32	57
1	D	297/326 (91%)	288 (97%)	9 (3%)	36	59
1	E	297/326 (91%)	287 (97%)	10 (3%)	32	57
All	All	1479/1630 (91%)	1431 (97%)	48 (3%)	34	58

All (48) 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	60	VAL
1	C	80	ASP
1	C	103	GLU
1	C	169	GLU
1	C	171	GLN
1	C	227	MET
1	C	232	LEU
1	A	32	PHE
1	A	47	SER
1	A	56	MET
1	A	60	VAL
1	A	80	ASP
1	A	103	GLU
1	A	169	GLU
1	A	171	GLN
1	A	227	MET
1	A	232	LEU
1	B	32	PHE

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Mol	Chain	Res	Type
1	B	47	SER
1	B	56	MET
1	B	60	VAL
1	B	115	ASN
1	B	169	GLU
1	B	171	GLN
1	B	227	MET
1	B	232	LEU
1	D	32	PHE
1	D	47	SER
1	D	56	MET
1	D	80	ASP
1	D	103	GLU
1	D	169	GLU
1	D	171	GLN
1	D	227	MET
1	D	232	LEU
1	E	32	PHE
1	E	47	SER
1	E	56	MET
1	E	60	VAL
1	E	80	ASP
1	E	103	GLU
1	E	169	GLU
1	E	171	GLN
1	E	227	MET
1	E	232	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	219	GLN
1	A	66	GLN
1	A	107	ASN
1	A	219	GLN
1	B	66	GLN
1	B	107	ASN
1	B	219	GLN
1	D	203	ASN
1	D	219	GLN
1	E	66	GLN
1	E	219	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	401	-	31,32,32	2.25	5 (16%)	41,50,50	2.05	11 (26%)
3	GLY	D	402	-	4,4,4	1.40	1 (25%)	3,4,4	2.25	1 (33%)
5	NAG	C	404	1	14,14,15	0.52	0	17,19,21	1.57	2 (11%)
3	GLY	C	402	-	4,4,4	1.17	1 (25%)	3,4,4	1.76	2 (66%)
3	GLY	A	402	-	4,4,4	1.27	1 (25%)	3,4,4	1.87	2 (66%)
2	7C6	D	401	-	31,32,32	2.42	6 (19%)	41,50,50	1.99	10 (24%)
2	7C6	E	401	-	31,32,32	2.10	5 (16%)	41,50,50	1.89	9 (21%)
3	GLY	B	402	-	4,4,4	1.15	1 (25%)	3,4,4	1.97	2 (66%)
3	GLY	E	402	-	4,4,4	1.30	1 (25%)	3,4,4	1.86	2 (66%)
2	7C6	B	401	-	31,32,32	2.12	6 (19%)	41,50,50	2.13	12 (29%)
2	7C6	C	401	-	31,32,32	1.98	5 (16%)	41,50,50	1.90	8 (19%)

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	A	401	-	-	0/12/50/50	0/5/5/5
3	GLY	D	402	-	-	2/2/2/2	-
5	NAG	C	404	1	-	1/6/23/26	0/1/1/1
3	GLY	C	402	-	-	0/2/2/2	-
3	GLY	A	402	-	-	0/2/2/2	-
2	7C6	D	401	-	-	0/12/50/50	0/5/5/5
2	7C6	E	401	-	-	0/12/50/50	0/5/5/5
3	GLY	B	402	-	-	2/2/2/2	-
3	GLY	E	402	-	-	0/2/2/2	-
2	7C6	B	401	-	-	0/12/50/50	0/5/5/5
2	7C6	C	401	-	-	0/12/50/50	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	7C6	O3-S1	7.29	1.51	1.43
2	B	401	7C6	O3-S1	7.22	1.51	1.43
2	E	401	7C6	O3-S1	7.15	1.51	1.43
2	D	401	7C6	O2-S1	6.91	1.50	1.43
2	E	401	7C6	O2-S1	6.63	1.50	1.43
2	B	401	7C6	O2-S1	6.46	1.50	1.43
2	D	401	7C6	C13-S1	-6.45	1.67	1.76
2	A	401	7C6	O3-S1	6.38	1.50	1.43
2	C	401	7C6	O3-S1	6.27	1.50	1.43
2	A	401	7C6	O2-S1	6.04	1.50	1.43
2	A	401	7C6	C13-S1	-6.03	1.68	1.76
2	C	401	7C6	O2-S1	6.00	1.49	1.43
2	C	401	7C6	C13-S1	-4.49	1.70	1.76
2	A	401	7C6	C1-N1	-4.24	1.47	1.50
2	E	401	7C6	C3-N2	3.53	1.42	1.36
2	D	401	7C6	S1-N1	3.33	1.68	1.63
2	B	401	7C6	C1-N1	-3.32	1.47	1.50
2	B	401	7C6	C13-S1	-2.97	1.72	1.76
2	A	401	7C6	O5-C16	-2.78	1.33	1.38
3	D	402	GLY	OXT-C	-2.76	1.21	1.30
2	B	401	7C6	C2-C3	2.53	1.55	1.51
3	E	402	GLY	OXT-C	-2.52	1.22	1.30
3	A	402	GLY	OXT-C	-2.46	1.22	1.30
2	B	401	7C6	C3-N2	2.39	1.40	1.36
2	D	401	7C6	O5-C16	-2.39	1.34	1.38
2	E	401	7C6	O5-C16	-2.26	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	GLY	OXT-C	-2.26	1.23	1.30
3	B	402	GLY	OXT-C	-2.25	1.23	1.30
2	C	401	7C6	C3-N2	2.18	1.40	1.36
2	E	401	7C6	C2-C3	2.17	1.54	1.51
2	C	401	7C6	C1-N1	-2.15	1.48	1.50
2	D	401	7C6	C2-C3	2.08	1.54	1.51

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	7C6	C1-N1-S1	-6.41	109.05	120.13
2	C	401	7C6	C1-N1-S1	-5.89	109.94	120.13
2	D	401	7C6	O3-S1-O2	-5.74	110.64	119.59
2	E	401	7C6	O3-S1-O2	-5.43	111.11	119.59
2	B	401	7C6	O3-S1-O2	-5.23	111.42	119.59
2	A	401	7C6	O3-S1-O2	-5.19	111.49	119.59
5	C	404	NAG	C1-O5-C5	4.93	118.80	112.19
2	B	401	7C6	C7-C8-C9	-4.90	120.08	125.03
2	A	401	7C6	C7-C8-C9	-4.84	120.14	125.03
2	C	401	7C6	O3-S1-O2	-4.63	112.36	119.59
2	E	401	7C6	C1-N1-S1	-4.59	112.19	120.13
2	C	401	7C6	C7-C8-C9	-4.57	120.41	125.03
2	D	401	7C6	C7-C8-C9	-4.45	120.53	125.03
2	D	401	7C6	O1-C3-N2	-4.13	118.33	122.35
2	C	401	7C6	C10-N1-S1	-4.03	110.79	118.80
2	E	401	7C6	C10-N1-S1	-3.95	110.94	118.80
2	A	401	7C6	C1-N1-S1	-3.86	113.45	120.13
2	D	401	7C6	C1-N1-S1	-3.82	113.53	120.13
2	E	401	7C6	C7-C8-C9	-3.81	121.18	125.03
3	D	402	GLY	OXT-C-O	-3.33	114.76	123.33
2	B	401	7C6	C13-S1-N1	3.29	113.11	107.36
2	A	401	7C6	O1-C3-N2	-3.26	119.17	122.35
2	A	401	7C6	C13-S1-N1	3.25	113.03	107.36
2	A	401	7C6	O5-C19-O4	-3.09	103.25	108.09
2	D	401	7C6	O5-C19-O4	-3.03	103.35	108.09
2	B	401	7C6	O4-C15-C14	3.02	131.88	127.86
2	B	401	7C6	O5-C19-O4	-2.95	103.47	108.09
2	D	401	7C6	C13-S1-N1	2.91	112.43	107.36
2	A	401	7C6	C19-O4-C15	-2.86	101.49	105.32
2	B	401	7C6	C10-N1-S1	-2.85	113.12	118.80
2	C	401	7C6	C13-S1-N1	2.79	112.23	107.36
2	B	401	7C6	C6-N3-C7	2.66	121.51	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	7C6	C10-N1-S1	-2.64	113.55	118.80
2	A	401	7C6	C10-N1-S1	-2.63	113.56	118.80
2	E	401	7C6	C12-N2-C3	2.61	120.17	117.69
2	A	401	7C6	O4-C15-C14	2.60	131.31	127.86
2	E	401	7C6	C13-S1-N1	2.59	111.88	107.36
3	A	402	GLY	OXT-C-O	-2.52	116.85	123.33
2	E	401	7C6	O4-C15-C14	2.51	131.19	127.86
3	E	402	GLY	OXT-C-O	-2.51	116.88	123.33
2	C	401	7C6	O4-C15-C14	2.48	131.16	127.86
3	B	402	GLY	OXT-C-CA	2.47	123.19	113.38
2	A	401	7C6	O2-S1-C13	-2.39	105.14	108.10
2	D	401	7C6	O4-C15-C14	2.34	130.97	127.86
5	C	404	NAG	O5-C1-C2	-2.30	107.73	111.29
2	D	401	7C6	O3-S1-N1	2.28	110.96	106.97
3	C	402	GLY	OXT-C-O	-2.28	117.47	123.33
2	B	401	7C6	O1-C3-N2	-2.25	120.16	122.35
3	B	402	GLY	OXT-C-O	-2.25	117.55	123.33
2	B	401	7C6	O3-S1-N1	2.24	110.89	106.97
2	D	401	7C6	C6-N3-C7	2.23	120.76	116.85
2	C	401	7C6	C6-N3-C7	2.19	120.69	116.85
2	A	401	7C6	C19-O5-C16	-2.17	102.41	105.32
2	C	401	7C6	O1-C3-N2	-2.13	120.28	122.35
2	B	401	7C6	C8-C7-N3	-2.13	121.02	124.41
2	E	401	7C6	O5-C19-O4	-2.11	104.79	108.09
2	E	401	7C6	C6-N3-C7	2.08	120.50	116.85
3	A	402	GLY	OXT-C-CA	2.02	121.42	113.38
2	B	401	7C6	C4-N2-C3	-2.02	120.34	122.58
3	C	402	GLY	OXT-C-CA	2.02	121.40	113.38
3	E	402	GLY	OXT-C-CA	2.01	121.37	113.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

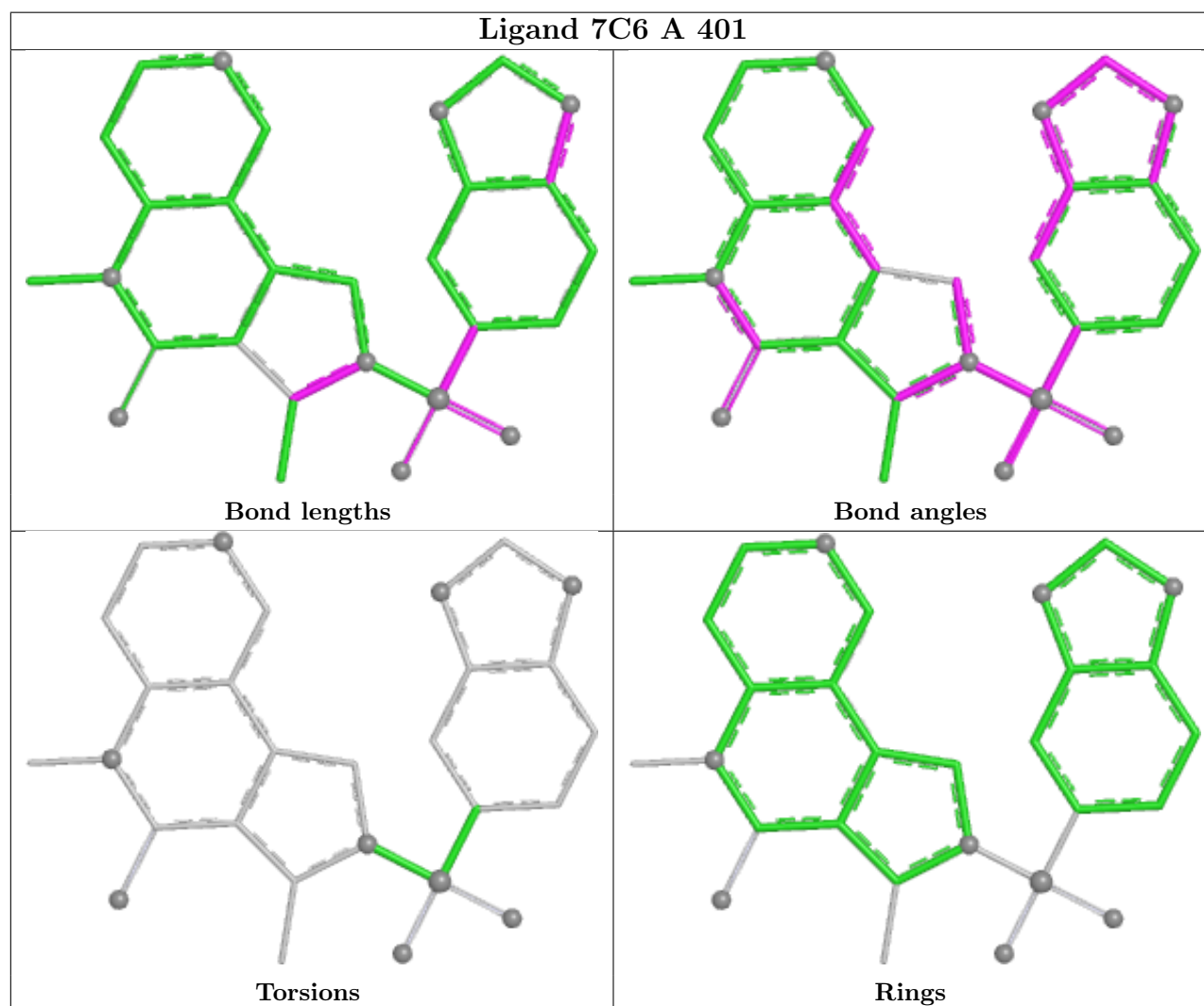
Mol	Chain	Res	Type	Atoms
3	B	402	GLY	O-C-CA-N
3	B	402	GLY	OXT-C-CA-N
3	D	402	GLY	O-C-CA-N
3	D	402	GLY	OXT-C-CA-N
5	C	404	NAG	O5-C5-C6-O6

There are no ring outliers.

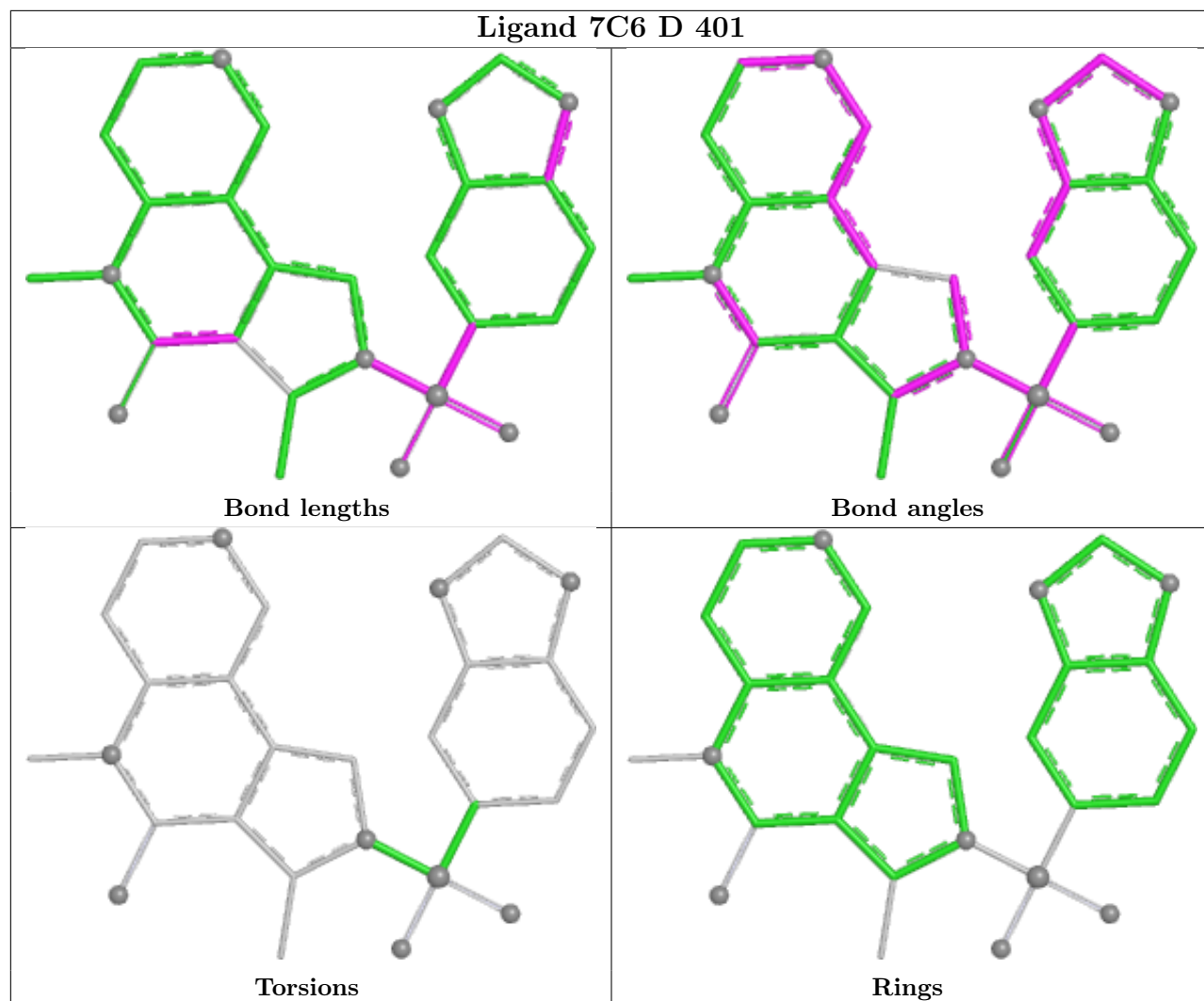
1 monomer is involved in 1 short contact:

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

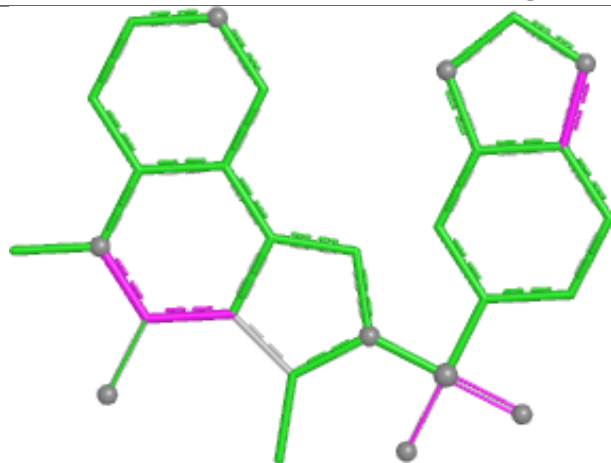
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



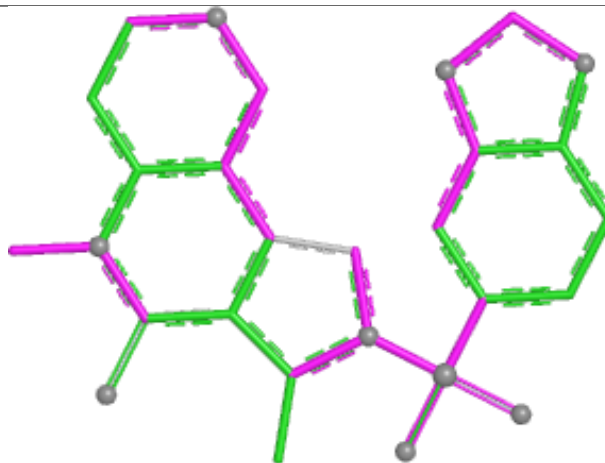
Ligand 7C6 D 401



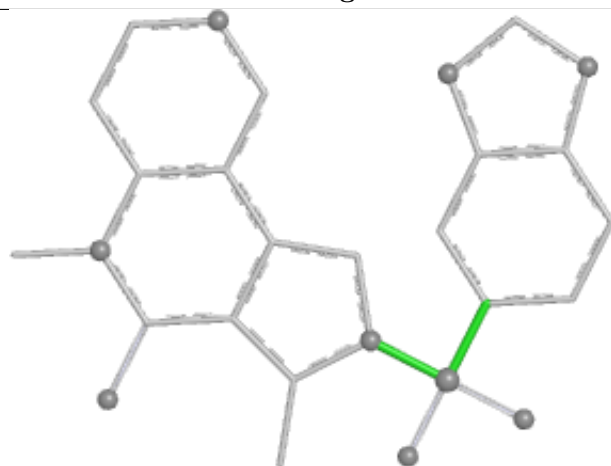
Ligand 7C6 E 401



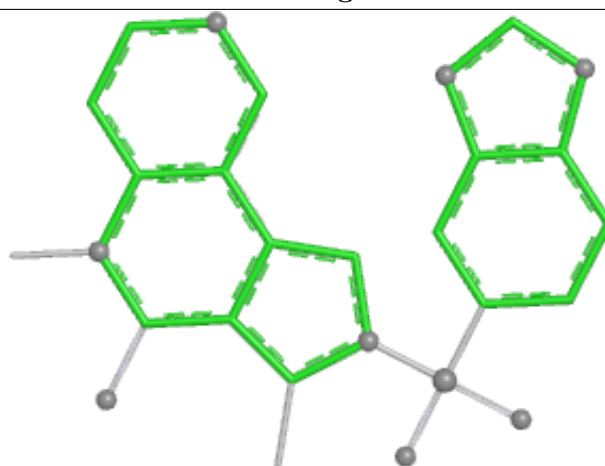
Bond lengths



Bond angles

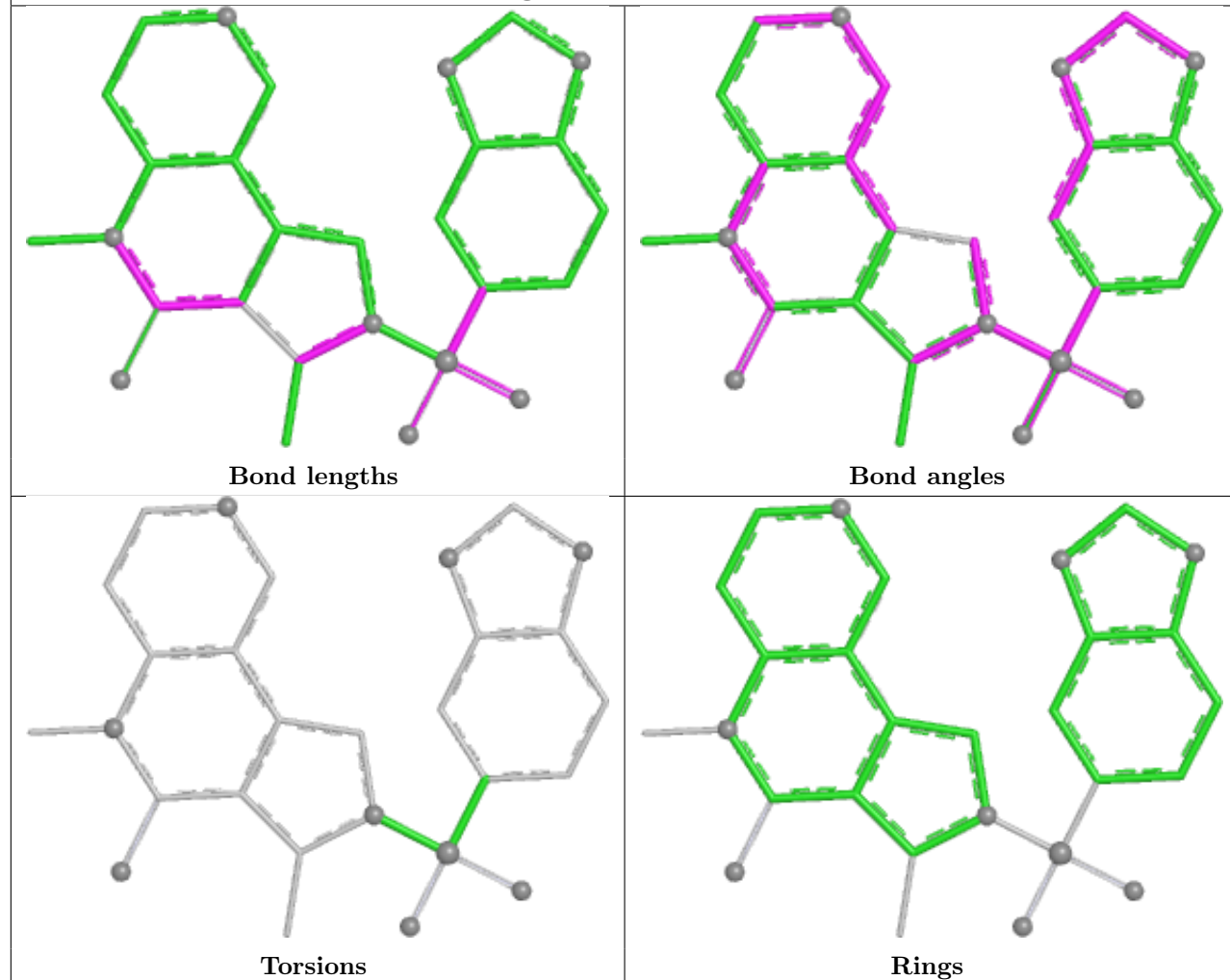


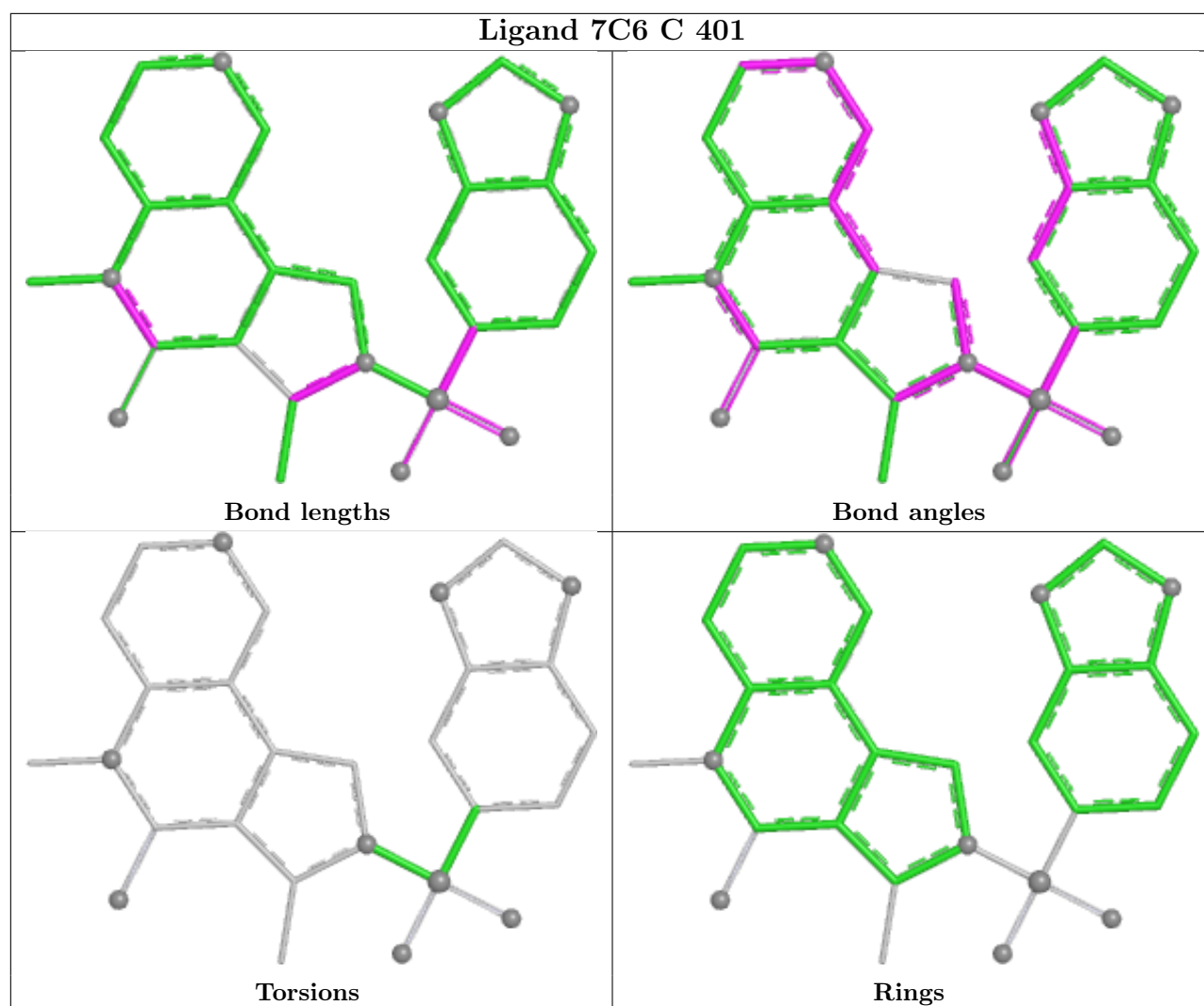
Torsions



Rings

Ligand 7C6 B 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%)	0.16	13 (3%)	44	29	57, 97, 193, 238	0
1	B	343/362 (94%)	0.24	18 (5%)	33	22	57, 99, 193, 250	0
1	C	338/362 (93%)	0.43	28 (8%)	17	13	59, 110, 241, 299	0
1	D	343/362 (94%)	0.49	37 (10%)	11	9	70, 116, 232, 284	0
1	E	338/362 (93%)	0.31	30 (8%)	15	12	64, 110, 205, 256	0
All	All	1700/1810 (93%)	0.33	126 (7%)	20	15	57, 107, 219, 299	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	253	VAL	8.3
1	C	181	GLY	5.8
1	D	254	ALA	5.7
1	D	249	ALA	5.6
1	B	219	GLN	5.2
1	C	278	SER	5.1
1	D	137	SER	5.0
1	E	330	PHE	4.9
1	C	182	LEU	4.9
1	D	312	THR	4.8
1	B	203	ASN	4.6
1	D	177	GLN	4.4
1	B	233	LEU	4.4
1	C	296	SER	4.3
1	C	242	PHE	4.2
1	D	256	GLY	4.2
1	E	188	LEU	4.2
1	C	249	ALA	4.2
1	E	251	ALA	4.2
1	E	293	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	179	ALA	4.1
1	D	250	PRO	4.1
1	D	147	MET	4.0
1	E	217	GLU	4.0
1	C	300	GLU	3.9
1	D	251	ALA	3.9
1	C	323	ASP	3.8
1	C	144	ASN	3.7
1	D	248	ALA	3.7
1	D	191	GLU	3.7
1	C	306	PHE	3.7
1	A	258	THR	3.6
1	D	176	VAL	3.6
1	C	46	ASN	3.6
1	D	138	CYS	3.5
1	E	334	PHE	3.5
1	D	219	GLN	3.4
1	B	197	TYR	3.4
1	B	310	ALA	3.4
1	C	183	THR	3.4
1	E	90	LEU	3.3
1	B	169	GLU	3.3
1	C	45	ILE	3.3
1	B	183	THR	3.3
1	D	174	ALA	3.3
1	E	93	ILE	3.2
1	E	337	PHE	3.2
1	B	234	ILE	3.2
1	E	183	THR	3.1
1	E	231	SER	3.1
1	E	319	ALA	3.1
1	C	303	ALA	3.1
1	B	40	THR	3.1
1	B	204	THR	3.1
1	C	178	VAL	3.0
1	D	324	THR	3.0
1	B	330	PHE	3.0
1	C	312	THR	3.0
1	E	280	VAL	2.9
1	D	139	PRO	2.9
1	A	314	VAL	2.9
1	C	299	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	219	GLN	2.9
1	E	91	ASP	2.9
1	C	248	ALA	2.9
1	D	313	LYS	2.9
1	E	335	LEU	2.9
1	A	261	LEU	2.8
1	A	336	ILE	2.8
1	D	225	ILE	2.8
1	C	280	VAL	2.8
1	D	314	VAL	2.8
1	D	166	LEU	2.8
1	E	333	ALA	2.7
1	E	311	GLY	2.7
1	D	58	TYR	2.7
1	D	342	TRP	2.7
1	A	188	LEU	2.7
1	C	240	VAL	2.7
1	D	178	VAL	2.7
1	E	328	ALA	2.7
1	E	110	GLU	2.6
1	A	270	SER	2.6
1	D	319	ALA	2.6
1	E	248	ALA	2.6
1	B	297	ALA	2.6
1	C	297	ALA	2.5
1	E	201	HIS	2.5
1	D	224	LEU	2.5
1	B	141	ASP	2.5
1	D	136	LEU	2.5
1	B	6	ALA	2.5
1	A	254	ALA	2.4
1	C	329	CYS	2.4
1	D	45	ILE	2.4
1	A	217	GLU	2.4
1	D	330	PHE	2.4
1	E	232	LEU	2.4
1	E	142	LEU	2.4
1	A	278	SER	2.4
1	D	3	SER	2.4
1	E	343	VAL	2.3
1	C	174	ALA	2.3
1	C	277	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	241	SER	2.3
1	A	71	PRO	2.3
1	E	127	LEU	2.3
1	A	31	ASN	2.3
1	D	221	GLY	2.2
1	A	312	THR	2.2
1	C	345	TYR	2.2
1	E	185	PRO	2.2
1	B	293	PHE	2.2
1	B	22	SER	2.2
1	E	92	SER	2.2
1	D	316	ILE	2.2
1	D	230	PRO	2.2
1	E	95	LYS	2.2
1	B	158	SER	2.2
1	D	257	ILE	2.2
1	D	255	LEU	2.2
1	A	186	GLN	2.1
1	E	73	LEU	2.1
1	D	208	THR	2.1
1	B	41	CYS	2.1
1	C	314	VAL	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, 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
4	ZN	D	403	1/1	0.56	0.08	150,150,150,150	1

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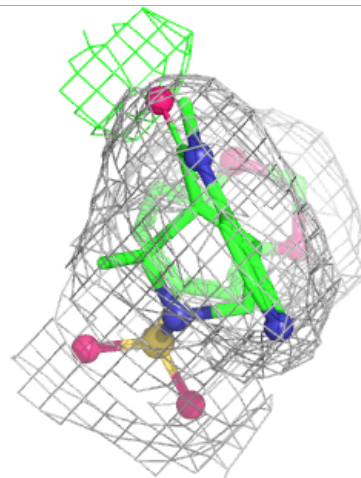
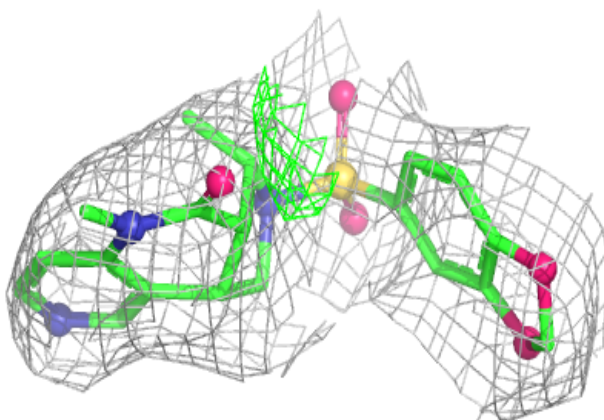
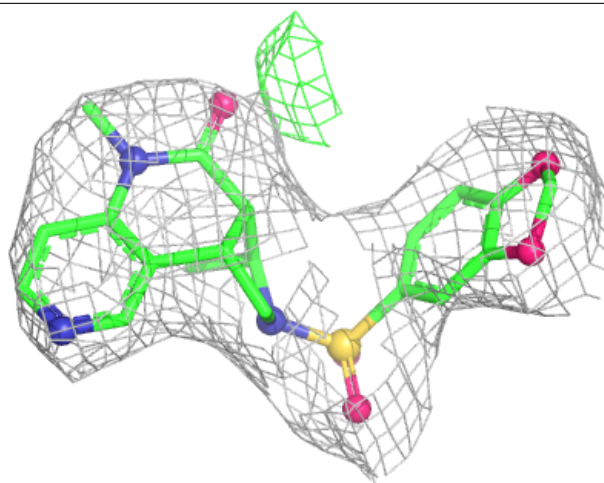
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	C	404	14/15	0.59	0.13	139,146,151,152	0
4	ZN	C	403	1/1	0.71	0.10	133,133,133,133	1
4	ZN	E	403	1/1	0.81	0.10	105,105,105,105	1
4	ZN	A	403	1/1	0.85	0.09	107,107,107,107	1
3	GLY	D	402	5/5	0.86	0.17	83,83,84,85	0
3	GLY	A	402	5/5	0.88	0.19	71,72,73,76	0
3	GLY	B	402	5/5	0.88	0.18	82,83,88,90	0
4	ZN	B	403	1/1	0.89	0.18	117,117,117,117	1
3	GLY	E	402	5/5	0.89	0.16	74,77,77,80	0
3	GLY	C	402	5/5	0.93	0.15	85,85,86,87	0
2	7C6	E	401	28/28	0.94	0.10	78,93,100,100	0
2	7C6	A	401	28/28	0.94	0.11	70,82,88,89	0
2	7C6	D	401	28/28	0.95	0.08	90,93,100,100	0
2	7C6	C	401	28/28	0.96	0.09	74,94,103,104	0
2	7C6	B	401	28/28	0.97	0.07	78,84,89,91	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.

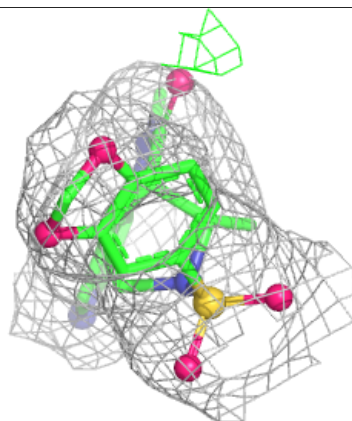
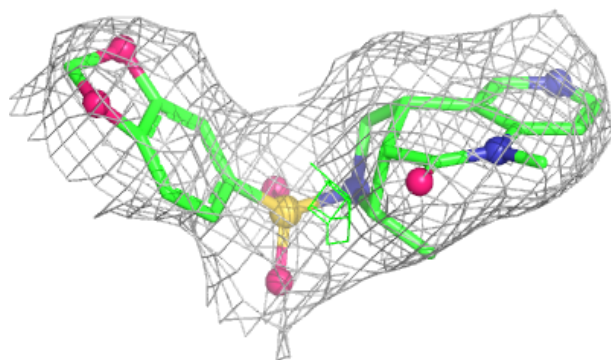
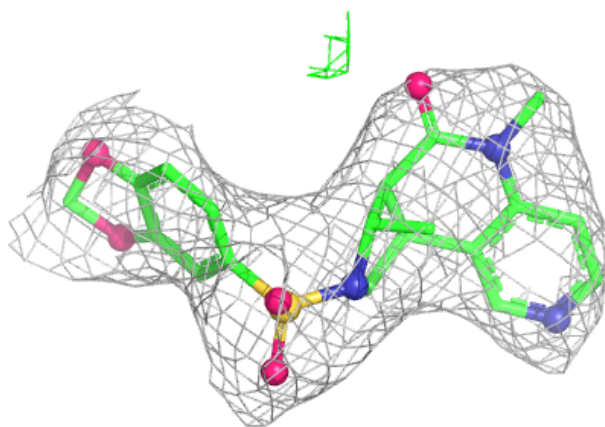
Electron density around 7C6 E 401:

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



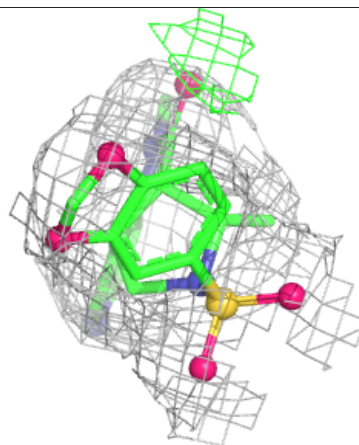
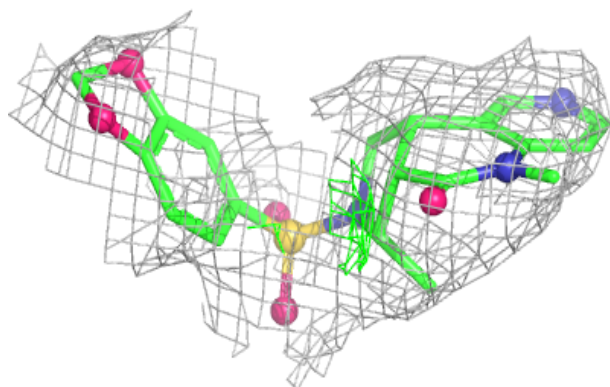
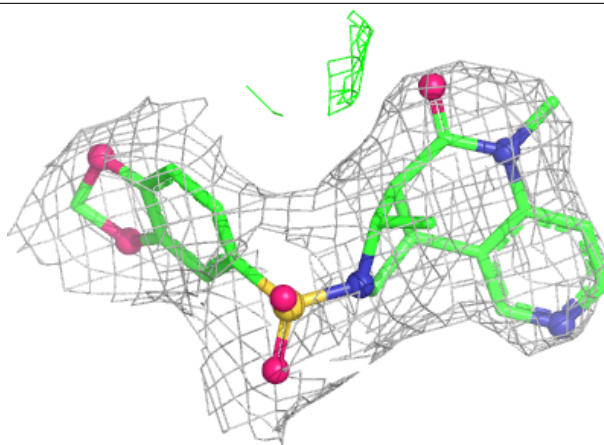
Electron density around 7C6 A 401:

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



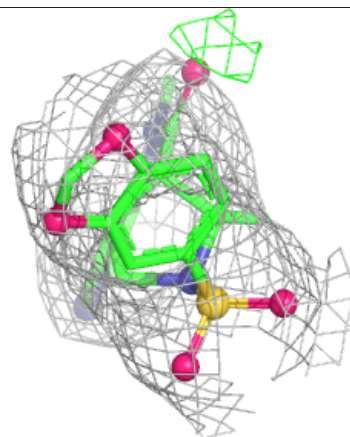
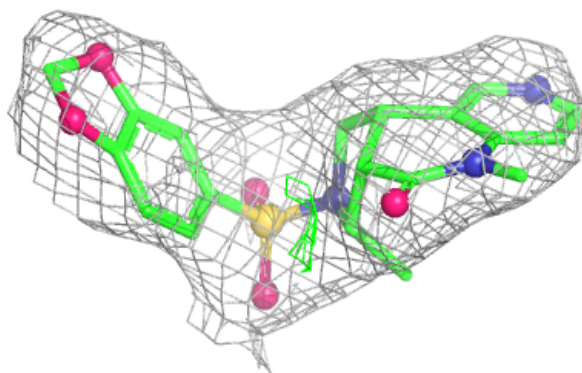
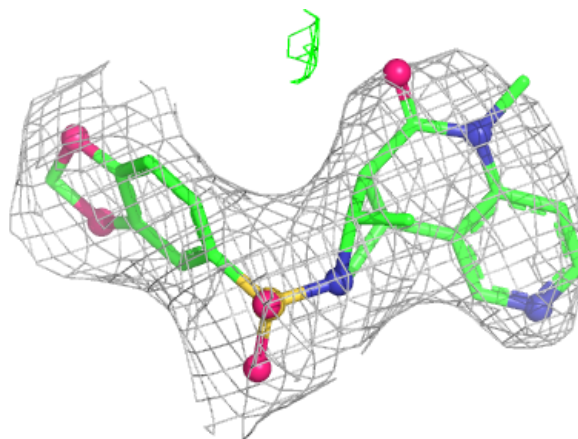
Electron density around 7C6 D 401:

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



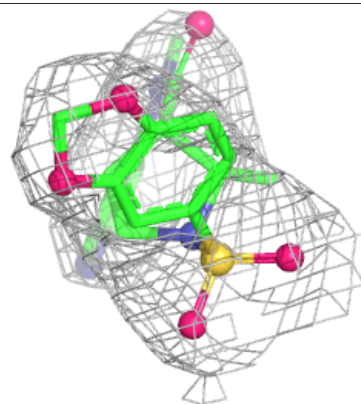
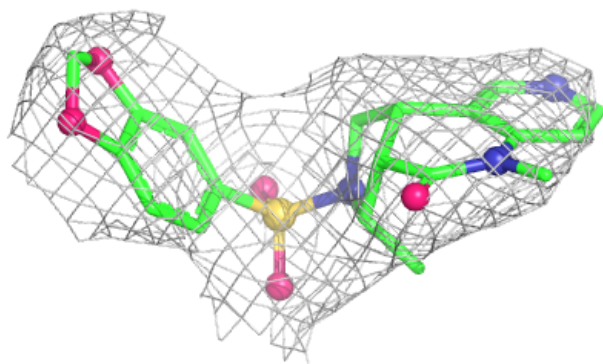
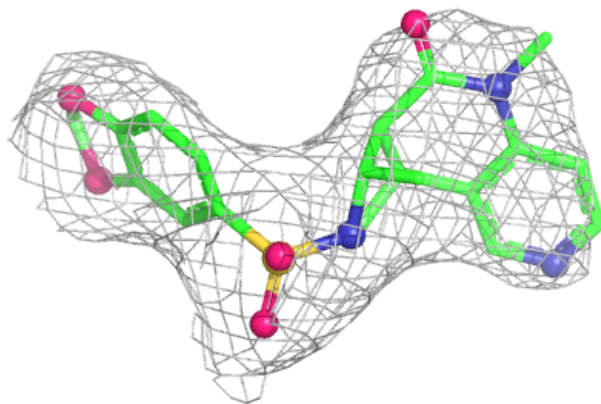
Electron density around 7C6 C 401:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.