



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:12 PM UTC

PDB ID : 5VDI / pdb_00005vdi
Title : Crystal Structure of Human Glycine Receptor alpha-3 Mutant N38Q Bound to AM-3607, Glycine, and Ivermectin
Authors : Shaffer, P.L.; Huang, X.; Chen, H.
Deposited on : 2017-04-03
Resolution : 3.10 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

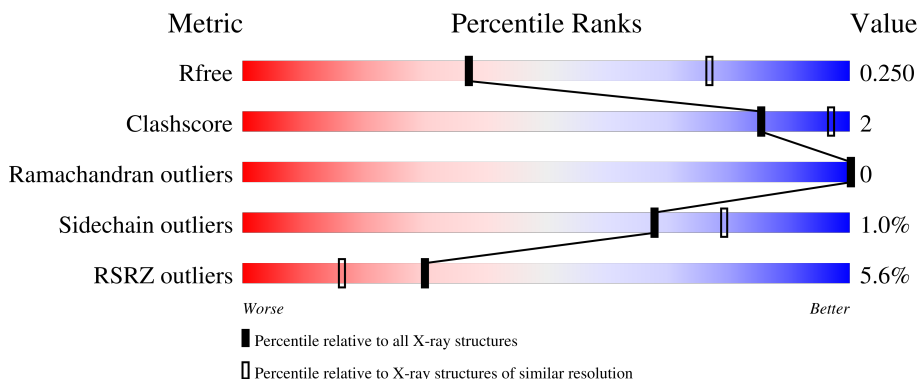
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	7% 87% 7% 7%
1	B	362	6% 88% 7% 5%
1	C	362	4% 88% 6% 7%
1	D	362	4% 87% 7% 6%
1	E	362	6% 88% 5% 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	C	402	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14105 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	A	338	Total	C	N	O	S	0	0	0
			2695	1759	431	485	20			
1	B	343	Total	C	N	O	S	0	0	0
			2714	1772	430	492	20			
1	C	338	Total	C	N	O	S	0	0	0
			2687	1755	425	487	20			
1	D	341	Total	C	N	O	S	0	0	0
			2720	1775	435	490	20			
1	E	338	Total	C	N	O	S	0	0	0
			2693	1758	428	487	20			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLN	ASN	engineered mutation	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
A	360	PHE	-	expression tag	UNP O75311
A	361	GLU	-	expression tag	UNP O75311
A	362	LYS	-	expression tag	UNP O75311
B	38	GLN	ASN	engineered mutation	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

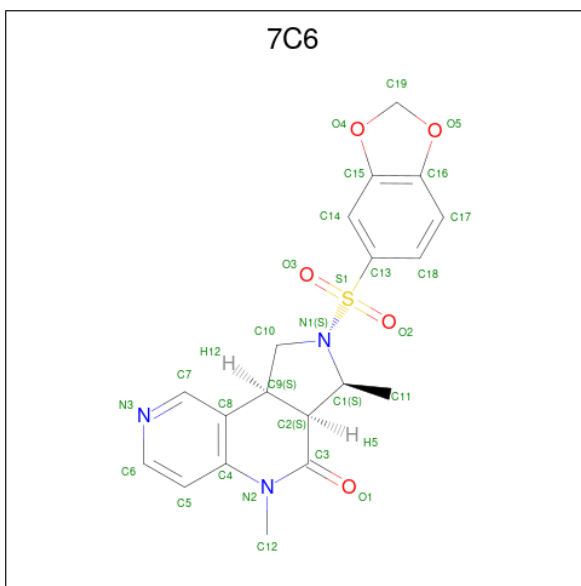
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Chain	Residue	Modelled	Actual	Comment	Reference
B	358	PRO	-	expression tag	UNP O75311
B	359	GLN	-	expression tag	UNP O75311
B	360	PHE	-	expression tag	UNP O75311
B	361	GLU	-	expression tag	UNP O75311
B	362	LYS	-	expression tag	UNP O75311
C	38	GLN	ASN	engineered mutation	UNP O75311
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
D	38	GLN	ASN	engineered mutation	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	38	GLN	ASN	engineered mutation	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

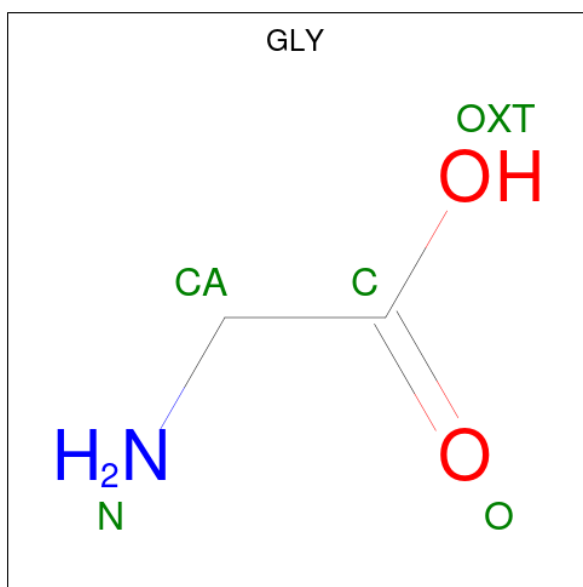
- Molecule 2 is (3S,3aS,9bS)-2-[(2H-1,3-benzodioxol-5-yl)sulfonyl]-3,5-dimethyl-1,2,3,3a,5,9b-h

exahydro-4H-pyrrolo[3,4-c][1,6]naphthyridin-4-one (CCD ID: 7C6) (formula: $C_{19}H_{19}N_3O_5S$).



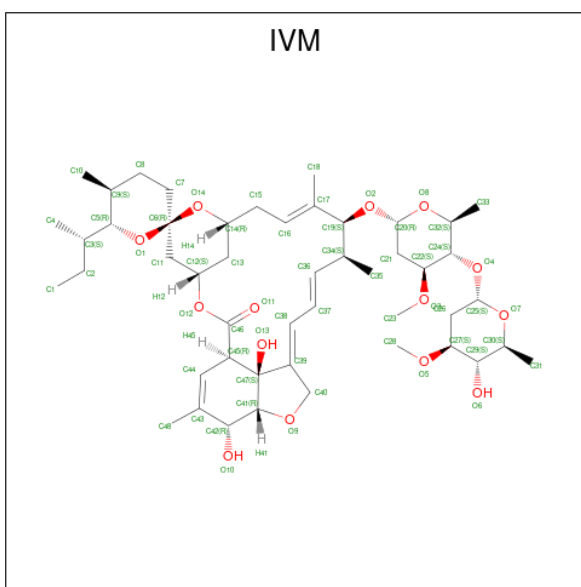
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	B	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	C	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	D	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	E	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	C	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 (2aE,4E,5'S,6S,6'R,7S,8E,11R,13R,15S,17aR,20R,20aR,20bS)-6'-[(2S)-butan-2-yl]-20,20b-dihydroxy-5',6,8,19-tetramethyl-17 -oxo-3',4',5',6,6',10,11,14,15,17,17a,20,20a,20b-tetradecahydro-2H,7H-spiro[11,15-methanofuro[4,3,2-pq][2,6]benzodioxacy cloctadecine-13,2'-pyran]-7-yl 2,6-dideoxy-4-O-(2,6-dideoxy-3-O-methyl-alpha-L-arabino-hexopyranosyl)-3-O-methyl-alpha-L-arabino-hexopyranoside (CCD ID: IVM) (formula: C₄₈H₇₄O₁₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			62	48	14		
4	B	1	Total	C	O	0	0
			62	48	14		
4	C	1	Total	C	O	0	0
			62	48	14		
4	D	1	Total	C	O	0	0
			62	48	14		
4	E	1	Total	C	O	0	0
			62	48	14		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

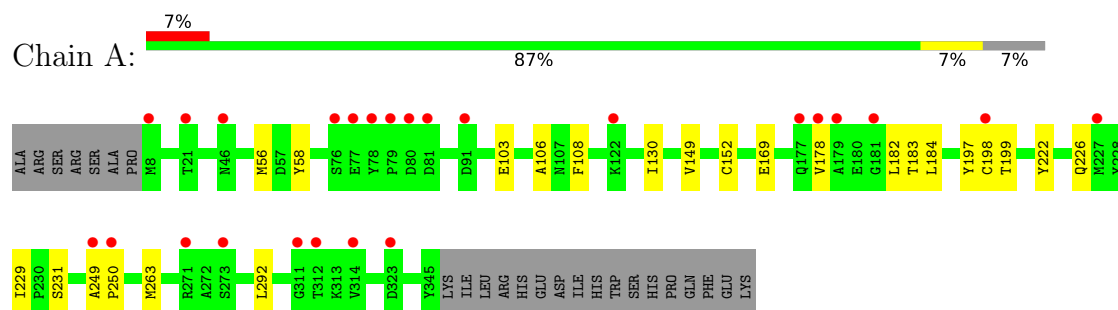
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total 25	O 25	0	0
6	B	23	Total 23	O 23	0	0
6	C	31	Total 31	O 31	0	0
6	D	20	Total 20	O 20	0	0
6	E	17	Total 17	O 17	0	0

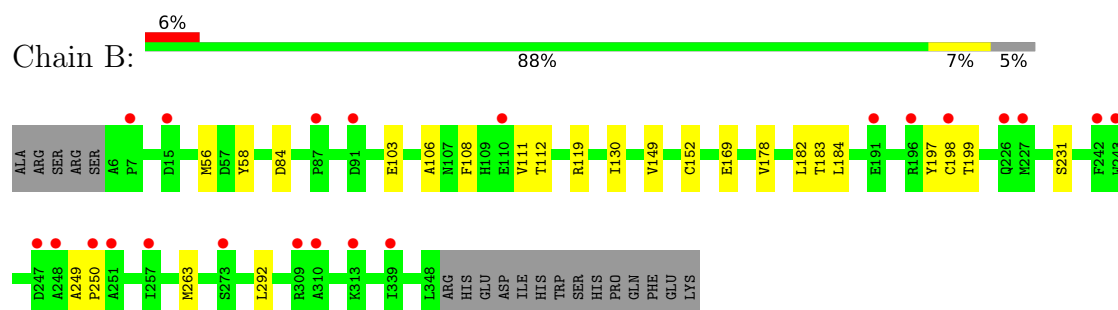
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

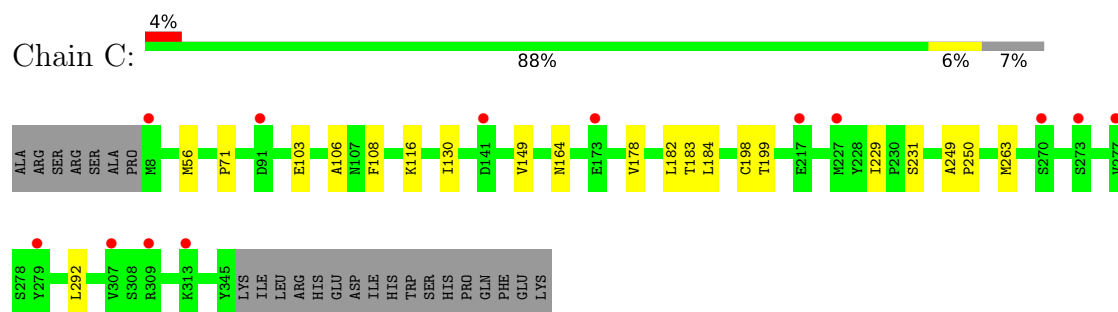
- Molecule 1: Glycine receptor subunit alpha-3



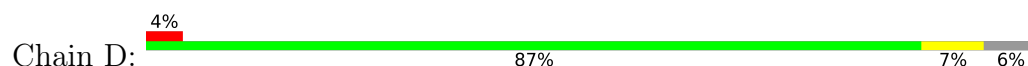
- Molecule 1: Glycine receptor subunit alpha-3

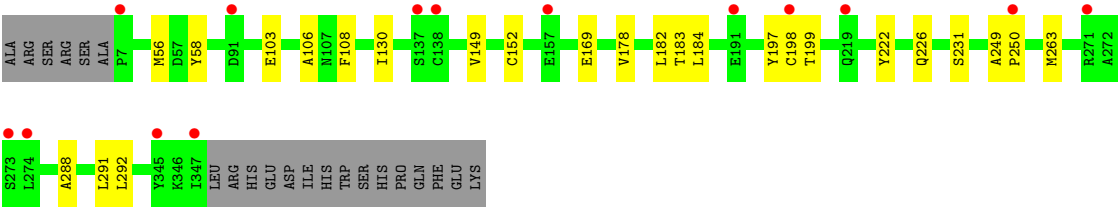


- Molecule 1: Glycine receptor subunit alpha-3

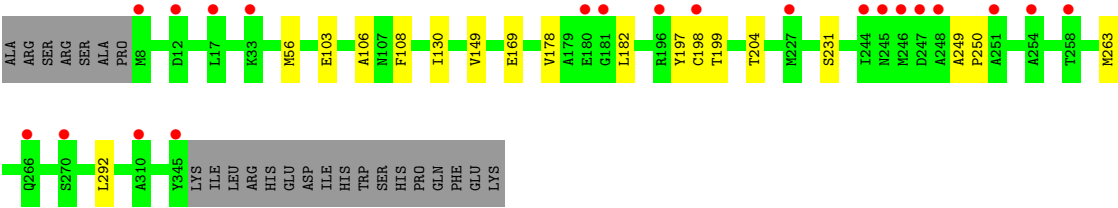
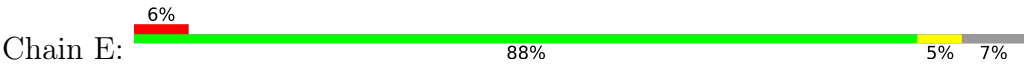


- Molecule 1: Glycine receptor subunit alpha-3





• Molecule 1: Glycine receptor subunit alpha-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.01Å 136.00Å 191.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-3.10) 99.7 (50.00-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.232 , 0.256 0.229 , 0.250	Depositor DCC
R_{free} test set	1225 reflections (1.12%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	1.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14105	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7C6, IVM, 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	0.46	0/2766	0.70	0/3767
1	B	0.48	0/2786	0.70	0/3798
1	C	0.49	0/2758	0.71	0/3758
1	D	0.46	0/2792	0.71	0/3801
1	E	0.46	0/2764	0.70	0/3765
All	All	0.47	0/13866	0.70	0/18889

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

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	2695	0	2645	11	0
1	B	2714	0	2645	11	0
1	C	2687	0	2627	11	0
1	D	2720	0	2672	12	0
1	E	2693	0	2638	8	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	0	0
3	A	5	0	2	0	0
3	B	5	0	2	1	0
3	C	5	0	2	0	0
3	D	5	0	2	1	0
3	E	5	0	2	1	0
4	A	62	0	74	1	0
4	B	62	0	74	2	0
4	C	62	0	74	2	0
4	D	62	0	74	4	0
4	E	62	0	74	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	25	0	0	0	0
6	B	23	0	0	0	0
6	C	31	0	0	3	0
6	D	20	0	0	1	0
6	E	17	0	0	0	0
All	All	14105	0	13607	61	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (61) 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)
4:C:403:IVM:H33	4:C:403:IVM:H25	1.43	1.00
4:C:403:IVM:H25	4:C:403:IVM:C33	2.17	0.75
1:A:229:ILE:HD11	4:E:403:IVM:H23B	1.70	0.73
4:B:403:IVM:H23B	1:C:229:ILE:HD11	1.73	0.69
3:B:402:GLY:N	6:C:603:HOH:O	2.36	0.57
1:E:204:THR:OG1	3:E:402:GLY:OXT	2.16	0.56
3:D:402:GLY:N	6:D:501:HOH:O	2.38	0.56
4:B:403:IVM:H30	4:B:403:IVM:H33	1.87	0.55
1:D:169:GLU:OE2	1:D:197:TYR:OH	2.22	0.53
1:A:222:TYR:CE2	1:A:226:GLN:HG3	2.43	0.52
1:A:169:GLU:OE2	1:A:197:TYR:OH	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:GLU:HG3	1:E:106:ALA:HB2	1.92	0.52
1:C:103:GLU:HG3	1:C:106:ALA:HB2	1.92	0.51
1:B:103:GLU:HG3	1:B:106:ALA:HB2	1.93	0.51
1:D:103:GLU:HG3	1:D:106:ALA:HB2	1.92	0.50
4:A:403:IVM:C33	4:A:403:IVM:H25	2.42	0.50
1:A:103:GLU:HG3	1:A:106:ALA:HB2	1.93	0.49
1:B:84:ASP:OD1	1:B:119:ARG:NE	2.42	0.47
1:D:288:ALA:HB1	4:D:403:IVM:H18B	1.95	0.47
1:C:71:PRO:HG2	6:C:629:HOH:O	2.14	0.47
1:C:198:CYS:O	1:C:199:THR:C	2.58	0.46
1:E:198:CYS:O	1:E:199:THR:C	2.59	0.46
1:A:198:CYS:O	1:A:199:THR:C	2.58	0.46
1:B:169:GLU:OE2	1:B:197:TYR:OH	2.25	0.46
1:B:249:ALA:N	1:B:250:PRO:HD2	2.31	0.46
1:D:178:VAL:HG13	1:D:182:LEU:HD23	1.98	0.45
1:E:178:VAL:HG13	1:E:182:LEU:HD23	1.97	0.45
1:C:178:VAL:HG13	1:C:182:LEU:HD23	1.99	0.45
1:A:249:ALA:N	1:A:250:PRO:HD2	2.31	0.45
1:D:249:ALA:N	1:D:250:PRO:HD2	2.31	0.45
1:E:249:ALA:N	1:E:250:PRO:HD2	2.31	0.45
1:B:198:CYS:O	1:B:199:THR:C	2.60	0.45
1:C:249:ALA:N	1:C:250:PRO:HD2	2.32	0.45
4:D:403:IVM:H25	4:D:403:IVM:H33	1.98	0.45
1:E:169:GLU:OE2	1:E:197:TYR:OH	2.24	0.45
1:C:108:PHE:CD1	1:C:130:ILE:HD11	2.52	0.45
1:B:231:SER:HB2	1:B:263:MET:HE1	1.99	0.45
1:B:178:VAL:HG13	1:B:182:LEU:HD23	1.98	0.44
1:A:178:VAL:HG13	1:A:182:LEU:HD23	1.98	0.44
1:A:231:SER:HB2	1:A:263:MET:HE1	1.99	0.44
4:D:403:IVM:H25	4:D:403:IVM:C33	2.48	0.44
1:E:108:PHE:CD1	1:E:130:ILE:HD11	2.53	0.44
1:D:198:CYS:O	1:D:199:THR:C	2.60	0.44
1:B:108:PHE:CD1	1:B:130:ILE:HD11	2.54	0.43
1:C:231:SER:HB2	1:C:263:MET:HE1	1.99	0.43
1:C:164:ASN:HB3	6:C:625:HOH:O	2.17	0.43
1:D:231:SER:HB2	1:D:263:MET:HE1	1.99	0.43
1:E:231:SER:HB2	1:E:263:MET:HE1	2.01	0.43
1:A:108:PHE:CD1	1:A:130:ILE:HD11	2.54	0.42
1:D:108:PHE:CD1	1:D:130:ILE:HD11	2.55	0.42
1:B:58:TYR:CE1	1:B:152:CYS:HB3	2.56	0.41
1:D:222:TYR:CE1	1:D:226:GLN:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:THR:C	1:A:184:LEU:HD12	2.46	0.41
1:D:291:LEU:HD23	4:D:403:IVM:C46	2.50	0.41
1:B:111:VAL:HA	1:B:112:THR:HA	1.91	0.41
1:C:116:LYS:HE2	1:C:130:ILE:HD12	2.03	0.41
1:C:183:THR:C	1:C:184:LEU:HD12	2.45	0.41
1:D:183:THR:C	1:D:184:LEU:HD12	2.46	0.41
1:B:183:THR:C	1:B:184:LEU:HD12	2.46	0.40
1:A:58:TYR:CE1	1:A:152:CYS:HB3	2.56	0.40
1:D:58:TYR:CE1	1:D:152:CYS:HB3	2.56	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%)	331 (97%)	10 (3%)	0	100	100
1	C	336/362 (93%)	327 (97%)	9 (3%)	0	100	100
1	D	339/362 (94%)	330 (97%)	9 (3%)	0	100	100
1	E	336/362 (93%)	330 (98%)	6 (2%)	0	100	100
All	All	1688/1810 (93%)	1647 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	294/326 (90%)	291 (99%)	3 (1%)	68	79
1	B	294/326 (90%)	291 (99%)	3 (1%)	68	79
1	C	293/326 (90%)	290 (99%)	3 (1%)	68	79
1	D	297/326 (91%)	294 (99%)	3 (1%)	68	79
1	E	294/326 (90%)	291 (99%)	3 (1%)	68	79
All	All	1472/1630 (90%)	1457 (99%)	15 (1%)	68	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	MET
1	A	149	VAL
1	A	292	LEU
1	B	56	MET
1	B	149	VAL
1	B	292	LEU
1	C	56	MET
1	C	149	VAL
1	C	292	LEU
1	D	56	MET
1	D	149	VAL
1	D	292	LEU
1	E	56	MET
1	E	149	VAL
1	E	292	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	219	GLN
1	B	66	GLN
1	B	107	ASN
1	B	219	GLN
1	C	219	GLN
1	D	66	GLN
1	D	144	ASN

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Mol	Chain	Res	Type
1	D	219	GLN
1	D	338	ASN
1	E	201	HIS
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 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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	B	401	-	31,32,32	2.10	4 (12%)	41,50,50	2.13	10 (24%)
3	GLY	A	402	-	4,4,4	1.22	1 (25%)	3,4,4	1.88	1 (33%)
2	7C6	D	401	-	31,32,32	2.01	5 (16%)	41,50,50	2.11	13 (31%)
3	GLY	D	402	-	4,4,4	1.29	1 (25%)	3,4,4	1.55	0
4	IVM	B	403	-	67,68,68	1.85	7 (10%)	87,102,102	1.34	11 (12%)
4	IVM	C	403	-	67,68,68	1.92	12 (17%)	87,102,102	1.65	19 (21%)
2	7C6	E	401	-	31,32,32	1.97	6 (19%)	41,50,50	1.96	9 (21%)
4	IVM	D	403	-	67,68,68	1.91	10 (14%)	87,102,102	1.58	18 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLY	E	402	-	4,4,4	1.33	1 (25%)	3,4,4	1.90	2 (66%)
4	IVM	E	403	-	67,68,68	1.87	8 (11%)	87,102,102	1.30	12 (13%)
2	7C6	A	401	-	31,32,32	1.98	6 (19%)	41,50,50	2.08	11 (26%)
3	GLY	B	402	-	4,4,4	1.23	1 (25%)	3,4,4	1.52	0
3	GLY	C	402	-	4,4,4	1.12	1 (25%)	3,4,4	1.79	2 (66%)
2	7C6	C	401	-	31,32,32	2.25	7 (22%)	41,50,50	1.88	12 (29%)
4	IVM	A	403	-	67,68,68	1.79	7 (10%)	87,102,102	1.58	16 (18%)

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	B	401	-	-	0/12/50/50	0/5/5/5
3	GLY	A	402	-	-	0/2/2/2	-
2	7C6	D	401	-	-	0/12/50/50	0/5/5/5
3	GLY	D	402	-	-	2/2/2/2	-
4	IVM	B	403	-	-	3/45/141/141	1/7/7/7
4	IVM	C	403	-	-	10/45/141/141	0/7/7/7
2	7C6	E	401	-	-	0/12/50/50	0/5/5/5
4	IVM	D	403	-	-	6/45/141/141	0/7/7/7
3	GLY	E	402	-	-	0/2/2/2	-
4	IVM	E	403	-	-	6/45/141/141	0/7/7/7
2	7C6	A	401	-	-	1/12/50/50	0/5/5/5
3	GLY	B	402	-	-	2/2/2/2	-
3	GLY	C	402	-	-	2/2/2/2	-
2	7C6	C	401	-	-	0/12/50/50	0/5/5/5
4	IVM	A	403	-	-	6/45/141/141	0/7/7/7

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	7C6	O3-S1	7.22	1.51	1.43
2	C	401	7C6	O3-S1	7.15	1.51	1.43
2	B	401	7C6	O3-S1	7.02	1.51	1.43
2	B	401	7C6	O2-S1	6.81	1.50	1.43
4	E	403	IVM	C40-C39	-6.70	1.39	1.50
4	C	403	IVM	C40-C39	-6.63	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	7C6	O2-S1	6.45	1.50	1.43
2	A	401	7C6	O3-S1	6.43	1.50	1.43
4	D	403	IVM	C40-C39	-6.40	1.40	1.50
2	C	401	7C6	O2-S1	6.37	1.50	1.43
4	B	403	IVM	C40-C39	-6.20	1.40	1.50
2	D	401	7C6	O2-S1	6.19	1.50	1.43
4	A	403	IVM	C40-C39	-6.17	1.40	1.50
2	E	401	7C6	O3-S1	6.14	1.50	1.43
2	E	401	7C6	O2-S1	6.12	1.50	1.43
4	A	403	IVM	C44-C43	6.11	1.40	1.33
4	E	403	IVM	C44-C43	5.97	1.40	1.33
4	E	403	IVM	C15-C16	-5.92	1.39	1.50
4	D	403	IVM	C15-C16	-5.89	1.39	1.50
4	D	403	IVM	C44-C43	5.86	1.40	1.33
4	A	403	IVM	C15-C16	-5.76	1.39	1.50
4	B	403	IVM	C44-C43	5.71	1.40	1.33
4	C	403	IVM	C15-C16	-5.64	1.39	1.50
4	B	403	IVM	C15-C16	-5.63	1.39	1.50
4	C	403	IVM	C44-C43	5.52	1.39	1.33
4	B	403	IVM	C16-C17	4.93	1.40	1.33
4	E	403	IVM	C16-C17	4.82	1.39	1.33
4	D	403	IVM	C16-C17	4.71	1.39	1.33
4	A	403	IVM	C16-C17	4.48	1.39	1.33
4	C	403	IVM	C16-C17	4.12	1.38	1.33
2	B	401	7C6	C13-S1	-4.10	1.70	1.76
2	C	401	7C6	C13-S1	-4.10	1.70	1.76
4	B	403	IVM	C38-C39	4.04	1.39	1.33
4	D	403	IVM	C38-C39	3.87	1.39	1.33
4	E	403	IVM	C45-C44	3.71	1.55	1.50
4	E	403	IVM	C38-C39	3.71	1.39	1.33
4	C	403	IVM	O9-C40	3.69	1.49	1.43
2	E	401	7C6	S1-N1	3.69	1.68	1.63
4	C	403	IVM	C38-C39	3.68	1.39	1.33
4	A	403	IVM	C38-C39	3.34	1.38	1.33
2	C	401	7C6	C3-N2	3.32	1.42	1.36
4	D	403	IVM	C45-C44	3.18	1.54	1.50
4	A	403	IVM	C45-C44	3.12	1.54	1.50
2	E	401	7C6	C3-N2	3.09	1.42	1.36
2	C	401	7C6	S1-N1	3.05	1.67	1.63
4	C	403	IVM	C45-C44	2.94	1.54	1.50
2	C	401	7C6	C1-N1	-2.93	1.48	1.50
4	D	403	IVM	O5-C27	2.90	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	7C6	C8-C9	2.75	1.56	1.52
2	D	401	7C6	C13-S1	-2.73	1.72	1.76
2	A	401	7C6	S1-N1	2.69	1.67	1.63
4	E	403	IVM	O5-C27	2.69	1.50	1.43
4	E	403	IVM	C26-C27	2.60	1.57	1.52
3	E	402	GLY	OXT-C	-2.58	1.22	1.30
4	B	403	IVM	C45-C44	2.56	1.53	1.50
3	D	402	GLY	OXT-C	-2.48	1.22	1.30
2	B	401	7C6	C2-C3	2.44	1.55	1.51
4	D	403	IVM	C26-C27	2.43	1.56	1.52
2	A	401	7C6	C2-C3	2.42	1.55	1.51
4	D	403	IVM	O9-C40	2.41	1.47	1.43
2	A	401	7C6	C3-N2	2.38	1.40	1.36
4	B	403	IVM	C41-C42	2.37	1.56	1.52
3	B	402	GLY	OXT-C	-2.34	1.23	1.30
3	A	402	GLY	OXT-C	-2.31	1.23	1.30
4	C	403	IVM	O7-C25	2.30	1.48	1.42
2	D	401	7C6	C3-N2	2.29	1.40	1.36
4	D	403	IVM	C42-C43	2.24	1.56	1.50
3	C	402	GLY	OXT-C	-2.17	1.23	1.30
2	C	401	7C6	C2-C3	2.12	1.54	1.51
4	A	403	IVM	C21-C22	2.12	1.56	1.52
2	E	401	7C6	C13-S1	-2.12	1.73	1.76
2	D	401	7C6	S1-N1	2.11	1.66	1.63
4	C	403	IVM	C11-C12	2.10	1.56	1.51
2	E	401	7C6	C8-C9	2.06	1.55	1.52
4	C	403	IVM	C21-C22	2.05	1.55	1.52
4	C	403	IVM	C13-C14	2.04	1.57	1.52
4	C	403	IVM	C24-C32	2.02	1.56	1.52

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	7C6	O3-S1-O2	-6.32	109.73	119.59
2	D	401	7C6	O3-S1-O2	-6.28	109.78	119.59
2	A	401	7C6	O3-S1-O2	-6.13	110.03	119.59
2	B	401	7C6	O1-C3-N2	-5.62	116.87	122.35
2	B	401	7C6	O3-S1-O2	-5.19	111.50	119.59
2	D	401	7C6	C7-C8-C9	-5.13	119.84	125.03
2	C	401	7C6	O3-S1-O2	-5.08	111.66	119.59
4	A	403	IVM	C13-C14-C15	-5.01	107.12	113.05
2	D	401	7C6	C10-N1-S1	-4.83	109.18	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	IVM	O12-C46-C45	4.74	118.11	110.91
4	D	403	IVM	C22-C24-C32	-4.60	104.06	110.56
2	B	401	7C6	C7-C8-C9	-4.49	120.49	125.03
4	D	403	IVM	C34-C19-C17	-4.48	105.02	113.19
4	C	403	IVM	O12-C46-C45	4.40	117.59	110.91
4	B	403	IVM	O12-C46-C45	4.40	117.59	110.91
4	D	403	IVM	O12-C46-C45	4.30	117.44	110.91
2	A	401	7C6	C7-C8-C9	-4.30	120.69	125.03
2	A	401	7C6	C1-N1-S1	-4.23	112.82	120.13
2	E	401	7C6	C7-C8-C9	-4.21	120.78	125.03
2	C	401	7C6	C7-C8-C9	-4.08	120.90	125.03
2	B	401	7C6	C10-N1-S1	-4.07	110.70	118.80
4	A	403	IVM	C37-C38-C39	-3.95	119.63	125.87
4	B	403	IVM	O14-C14-C15	3.91	111.08	106.53
4	C	403	IVM	C13-C14-C15	-3.91	108.42	113.05
4	A	403	IVM	O7-C30-C29	-3.84	102.64	109.55
2	D	401	7C6	C1-N1-S1	-3.84	113.50	120.13
4	C	403	IVM	O14-C14-C13	3.81	115.72	109.02
2	B	401	7C6	C1-N1-S1	-3.79	113.59	120.13
2	E	401	7C6	C13-S1-N1	3.77	113.94	107.36
4	C	403	IVM	C38-C37-C36	-3.72	115.81	124.43
4	E	403	IVM	O12-C46-C45	3.63	116.42	110.91
4	D	403	IVM	O14-C6-C11	-3.60	106.40	110.79
2	C	401	7C6	C13-S1-N1	3.50	113.47	107.36
2	A	401	7C6	O1-C3-N2	-3.42	119.02	122.35
4	B	403	IVM	C37-C38-C39	-3.30	120.65	125.87
2	C	401	7C6	O5-C19-O4	-3.30	102.92	108.09
4	C	403	IVM	C8-C9-C5	3.27	112.88	108.33
4	C	403	IVM	C34-C19-C17	-3.20	107.35	113.19
2	B	401	7C6	C6-N3-C7	3.17	122.41	116.85
2	C	401	7C6	C10-N1-S1	-3.16	112.52	118.80
2	E	401	7C6	O5-C19-O4	-3.15	103.14	108.09
4	C	403	IVM	C47-C45-C46	3.15	112.30	109.05
2	B	401	7C6	O5-C19-O4	-3.15	103.16	108.09
2	A	401	7C6	O4-C15-C14	3.14	132.04	127.86
2	A	401	7C6	C10-N1-S1	-3.11	112.61	118.80
2	C	401	7C6	C6-N3-C7	3.04	122.18	116.85
4	D	403	IVM	C8-C9-C5	3.02	112.53	108.33
4	C	403	IVM	O14-C14-C15	3.01	110.04	106.53
4	C	403	IVM	C26-C27-C29	-2.99	104.17	110.59
4	C	403	IVM	O4-C24-C32	2.96	114.32	106.77
4	A	403	IVM	C34-C19-C17	-2.95	107.82	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	7C6	C6-N3-C7	2.89	121.91	116.85
4	A	403	IVM	O11-C46-C45	-2.88	120.69	125.06
2	A	401	7C6	O5-C19-O4	-2.88	103.57	108.09
4	D	403	IVM	C8-C7-C6	2.87	115.08	111.70
2	E	401	7C6	O4-C15-C14	2.86	131.66	127.86
2	D	401	7C6	C12-N2-C3	2.86	120.40	117.69
4	B	403	IVM	C34-C19-C17	-2.83	108.03	113.19
4	D	403	IVM	C47-C45-C46	2.82	111.96	109.05
4	C	403	IVM	O11-C46-C45	-2.82	120.78	125.06
4	A	403	IVM	C26-C27-C29	-2.82	104.53	110.59
2	E	401	7C6	C1-N1-S1	-2.80	115.30	120.13
4	B	403	IVM	O8-C32-C24	2.77	114.33	109.19
2	B	401	7C6	C8-C7-N3	-2.76	120.01	124.41
4	E	403	IVM	O11-C46-C45	-2.74	120.91	125.06
4	D	403	IVM	C38-C37-C36	-2.70	118.17	124.43
4	A	403	IVM	O14-C14-C15	2.68	109.65	106.53
4	D	403	IVM	C48-C43-C42	2.68	120.93	116.51
4	E	403	IVM	C38-C37-C36	-2.67	118.25	124.43
4	D	403	IVM	C48-C43-C44	-2.64	117.11	123.36
2	B	401	7C6	O4-C15-C14	2.63	131.36	127.86
2	D	401	7C6	C8-C7-N3	-2.62	120.23	124.41
2	C	401	7C6	O4-C15-C14	2.62	131.34	127.86
2	D	401	7C6	O4-C15-C14	2.62	131.34	127.86
2	C	401	7C6	C8-C7-N3	-2.62	120.24	124.41
4	E	403	IVM	C37-C38-C39	-2.62	121.73	125.87
2	A	401	7C6	C13-S1-N1	2.60	111.90	107.36
2	A	401	7C6	C6-N3-C7	2.60	121.41	116.85
4	C	403	IVM	O7-C30-C29	-2.58	104.92	109.55
4	E	403	IVM	C8-C7-C6	2.57	114.74	111.70
2	E	401	7C6	C10-N1-S1	-2.57	113.69	118.80
4	B	403	IVM	C38-C37-C36	-2.55	118.51	124.43
4	B	403	IVM	C34-C36-C37	-2.53	120.89	126.11
4	E	403	IVM	C8-C9-C5	2.52	111.83	108.33
3	E	402	GLY	OXT-C-O	-2.51	116.87	123.33
4	A	403	IVM	C38-C37-C36	-2.50	118.63	124.43
2	C	401	7C6	C11-C1-N1	-2.49	107.57	111.61
3	A	402	GLY	OXT-C-CA	2.49	123.28	113.38
2	D	401	7C6	O1-C3-N2	-2.48	119.93	122.35
4	C	403	IVM	O8-C32-C24	2.47	113.77	109.19
2	C	401	7C6	C1-N1-S1	-2.47	115.86	120.13
2	E	401	7C6	C12-N2-C3	2.44	120.01	117.69
4	B	403	IVM	O11-C46-C45	-2.41	121.40	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	IVM	O8-C20-C21	-2.40	107.13	110.84
4	E	403	IVM	C13-C14-C15	-2.39	110.22	113.05
4	D	403	IVM	O5-C27-C29	2.39	117.47	109.35
4	D	403	IVM	O11-C46-C45	-2.38	121.45	125.06
2	E	401	7C6	C6-N3-C7	2.36	120.99	116.85
4	D	403	IVM	O4-C25-C26	2.36	112.82	108.28
2	A	401	7C6	O5-C16-C17	2.35	132.24	127.72
4	E	403	IVM	O14-C6-C11	-2.32	107.96	110.79
4	D	403	IVM	O2-C19-C17	2.32	115.97	111.69
2	D	401	7C6	C13-S1-N1	2.31	111.40	107.36
4	C	403	IVM	O5-C27-C29	2.30	117.18	109.35
2	B	401	7C6	C10-N1-C1	-2.29	107.75	110.68
4	C	403	IVM	C22-C24-C32	-2.25	107.38	110.56
2	D	401	7C6	C10-N1-C1	-2.25	107.80	110.68
3	C	402	GLY	OXT-C-CA	2.24	122.27	113.38
4	D	403	IVM	O4-C24-C32	2.23	112.46	106.77
4	D	403	IVM	O8-C32-C33	2.20	111.63	106.74
4	A	403	IVM	O5-C27-C29	2.20	116.85	109.35
4	A	403	IVM	C33-C32-C24	2.20	116.67	113.39
4	E	403	IVM	C22-C24-C32	-2.18	107.47	110.56
4	C	403	IVM	C34-C36-C37	-2.18	121.60	126.11
4	C	403	IVM	O14-C6-C11	-2.18	108.13	110.79
4	B	403	IVM	O7-C30-C31	2.17	111.56	106.74
2	C	401	7C6	C12-N2-C3	2.16	119.74	117.69
2	D	401	7C6	O5-C19-O4	-2.13	104.75	108.09
4	E	403	IVM	O7-C30-C31	2.13	111.45	106.74
4	C	403	IVM	C18-C17-C19	2.12	120.14	115.96
3	E	402	GLY	OXT-C-CA	2.12	121.80	113.38
4	E	403	IVM	C6-C11-C12	-2.11	108.02	111.33
2	C	401	7C6	O1-C3-N2	-2.10	120.31	122.35
4	A	403	IVM	C40-O9-C41	-2.08	103.94	107.07
4	B	403	IVM	C33-C32-C24	-2.07	110.31	113.39
3	C	402	GLY	OXT-C-O	-2.07	118.02	123.33
4	A	403	IVM	C34-C36-C37	-2.06	121.86	126.11
4	A	403	IVM	O7-C30-C31	2.05	111.30	106.74
2	D	401	7C6	C4-N2-C3	-2.05	120.31	122.58
4	D	403	IVM	C34-C36-C37	-2.05	121.88	126.11
2	A	401	7C6	C4-N2-C3	-2.04	120.31	122.58
4	E	403	IVM	O12-C12-C11	2.04	112.85	107.64
4	A	403	IVM	O4-C24-C32	2.02	111.92	106.77
4	C	403	IVM	O3-C22-C21	2.02	116.57	110.61
4	D	403	IVM	C37-C38-C39	-2.02	122.68	125.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	IVM	O10-C42-C43	-2.01	107.17	110.60

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	GLY	OXT-C-CA-N
3	C	402	GLY	O-C-CA-N
3	C	402	GLY	OXT-C-CA-N
3	D	402	GLY	O-C-CA-N
3	B	402	GLY	O-C-CA-N
3	D	402	GLY	OXT-C-CA-N
4	C	403	IVM	C21-C22-O3-C23
4	E	403	IVM	C26-C25-O4-C24
4	E	403	IVM	C1-C2-C3-C4
4	D	403	IVM	C21-C22-O3-C23
4	C	403	IVM	C1-C2-C3-C4
4	A	403	IVM	C26-C25-O4-C24
4	A	403	IVM	O7-C25-O4-C24
4	C	403	IVM	O7-C25-O4-C24
4	D	403	IVM	O7-C25-O4-C24
4	E	403	IVM	O7-C25-O4-C24
4	A	403	IVM	C21-C22-O3-C23
4	C	403	IVM	C26-C27-O5-C28
4	B	403	IVM	C1-C2-C3-C4
4	C	403	IVM	C26-C25-O4-C24
4	D	403	IVM	C26-C25-O4-C24
4	C	403	IVM	O8-C20-O2-C19
4	B	403	IVM	C1-C2-C3-C5
4	C	403	IVM	C1-C2-C3-C5
4	E	403	IVM	C1-C2-C3-C5
4	C	403	IVM	C22-C24-O4-C25
4	A	403	IVM	C19-C34-C36-C37
4	C	403	IVM	C32-C24-O4-C25
4	D	403	IVM	C19-C34-C36-C37
4	E	403	IVM	C19-C34-C36-C37
4	D	403	IVM	O11-C46-O12-C12
4	C	403	IVM	C34-C19-O2-C20
4	D	403	IVM	C22-C24-O4-C25
4	A	403	IVM	C32-C24-O4-C25
4	E	403	IVM	C4-C3-C5-C9
4	A	403	IVM	C22-C24-O4-C25

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Mol	Chain	Res	Type	Atoms
2	A	401	7C6	C10-N1-S1-O3
4	B	403	IVM	C26-C27-O5-C28

All (1) ring outliers are listed below:

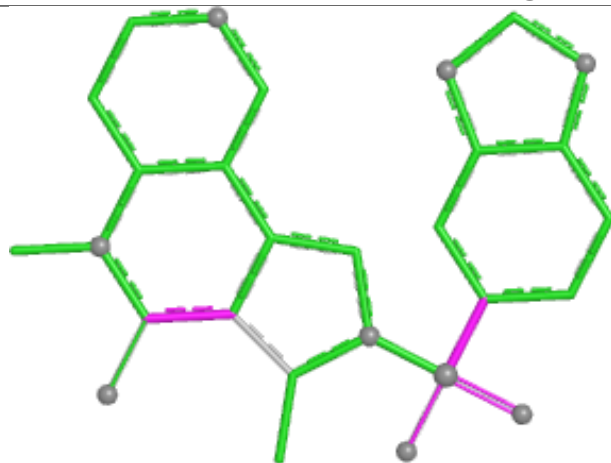
Mol	Chain	Res	Type	Atoms
4	B	403	IVM	C5-C6-C7-C8-C9-O1

8 monomers are involved in 13 short contacts:

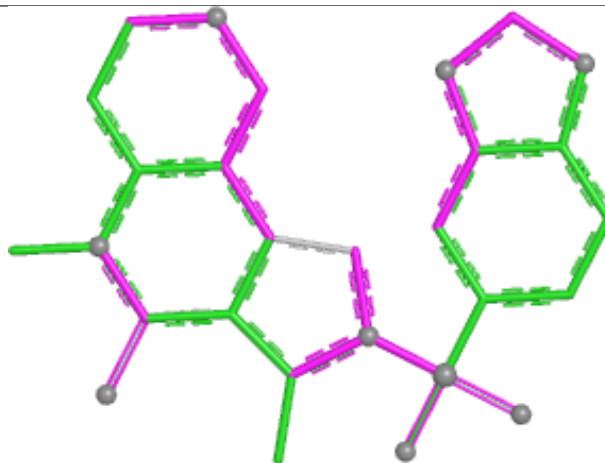
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	GLY	1	0
4	B	403	IVM	2	0
4	C	403	IVM	2	0
4	D	403	IVM	4	0
3	E	402	GLY	1	0
4	E	403	IVM	1	0
3	B	402	GLY	1	0
4	A	403	IVM	1	0

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.

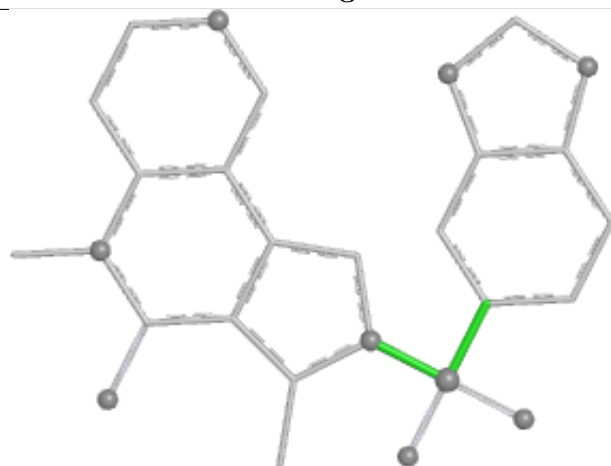
Ligand 7C6 B 401



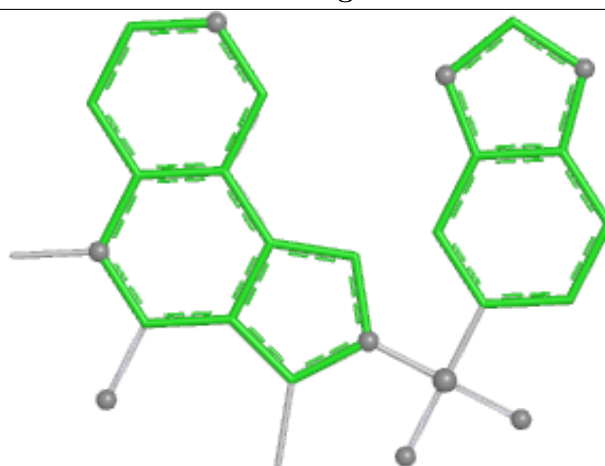
Bond lengths



Bond angles

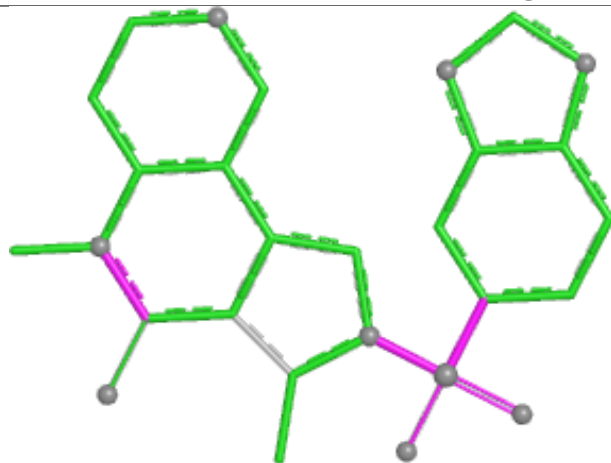


Torsions

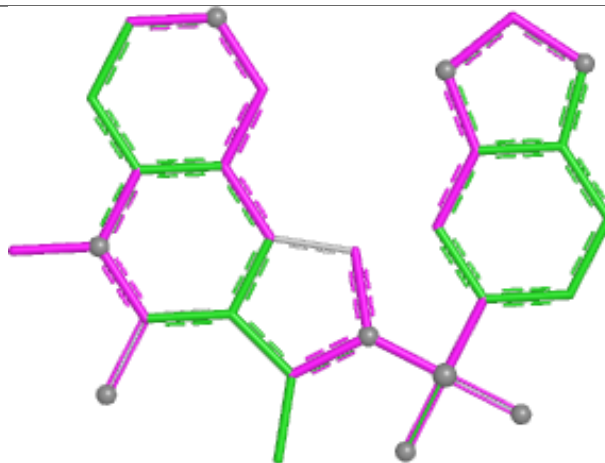


Rings

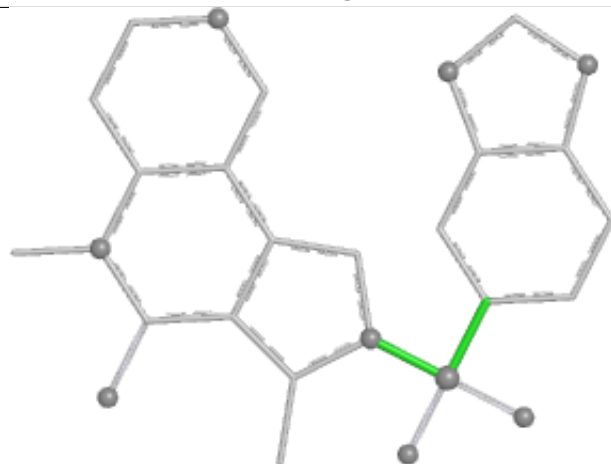
Ligand 7C6 D 401



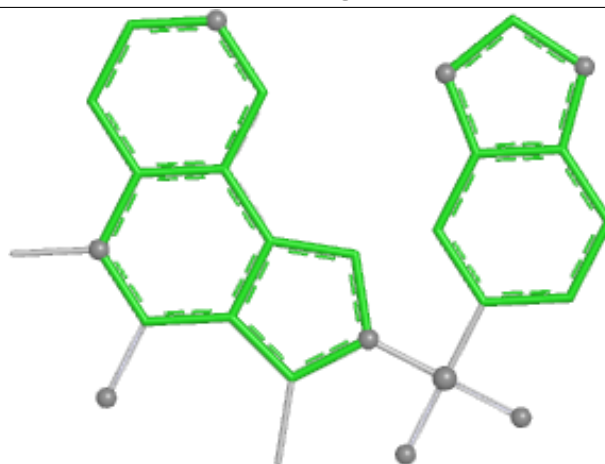
Bond lengths



Bond angles

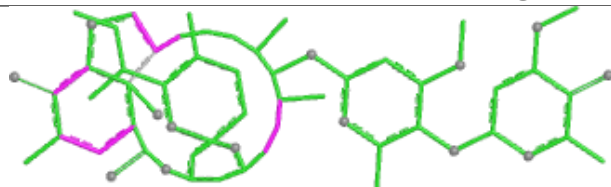


Torsions

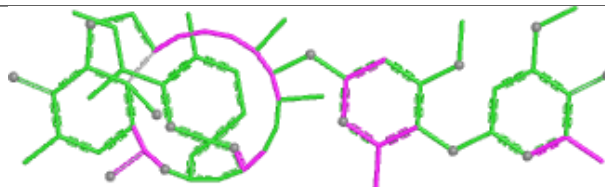


Rings

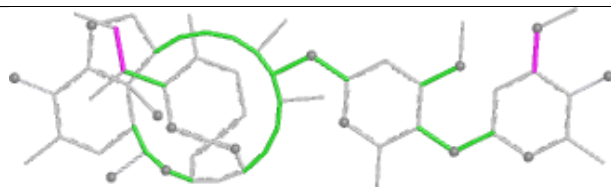
Ligand IVM B 403



Bond lengths



Bond angles

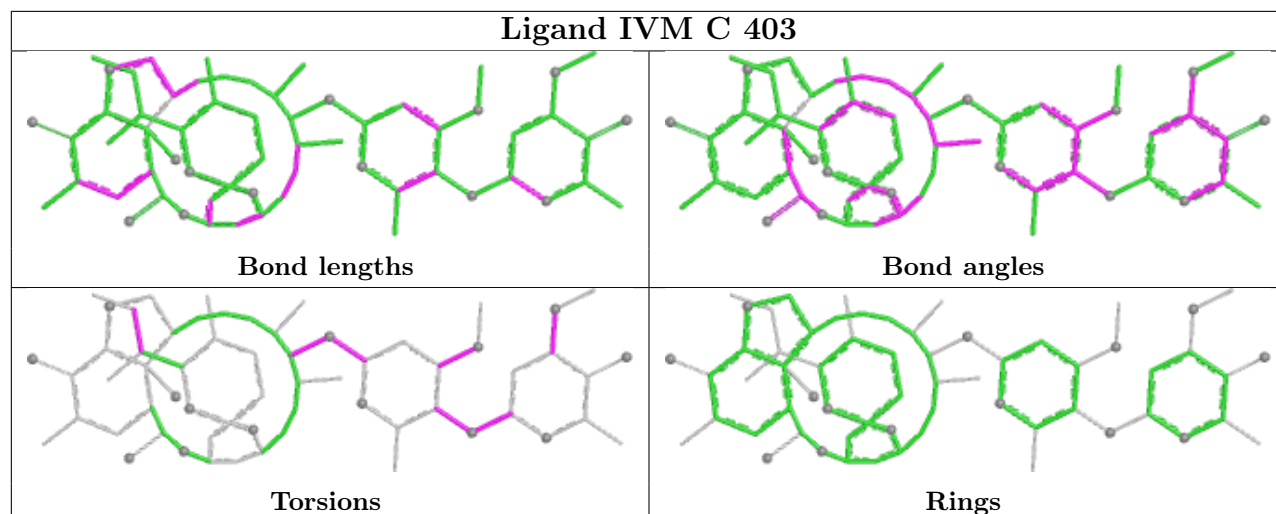


Torsions

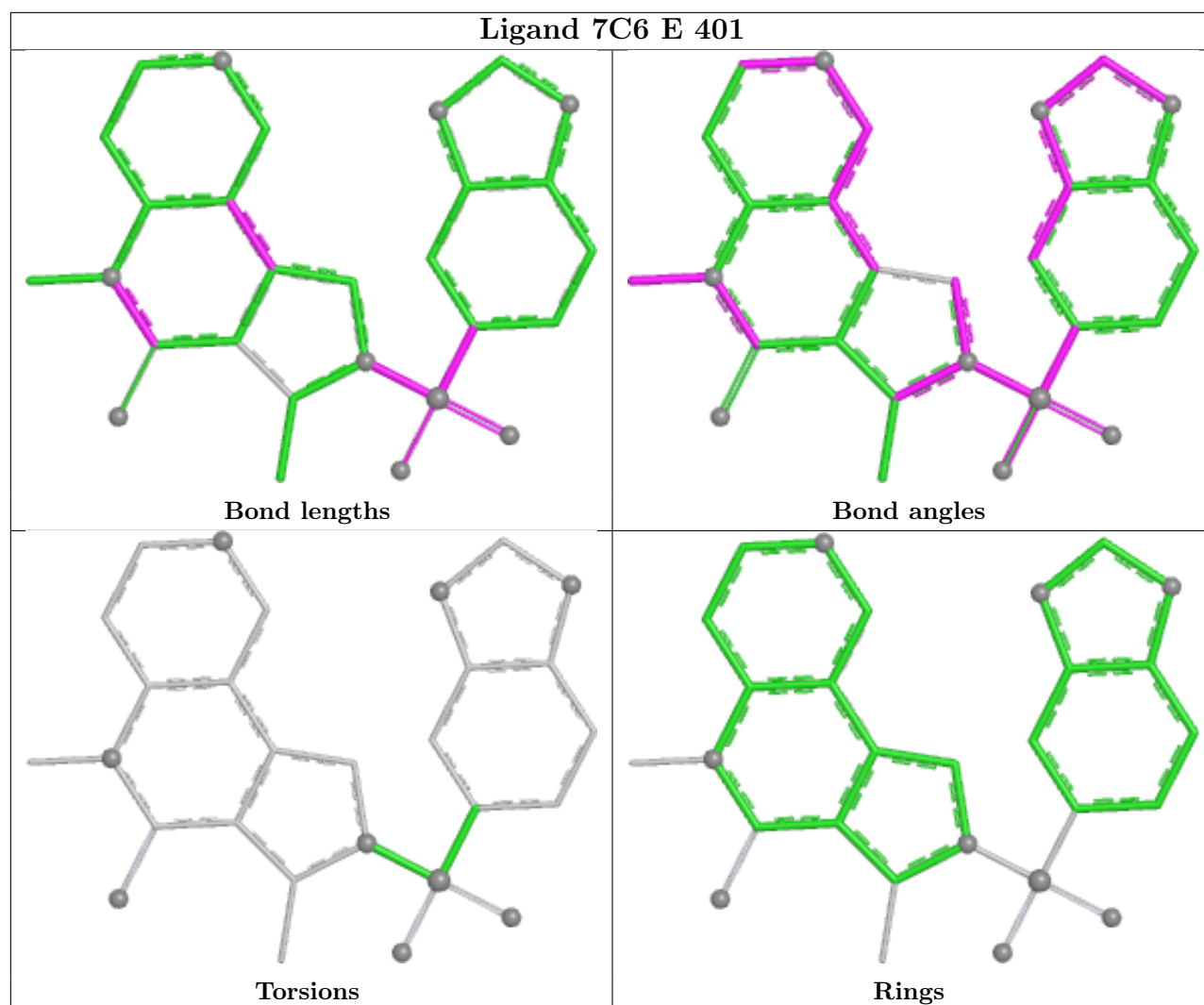


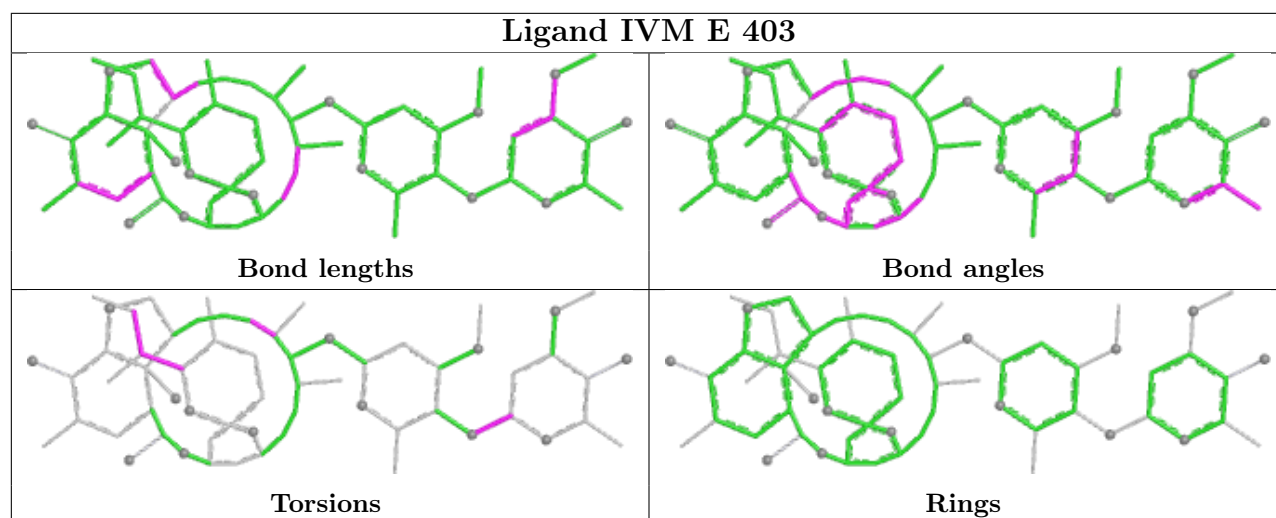
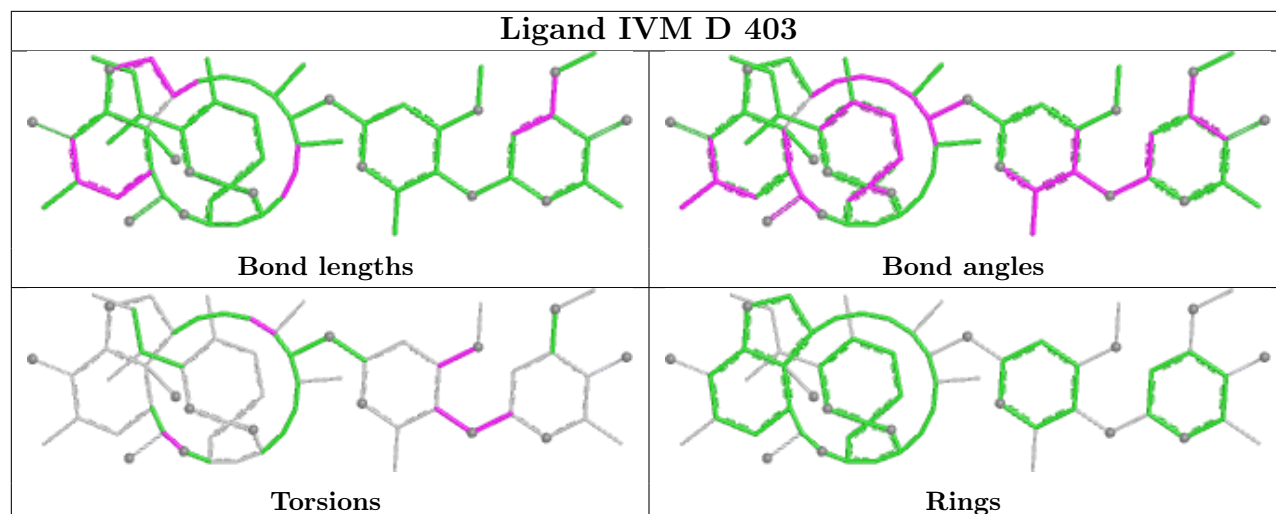
Rings

Ligand IVM C 403

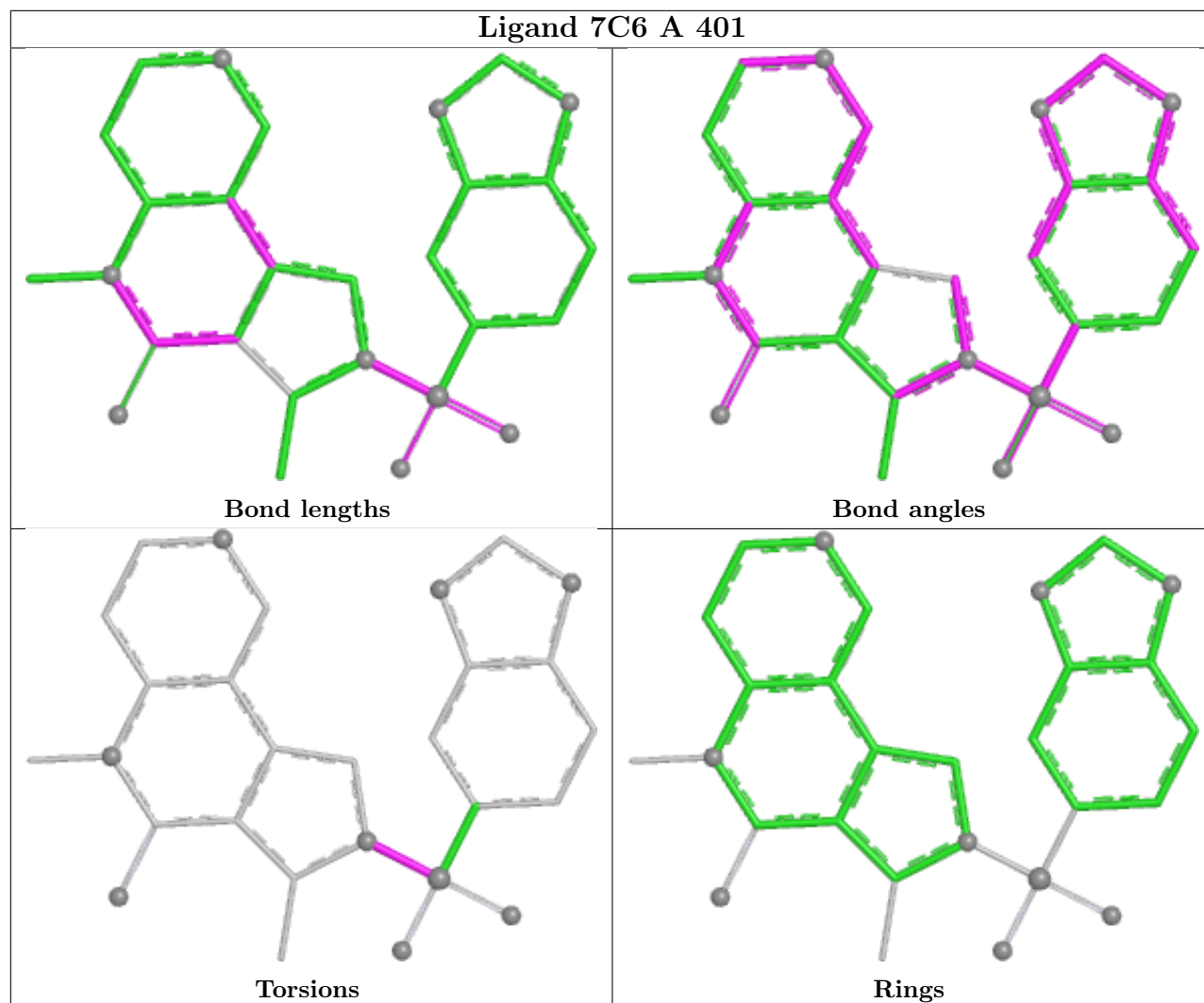


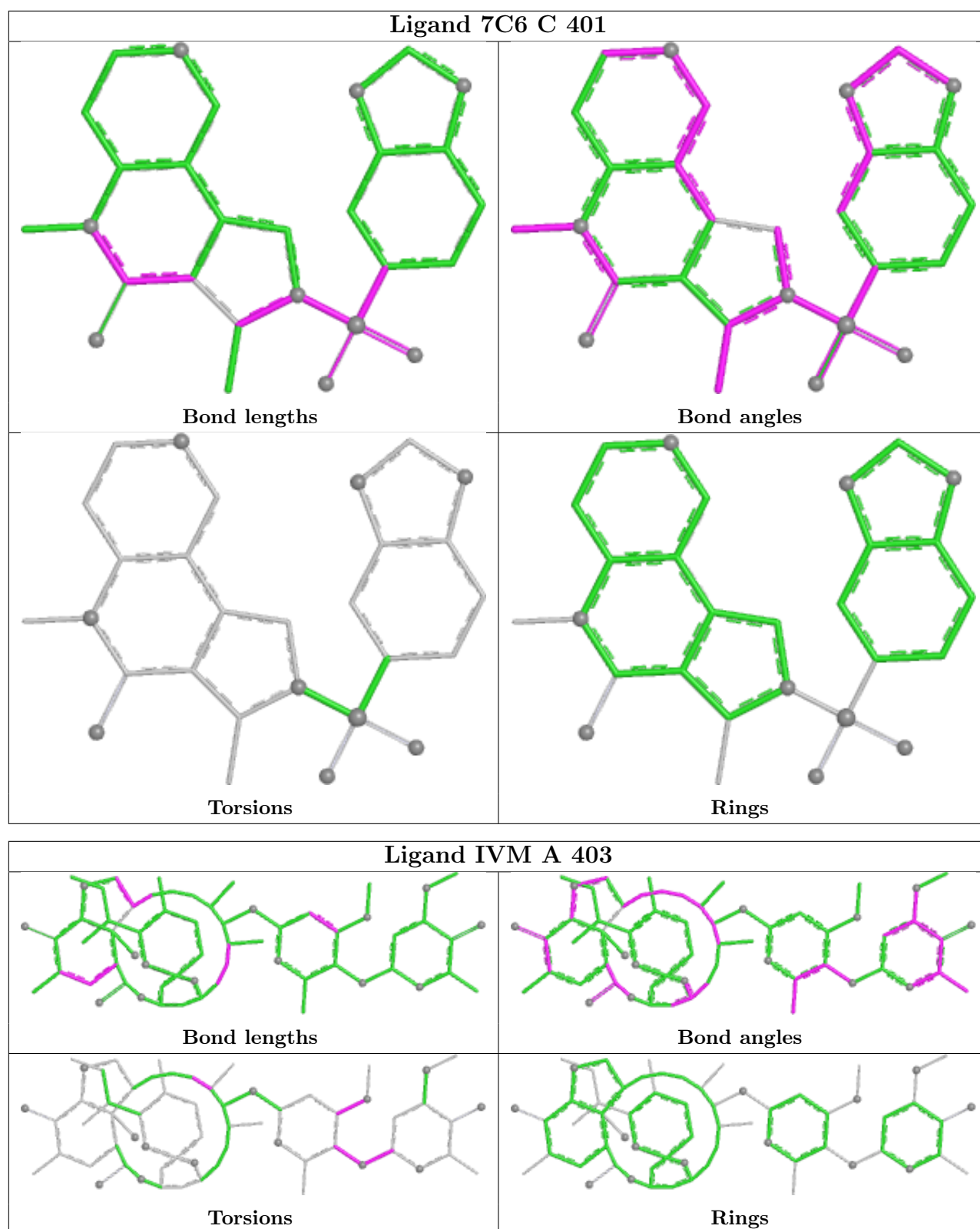
Ligand 7C6 E 401





Ligand 7C6 A 401





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.57	25 (7%)	20 11	40, 63, 90, 108	0
1	B	343/362 (94%)	0.48	22 (6%)	25 14	41, 58, 89, 110	0
1	C	338/362 (93%)	0.43	13 (3%)	44 25	41, 56, 83, 103	0
1	D	341/362 (94%)	0.38	14 (4%)	41 23	44, 63, 77, 101	0
1	E	338/362 (93%)	0.54	21 (6%)	26 14	45, 68, 91, 115	0
All	All	1698/1810 (93%)	0.48	95 (5%)	30 16	40, 63, 88, 115	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	ASP	7.8
1	A	79	PRO	5.8
1	A	76	SER	5.2
1	C	141	ASP	5.2
1	A	80	ASP	4.8
1	D	138	CYS	4.2
1	D	7	PRO	3.7
1	E	254	ALA	3.7
1	E	248	ALA	3.6
1	A	250	PRO	3.6
1	C	273	SER	3.5
1	A	179	ALA	3.5
1	B	91	ASP	3.4
1	C	91	ASP	3.4
1	B	243	TRP	3.2
1	B	310	ALA	3.2
1	A	178	VAL	3.2
1	A	77	GLU	3.1
1	E	258	THR	3.1
1	C	307	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	227	MET	3.1
1	C	8	MET	3.1
1	B	251	ALA	3.0
1	E	33	LYS	3.0
1	E	310	ALA	3.0
1	D	271	ARG	3.0
1	A	122	LYS	2.9
1	A	181	GLY	2.9
1	B	198	CYS	2.9
1	E	8	MET	2.9
1	A	198	CYS	2.8
1	A	227	MET	2.8
1	E	180	GLU	2.8
1	D	157	GLU	2.8
1	B	15	ASP	2.8
1	C	309	ARG	2.7
1	E	246	MET	2.7
1	C	313	LYS	2.7
1	B	191	GLU	2.7
1	C	173	GLU	2.7
1	E	251	ALA	2.6
1	D	91	ASP	2.6
1	A	8	MET	2.6
1	D	345	TYR	2.5
1	A	323	ASP	2.5
1	E	227	MET	2.5
1	A	249	ALA	2.5
1	D	137	SER	2.5
1	B	339	ILE	2.5
1	C	277	VAL	2.5
1	B	273	SER	2.4
1	D	250	PRO	2.4
1	D	191	GLU	2.4
1	B	247	ASP	2.4
1	A	273	SER	2.4
1	E	270	SER	2.4
1	B	87	PRO	2.4
1	A	46	ASN	2.3
1	E	12	ASP	2.3
1	E	266	GLN	2.3
1	D	273	SER	2.3
1	A	311	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	227	MET	2.3
1	D	274	LEU	2.3
1	A	177	GLN	2.3
1	E	245	ASN	2.3
1	D	347	ILE	2.2
1	B	196	ARG	2.2
1	B	7	PRO	2.2
1	A	314	VAL	2.2
1	E	198	CYS	2.2
1	E	247	ASP	2.2
1	B	248	ALA	2.2
1	B	242	PHE	2.2
1	B	226	GLN	2.2
1	E	17	LEU	2.2
1	C	217	GLU	2.2
1	C	279	TYR	2.1
1	E	181	GLY	2.1
1	A	91	ASP	2.1
1	A	21	THR	2.1
1	D	219	GLN	2.1
1	D	198	CYS	2.1
1	B	250	PRO	2.1
1	E	244	ILE	2.1
1	B	257	ILE	2.0
1	E	345	TYR	2.0
1	B	110	GLU	2.0
1	E	196	ARG	2.0
1	C	270	SER	2.0
1	A	78	TYR	2.0
1	A	312	THR	2.0
1	B	313	LYS	2.0
1	A	271	ARG	2.0
1	B	309	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

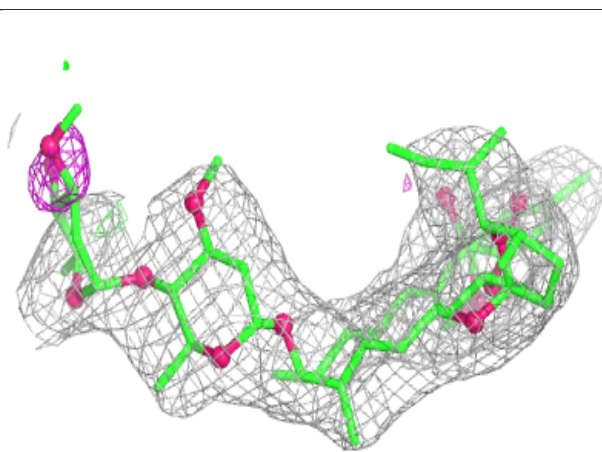
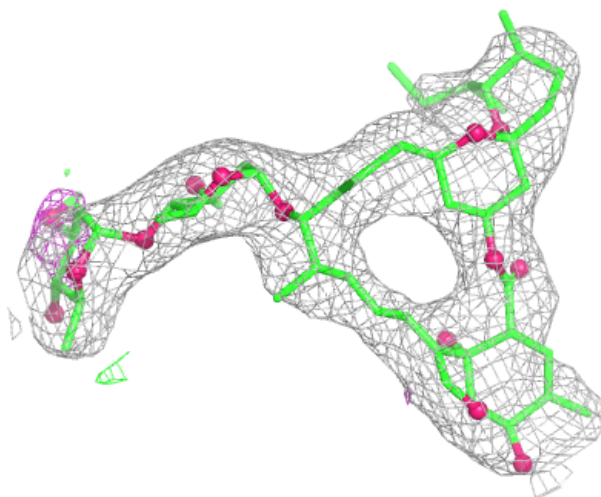
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ZN	D	404	1/1	0.52	0.26	106,106,106,106	1
5	ZN	C	404	1/1	0.72	0.12	79,79,79,79	1
5	ZN	B	404	1/1	0.75	0.14	71,71,71,71	1
5	ZN	E	404	1/1	0.75	0.16	88,88,88,88	1
5	ZN	A	404	1/1	0.81	0.12	66,66,66,66	1
4	IVM	E	403	62/62	0.89	0.16	61,72,102,106	0
4	IVM	D	403	62/62	0.90	0.14	62,68,100,103	0
4	IVM	C	403	62/62	0.91	0.13	59,63,99,104	0
2	7C6	E	401	28/28	0.91	0.14	65,68,70,71	0
4	IVM	A	403	62/62	0.92	0.15	60,67,118,126	0
4	IVM	B	403	62/62	0.92	0.12	57,66,87,88	0
3	GLY	E	402	5/5	0.94	0.12	54,54,54,55	0
3	GLY	A	402	5/5	0.95	0.09	42,42,43,43	0
2	7C6	D	401	28/28	0.95	0.10	65,68,71,72	0
2	7C6	B	401	28/28	0.96	0.09	50,53,56,57	0
2	7C6	C	401	28/28	0.96	0.10	48,49,52,52	0
3	GLY	B	402	5/5	0.96	0.10	44,44,45,45	0
3	GLY	D	402	5/5	0.96	0.16	46,47,47,48	0
2	7C6	A	401	28/28	0.96	0.09	42,46,49,49	0
3	GLY	C	402	5/5	0.97	0.10	52,52,53,53	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.

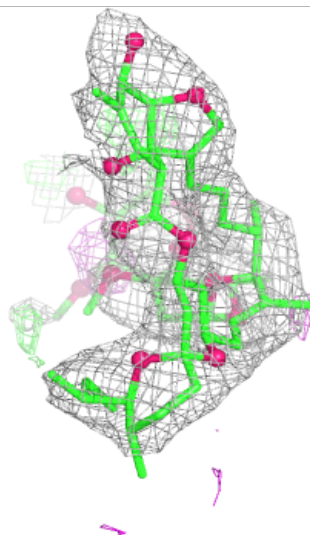
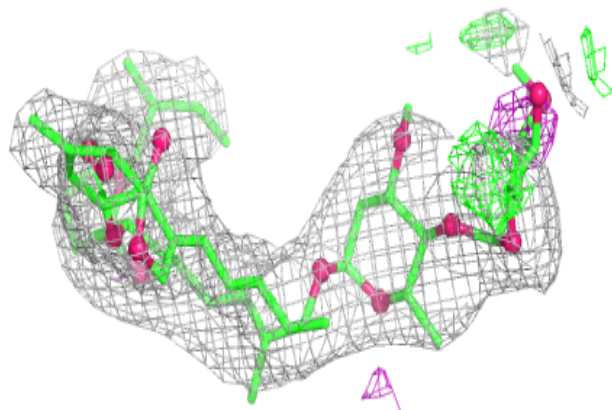
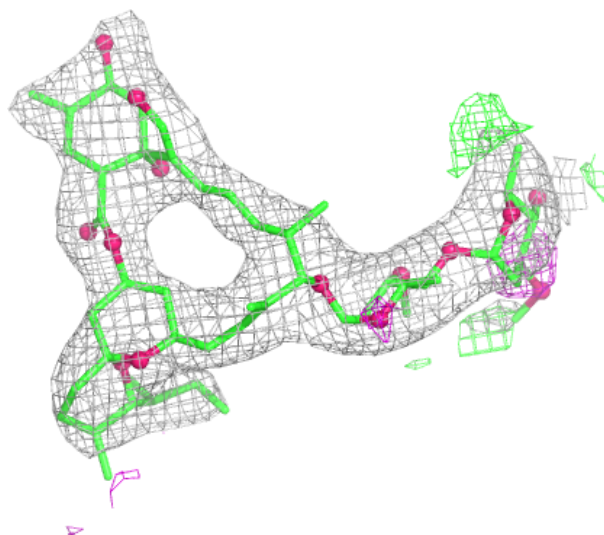
Electron density around IVM E 403:

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



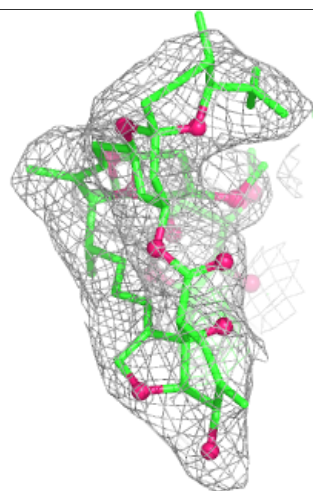
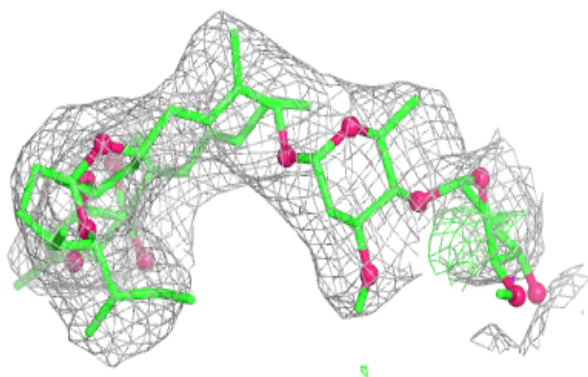
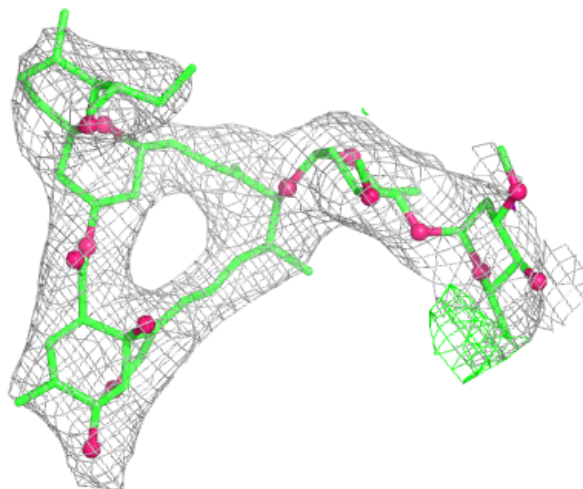
Electron density around IVM D 403:

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



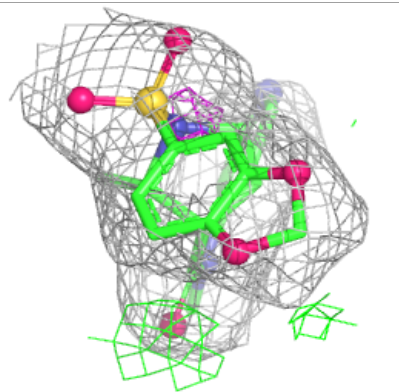
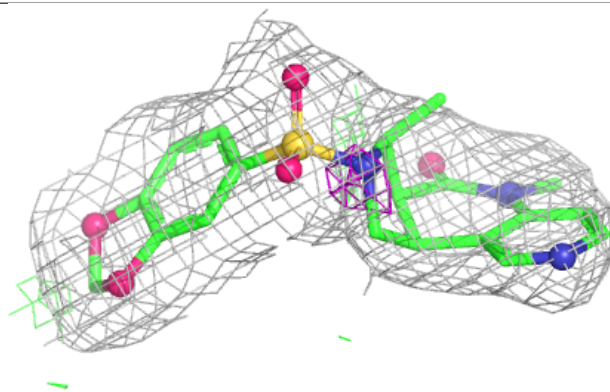
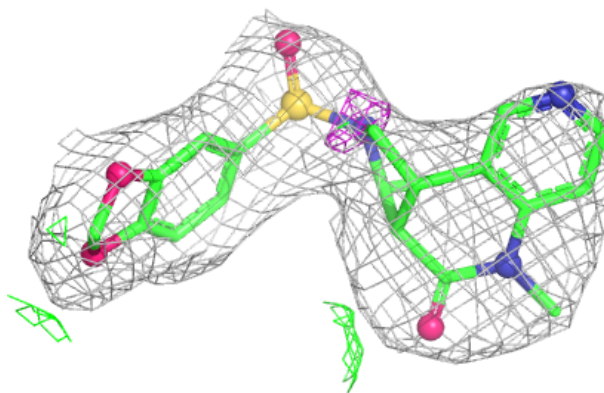
Electron density around IVM C 403:

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



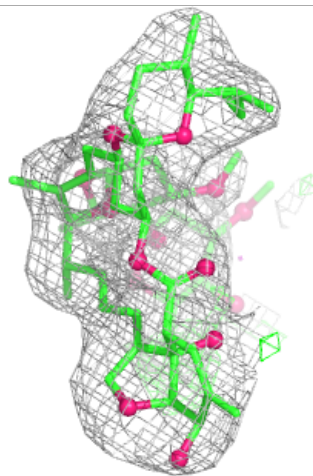
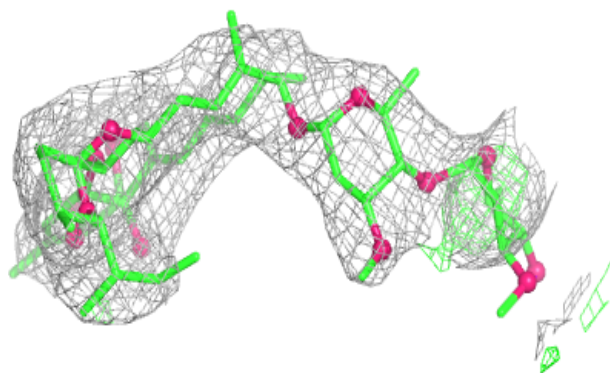
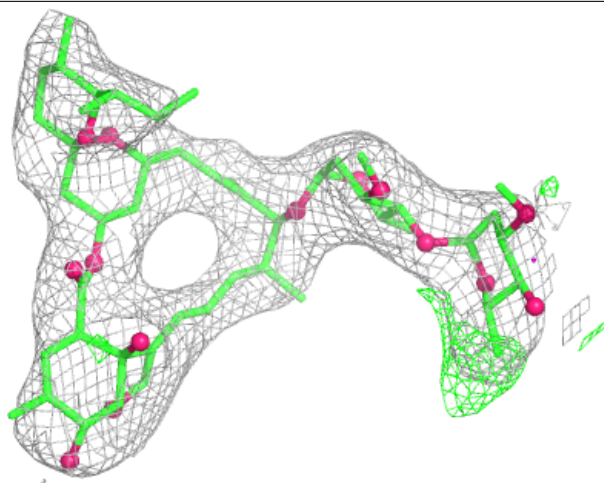
Electron density around 7C6 E 401:

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



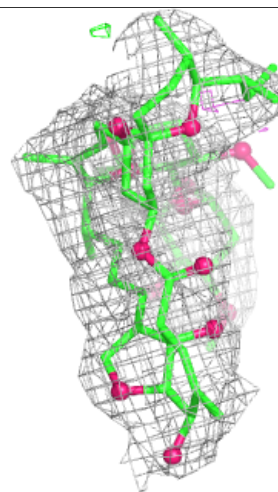
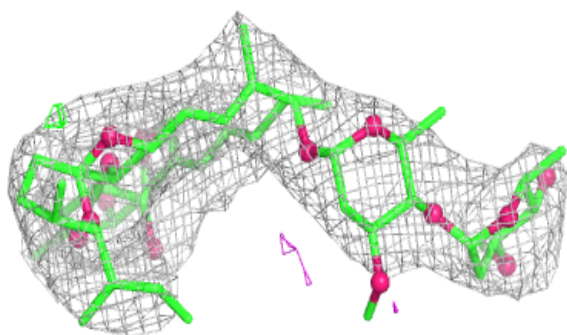
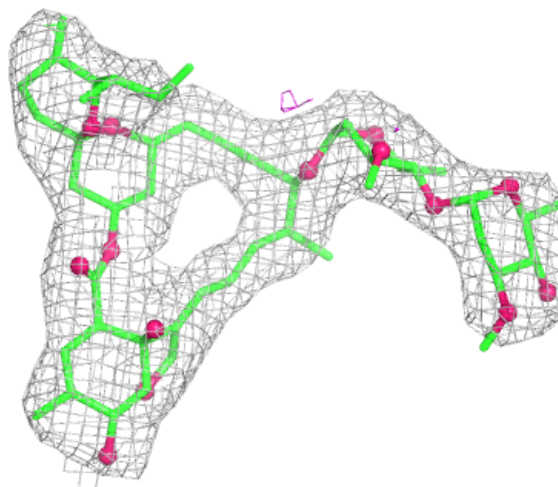
Electron density around IVM A 403:

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



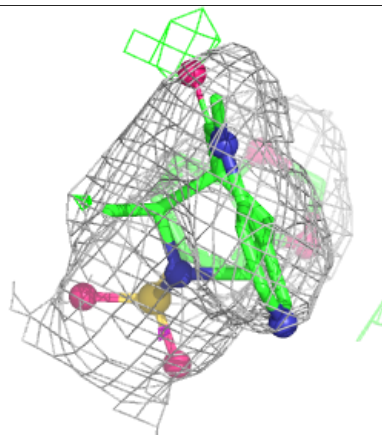
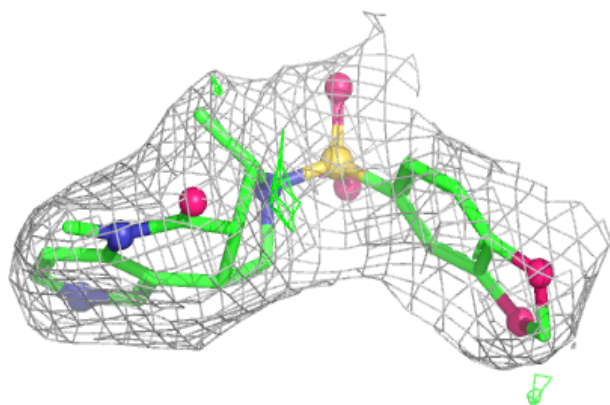
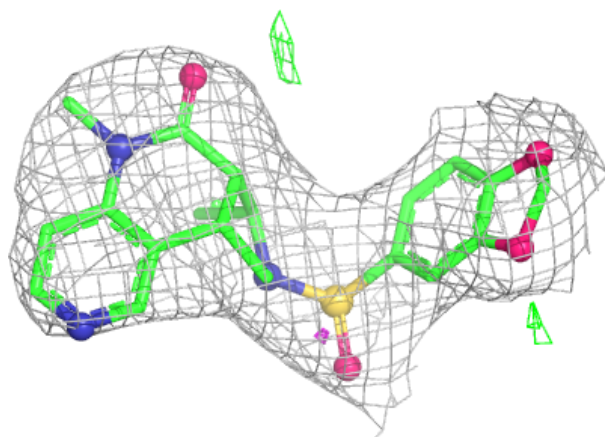
Electron density around IVM B 403:

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



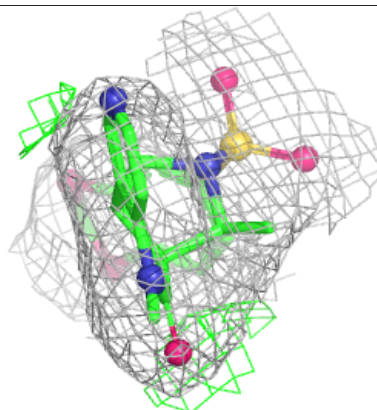
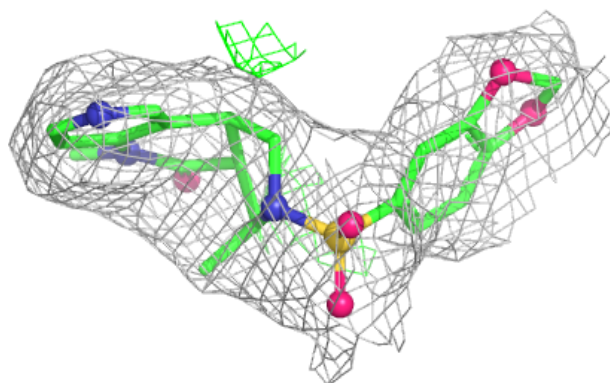
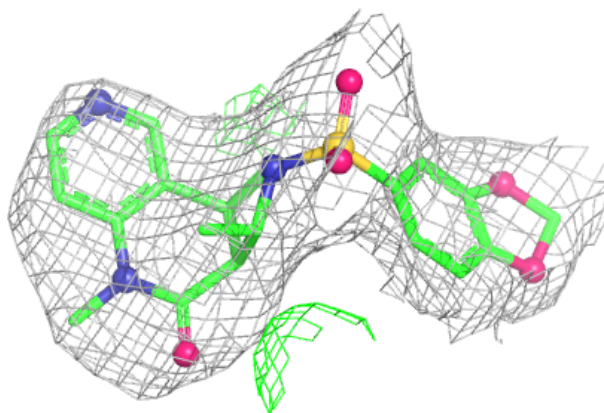
Electron density around 7C6 D 401:

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

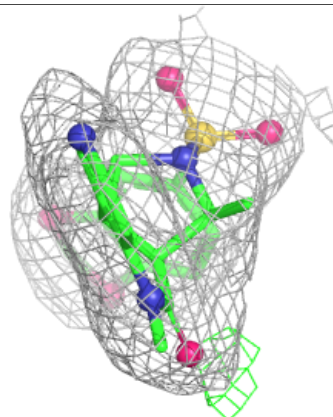
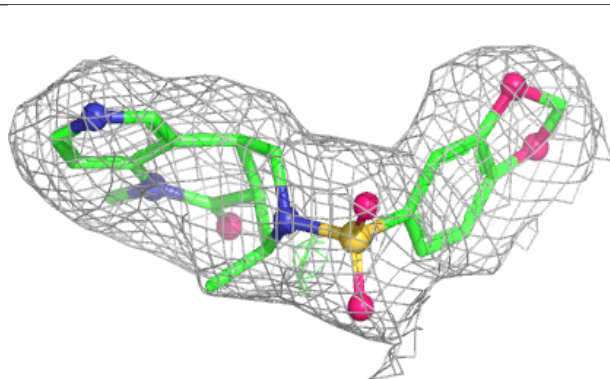
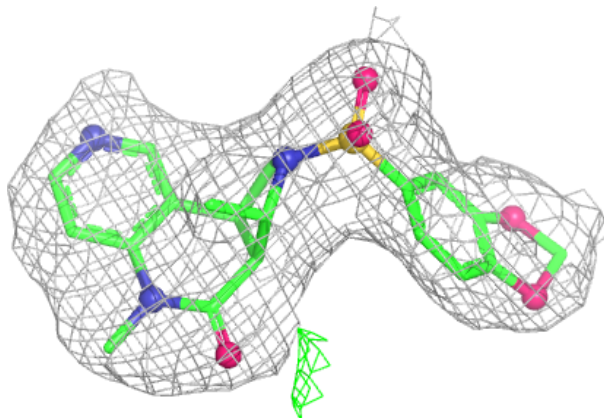


Electron density around 7C6 B 401:

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

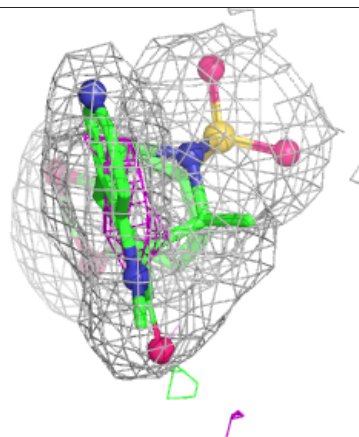
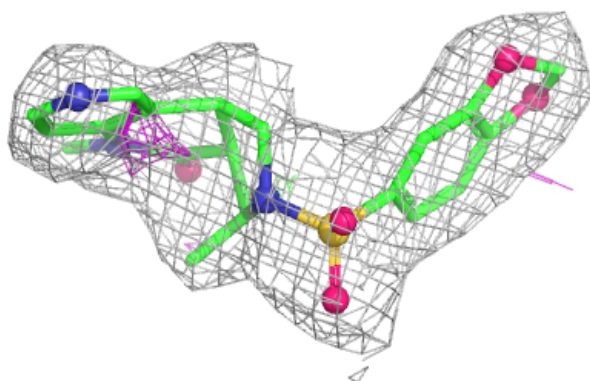
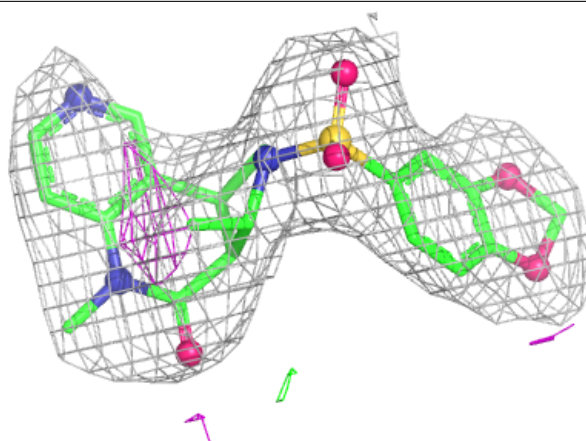
**Electron density around 7C6 C 401:**

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



Electron density around 7C6 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.