



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 07:53 PM BST

PDB ID : 5VDH
Title : Crystal Structure of Human Glycine Receptor alpha-3 Bound to AM-3607, Glycine, and Ivermectin
Authors : Shaffer, P.L.; Huang, X.; Chen, H.
Deposited on : 2017-04-03
Resolution : 2.85 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

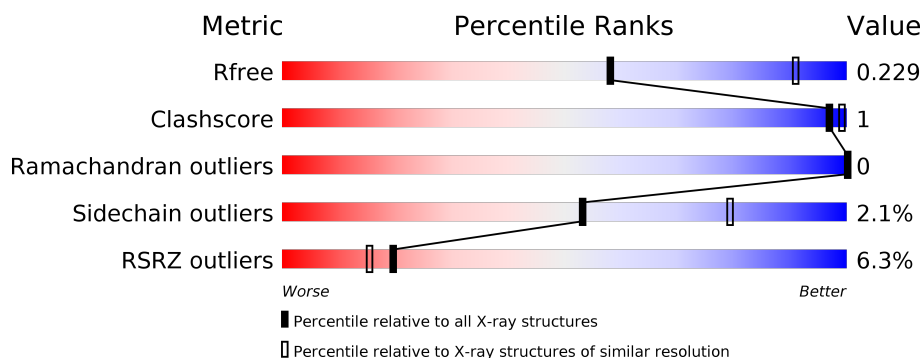
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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>3%</div> <div> <div></div> <div>90%</div> <div>7%</div> </div> </div>
1	B	362	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
1	C	362	<div> <div>11%</div> <div> <div></div> <div>90%</div> <div>7%</div> </div> </div>
1	D	362	<div> <div>7%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	E	362	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>7%</div> </div> </div>

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
5	ZN	D	404	-	-	-	X
6	CL	A	405	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14064 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
			2696	1759	428	489	20			
1	B	343	Total	C	N	O	S	0	0	0
			2713	1771	430	492	20			
1	C	338	Total	C	N	O	S	0	0	0
			2686	1754	425	487	20			
1	D	343	Total	C	N	O	S	0	0	0
			2718	1772	433	494	19			
1	E	338	Total	C	N	O	S	0	0	0
			2700	1762	429	489	20			

There are 55 discrepancies between the modelled and reference sequences:

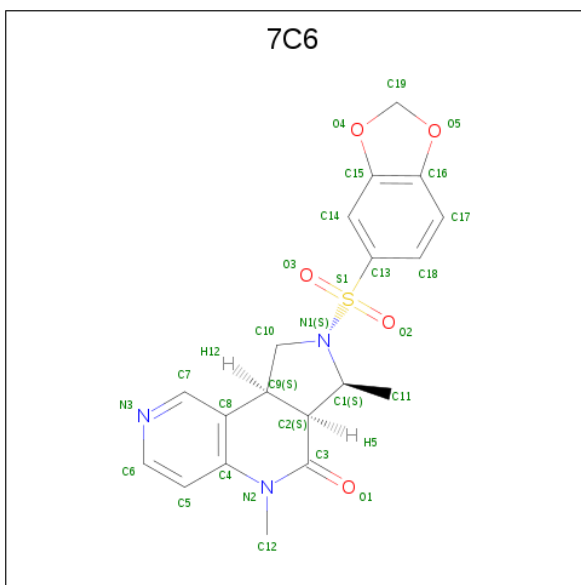
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	ALA	-	linker	UNP O75311
A	311	GLY	-	linker	UNP O75311
A	312	THR	-	linker	UNP O75311
A	355	TRP	-	expression tag	UNP O75311
A	356	SER	-	expression tag	UNP O75311
A	357	HIS	-	expression tag	UNP O75311
A	358	PRO	-	expression tag	UNP O75311
A	359	GLN	-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

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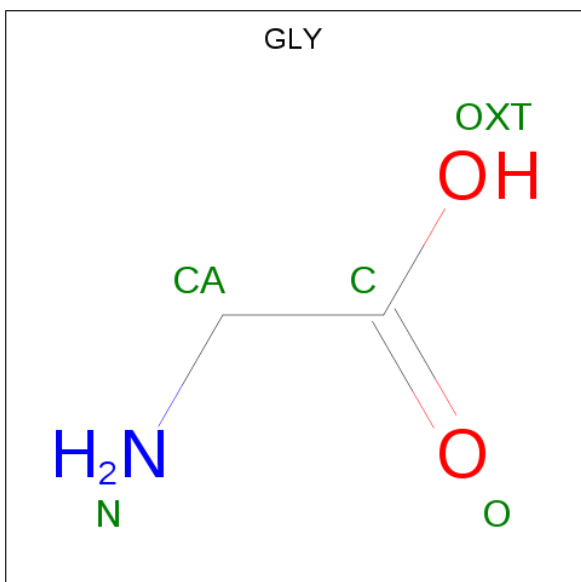
Chain	Residue	Modelled	Actual	Comment	Reference
B	360	PHE	-	expression tag	UNP O75311
B	361	GLU	-	expression tag	UNP O75311
B	362	LYS	-	expression tag	UNP O75311
C	310	ALA	-	linker	UNP O75311
C	311	GLY	-	linker	UNP O75311
C	312	THR	-	linker	UNP O75311
C	355	TRP	-	expression tag	UNP O75311
C	356	SER	-	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	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).



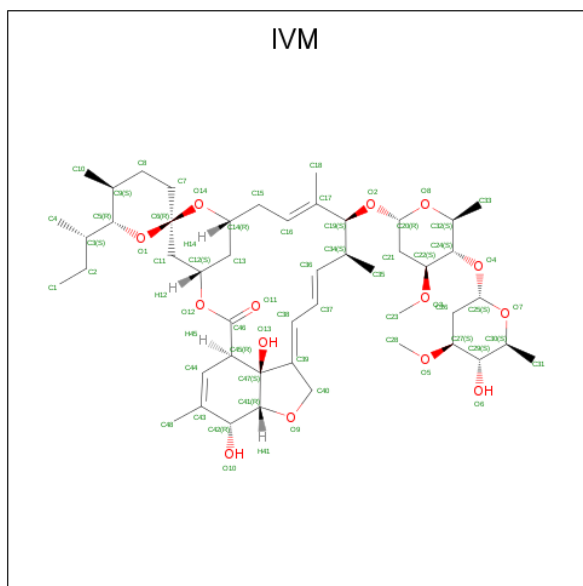
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	B	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	C	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	D	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	E	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

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



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 (three-letter code: 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		

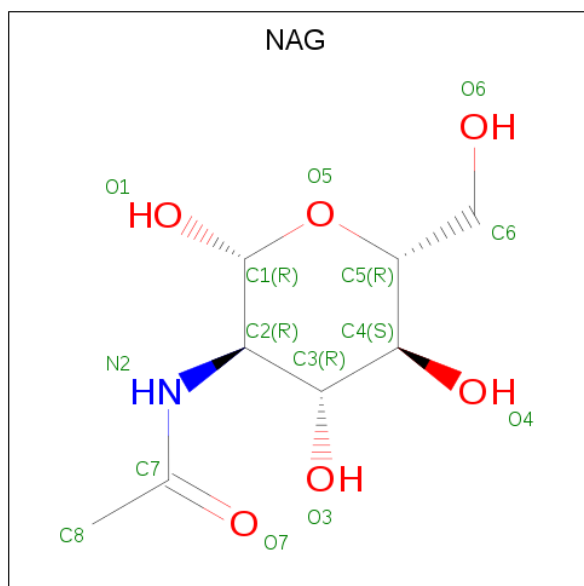
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	18	Total 18	O 18	0	0
8	B	11	Total 11	O 11	0	0
8	C	10	Total 10	O 10	0	0
8	D	8	Total 8	O 8	0	0
8	E	9	Total 9	O 9	0	0

Chain E:

Position	Residue	Information Content (bits)
1	ALA	0.95
2	ARG	0.95
3	ARG	0.95
4	ARG	0.95
5	SER	0.95
6	ALA	0.95
7	ALA	0.95
8	PRO	0.95
9	PRO	0.95
10	PRO	0.95
11	D12	0.95
12	T21	0.95
13	F32	0.95
14	S47	0.95
15	R65	0.95
16	L73	0.95
17	D80	0.95
18	E103	0.95
19	A106	0.95
20	N115	0.95
21	E169	0.95
22	Q170	0.95
23	Q171	0.95
24	P175	0.95
25	T183	0.95
26	L188	0.95
27	L189	0.95
28	E192	0.95
29	L195	0.95
30	R196	0.95
31	R213	0.95
32	F214	0.95
33	E217	0.95
34	L233	0.95
35	T258	0.95
36	L261	0.95
37	T262	0.95
38	M263	0.95
39	T264	0.95
40	T265	0.95

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.06 Å 119.06 Å 429.93 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 49.62 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.85) 99.8 (49.62-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.86 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.226 , 0.236 0.223 , 0.229	Depositor DCC
R_{free} test set	3666 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14064	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: IVM, ZN, CL, 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	0.28	0/2767	0.48	0/3769
1	B	0.28	0/2785	0.47	0/3797
1	C	0.28	0/2757	0.50	2/3757 (0.1%)
1	D	0.27	0/2790	0.47	0/3803
1	E	0.28	0/2771	0.47	0/3773
All	All	0.28	0/13870	0.48	2/18899 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	C	59	ARG	NE-CZ-NH2	-5.60	117.50	120.30

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	2696	0	2640	4	0
1	B	2713	0	2643	4	0
1	C	2686	0	2624	5	0
1	D	2718	0	2653	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2700	0	2651	6	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
2	C	28	0	0	0	0
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	0	0
3	E	5	0	2	0	0
4	A	62	0	74	3	0
4	B	62	0	74	3	0
4	C	62	0	74	2	0
4	D	62	0	74	2	0
4	E	62	0	74	0	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	1	0	0	0	0
7	C	14	0	13	0	0
8	A	18	0	0	0	0
8	B	11	0	0	0	0
8	C	10	0	0	1	0
8	D	8	0	0	0	0
8	E	9	0	0	0	0
All	All	14064	0	13604	25	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 (25) 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)
3:B:402:GLY:N	8:C:501:HOH:O	2.37	0.56
4:B:403:IVM:H33	4:B:403:IVM:H30	1.90	0.54
4:D:403:IVM:H8	1:E:233:LEU:HD13	1.93	0.51
4:B:403:IVM:H8	1:C:233:LEU:HD13	1.93	0.50
1:A:103:GLU:HG3	1:A:106:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:GLU:HG3	1:C:106:ALA:HB2	1.95	0.48
1:B:103:GLU:HG3	1:B:106:ALA:HB2	1.96	0.47
4:B:403:IVM:H8	1:C:233:LEU:CD1	2.44	0.47
1:E:103:GLU:HG3	1:E:106:ALA:HB2	1.95	0.47
1:D:103:GLU:HG3	1:D:106:ALA:HB2	1.95	0.47
4:A:403:IVM:H8	1:B:233:LEU:HD13	1.96	0.46
4:C:403:IVM:H8	1:D:233:LEU:HD13	1.97	0.46
1:E:196:ARG:HD2	1:E:213:ARG:HE	1.83	0.44
1:D:196:ARG:HD2	1:D:213:ARG:HE	1.83	0.44
4:D:403:IVM:H8	1:E:233:LEU:CD1	2.49	0.43
1:A:196:ARG:HD2	1:A:213:ARG:HE	1.83	0.43
4:A:403:IVM:H23A	1:B:229:ILE:HD11	2.01	0.42
4:A:403:IVM:H8	1:B:233:LEU:CD1	2.49	0.42
1:C:203:ASN:C	1:C:203:ASN:HD22	2.23	0.41
4:C:403:IVM:H8	1:D:233:LEU:CD1	2.50	0.41
1:A:175:PRO:HG2	1:A:195:LEU:HD11	2.03	0.41
1:D:203:ASN:HD21	1:E:65:ARG:NH1	2.19	0.41
1:C:175:PRO:HG2	1:C:195:LEU:HD11	2.03	0.41
1:E:175:PRO:HG2	1:E:195:LEU:HD11	2.03	0.41
1:A:108:PHE:CD1	1:A:130:ILE:HD11	2.57	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%)	330 (98%)	6 (2%)	0	100	100
1	B	341/362 (94%)	335 (98%)	6 (2%)	0	100	100
1	C	336/362 (93%)	330 (98%)	6 (2%)	0	100	100
1	D	341/362 (94%)	335 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	336/362 (93%)	330 (98%)	6 (2%)	0	100	100
All	All	1690/1810 (93%)	1660 (98%)	30 (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	295/326 (90%)	289 (98%)	6 (2%)	55	80
1	B	294/326 (90%)	288 (98%)	6 (2%)	55	80
1	C	293/326 (90%)	286 (98%)	7 (2%)	49	77
1	D	296/326 (91%)	290 (98%)	6 (2%)	55	80
1	E	296/326 (91%)	290 (98%)	6 (2%)	55	80
All	All	1474/1630 (90%)	1443 (98%)	31 (2%)	53	79

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	PHE
1	A	47	SER
1	A	80	ASP
1	A	115	ASN
1	A	169	GLU
1	A	171	GLN
1	B	32	PHE
1	B	47	SER
1	B	80	ASP
1	B	115	ASN
1	B	169	GLU
1	B	171	GLN
1	C	32	PHE
1	C	47	SER

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Mol	Chain	Res	Type
1	C	80	ASP
1	C	115	ASN
1	C	169	GLU
1	C	171	GLN
1	C	203	ASN
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	E	32	PHE
1	E	47	SER
1	E	80	ASP
1	E	115	ASN
1	E	169	GLU
1	E	171	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	203	ASN
1	D	203	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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$
4	IVM	B	403	-	65,68,68	1.83	8 (12%)	82,102,102	1.36	10 (12%)
4	IVM	D	403	-	65,68,68	1.84	8 (12%)	82,102,102	1.35	11 (13%)
2	7C6	E	401	-	31,32,32	1.94	3 (9%)	41,50,50	1.91	8 (19%)
2	7C6	A	401	-	31,32,32	1.98	6 (19%)	41,50,50	1.94	8 (19%)
2	7C6	B	401	-	31,32,32	1.86	4 (12%)	41,50,50	2.04	10 (24%)
2	7C6	C	401	-	31,32,32	1.87	4 (12%)	41,50,50	1.92	9 (21%)
4	IVM	A	403	-	65,68,68	1.86	8 (12%)	82,102,102	1.28	9 (10%)
4	IVM	C	403	-	65,68,68	1.83	8 (12%)	82,102,102	1.39	13 (15%)
4	IVM	E	403	-	65,68,68	1.81	8 (12%)	82,102,102	1.34	11 (13%)
2	7C6	D	401	-	31,32,32	1.99	5 (16%)	41,50,50	2.01	9 (21%)
7	NAG	C	405	1	14,14,15	0.51	0	17,19,21	1.15	2 (11%)

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
4	IVM	B	403	-	-	2/45/141/141	0/6/7/7
4	IVM	D	403	-	-	3/45/141/141	0/6/7/7
2	7C6	E	401	-	-	0/12/50/50	0/5/5/5
2	7C6	A	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
4	IVM	A	403	-	-	4/45/141/141	1/6/7/7
4	IVM	C	403	-	-	5/45/141/141	1/6/7/7
4	IVM	E	403	-	-	5/45/141/141	0/6/7/7
2	7C6	D	401	-	-	0/12/50/50	0/5/5/5
7	NAG	C	405	1	-	1/6/23/26	0/1/1/1

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	7C6	O3-S1	7.20	1.51	1.43
2	D	401	7C6	O3-S1	6.66	1.50	1.43
2	D	401	7C6	O2-S1	6.63	1.50	1.43
2	A	401	7C6	O3-S1	6.47	1.50	1.43
2	B	401	7C6	O3-S1	6.41	1.50	1.43
2	C	401	7C6	O3-S1	6.35	1.50	1.43
2	E	401	7C6	O2-S1	6.17	1.50	1.43
4	A	403	IVM	C44-C43	6.15	1.40	1.33
2	B	401	7C6	O2-S1	6.07	1.50	1.43
4	B	403	IVM	C44-C43	6.04	1.40	1.33
2	C	401	7C6	O2-S1	6.01	1.50	1.43
4	E	403	IVM	C44-C43	5.89	1.40	1.33
2	A	401	7C6	O2-S1	5.86	1.50	1.43
4	C	403	IVM	C44-C43	5.85	1.40	1.33
4	D	403	IVM	C44-C43	5.84	1.40	1.33
4	C	403	IVM	C40-C39	-5.73	1.40	1.50
4	D	403	IVM	C40-C39	-5.70	1.40	1.50
4	A	403	IVM	C40-C39	-5.66	1.40	1.50
4	D	403	IVM	C15-C16	-5.59	1.39	1.50
4	A	403	IVM	C15-C16	-5.55	1.39	1.50
4	B	403	IVM	C40-C39	-5.53	1.40	1.50
4	E	403	IVM	C15-C16	-5.52	1.39	1.50
4	B	403	IVM	C15-C16	-5.50	1.39	1.50
4	C	403	IVM	C15-C16	-5.50	1.39	1.50
4	E	403	IVM	C40-C39	-5.49	1.40	1.50
4	D	403	IVM	C16-C17	5.29	1.39	1.33
4	E	403	IVM	C16-C17	5.20	1.39	1.33
4	B	403	IVM	C16-C17	5.19	1.39	1.33
4	A	403	IVM	C16-C17	5.18	1.39	1.33
4	C	403	IVM	C16-C17	5.01	1.39	1.33
4	C	403	IVM	C38-C39	4.47	1.39	1.33
4	B	403	IVM	C38-C39	4.43	1.39	1.33
4	D	403	IVM	C38-C39	4.41	1.39	1.33
4	A	403	IVM	C38-C39	4.34	1.39	1.33
4	E	403	IVM	C38-C39	4.27	1.39	1.33
4	A	403	IVM	C45-C44	3.68	1.55	1.51
4	B	403	IVM	C45-C44	3.67	1.55	1.51
4	C	403	IVM	C45-C44	3.46	1.55	1.51
2	A	401	7C6	S1-N1	3.41	1.68	1.63
4	D	403	IVM	C45-C44	3.41	1.54	1.51
4	E	403	IVM	C45-C44	3.28	1.54	1.51
2	B	401	7C6	C2-C3	2.89	1.55	1.51
2	A	401	7C6	C2-C3	2.77	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	IVM	C41-C42	2.60	1.55	1.51
2	C	401	7C6	C2-C3	2.58	1.54	1.51
2	A	401	7C6	C13-S1	-2.53	1.72	1.76
2	E	401	7C6	C2-C3	2.49	1.54	1.51
2	D	401	7C6	C13-S1	-2.47	1.73	1.76
4	B	403	IVM	C41-C42	2.37	1.55	1.51
4	D	403	IVM	C41-C42	2.36	1.55	1.51
4	A	403	IVM	C41-C42	2.34	1.55	1.51
4	E	403	IVM	O9-C40	2.34	1.47	1.43
2	D	401	7C6	C2-C3	2.31	1.54	1.51
4	A	403	IVM	O9-C40	2.22	1.47	1.43
2	D	401	7C6	C3-N2	2.19	1.40	1.36
2	C	401	7C6	C3-N2	2.19	1.40	1.36
4	C	403	IVM	O9-C40	2.18	1.47	1.43
2	A	401	7C6	C3-N2	2.16	1.40	1.36
4	D	403	IVM	O9-C40	2.14	1.47	1.43
2	B	401	7C6	C3-N2	2.06	1.40	1.36
4	B	403	IVM	O9-C40	2.06	1.46	1.43
4	E	403	IVM	C11-C12	2.02	1.55	1.51

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	7C6	O3-S1-O2	-6.11	109.63	119.52
2	E	401	7C6	O3-S1-O2	-6.05	109.72	119.52
2	C	401	7C6	O3-S1-O2	-5.57	110.49	119.52
2	D	401	7C6	O3-S1-O2	-5.49	110.63	119.52
4	D	403	IVM	O12-C46-C45	5.25	118.57	110.97
4	C	403	IVM	O12-C46-C45	5.17	118.45	110.97
4	B	403	IVM	O12-C46-C45	5.11	118.36	110.97
2	A	401	7C6	O3-S1-O2	-4.81	111.73	119.52
4	E	403	IVM	O12-C46-C45	4.79	117.90	110.97
2	D	401	7C6	C1-N1-S1	-4.74	111.79	120.06
4	A	403	IVM	O12-C46-C45	4.72	117.80	110.97
2	B	401	7C6	C1-N1-S1	-4.68	111.90	120.06
4	C	403	IVM	O14-C14-C15	4.56	110.22	105.82
2	A	401	7C6	C7-C8-C9	-4.54	120.36	125.03
2	C	401	7C6	C1-N1-S1	-4.46	112.30	120.06
2	D	401	7C6	C7-C8-C9	-4.36	120.55	125.03
2	D	401	7C6	C10-N1-S1	-4.36	110.32	118.80
2	B	401	7C6	C10-N1-S1	-4.32	110.39	118.80
2	A	401	7C6	C10-N1-S1	-4.16	110.70	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	7C6	C10-N1-S1	-4.16	110.71	118.80
2	E	401	7C6	C7-C8-C9	-4.13	120.79	125.03
2	B	401	7C6	C7-C8-C9	-4.10	120.81	125.03
2	C	401	7C6	C7-C8-C9	-4.06	120.86	125.03
2	E	401	7C6	C1-N1-S1	-3.91	113.25	120.06
2	A	401	7C6	C1-N1-S1	-3.91	113.25	120.06
2	A	401	7C6	O1-C3-N2	-3.72	118.69	122.44
2	B	401	7C6	O1-C3-N2	-3.69	118.72	122.44
4	E	403	IVM	O14-C14-C15	3.69	109.37	105.82
4	B	403	IVM	O14-C14-C15	3.64	109.32	105.82
2	E	401	7C6	C10-N1-S1	-3.52	111.95	118.80
2	C	401	7C6	O1-C3-N2	-3.44	118.97	122.44
2	E	401	7C6	O1-C3-N2	-3.18	119.23	122.44
2	D	401	7C6	O1-C3-N2	-3.17	119.24	122.44
4	A	403	IVM	C3-C5-C9	-3.11	110.95	116.50
7	C	405	NAG	C1-O5-C5	3.10	116.39	112.19
4	E	403	IVM	C34-C36-C37	-2.96	119.93	126.16
2	B	401	7C6	C6-N3-C7	2.94	121.93	116.85
2	D	401	7C6	C6-N3-C7	2.86	121.79	116.85
4	D	403	IVM	C37-C38-C39	-2.84	121.09	130.07
4	C	403	IVM	C3-C5-C9	-2.83	111.45	116.50
4	C	403	IVM	C34-C36-C37	-2.82	120.23	126.16
2	E	401	7C6	C6-N3-C7	2.82	121.73	116.85
4	D	403	IVM	C3-C5-C9	-2.80	111.49	116.50
4	E	403	IVM	C3-C5-C9	-2.80	111.49	116.50
4	D	403	IVM	C34-C36-C37	-2.79	120.28	126.16
4	A	403	IVM	O14-C14-C15	2.78	108.50	105.82
2	A	401	7C6	C6-N3-C7	2.78	121.65	116.85
4	C	403	IVM	C13-C14-C15	-2.77	109.49	113.21
4	E	403	IVM	C37-C38-C39	-2.75	121.36	130.07
2	D	401	7C6	O4-C15-C14	2.74	131.52	127.85
4	E	403	IVM	C34-C19-C17	-2.72	108.46	113.89
4	B	403	IVM	C3-C5-C9	-2.71	111.65	116.50
4	D	403	IVM	O1-C5-C3	2.70	110.24	106.12
4	A	403	IVM	C37-C38-C39	-2.64	121.72	130.07
2	A	401	7C6	O4-C15-C14	2.61	131.35	127.85
4	C	403	IVM	C37-C38-C39	-2.61	121.83	130.07
4	B	403	IVM	O11-C46-C45	-2.60	120.60	125.05
4	B	403	IVM	C37-C38-C39	-2.60	121.86	130.07
2	A	401	7C6	C10-N1-C1	-2.59	107.36	110.68
2	C	401	7C6	C6-N3-C7	2.57	121.30	116.85
4	E	403	IVM	O11-C46-C45	-2.55	120.68	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	IVM	C38-C37-C36	-2.52	118.42	124.53
4	A	403	IVM	C34-C36-C37	-2.52	120.86	126.16
4	D	403	IVM	O11-C46-C45	-2.52	120.74	125.05
2	B	401	7C6	O4-C15-C14	2.50	131.19	127.85
2	D	401	7C6	O5-C19-O4	-2.49	104.10	108.08
4	D	403	IVM	C34-C19-C17	-2.49	108.93	113.89
2	C	401	7C6	O4-C15-C14	2.48	131.17	127.85
4	C	403	IVM	O11-C46-C45	-2.46	120.83	125.05
4	B	403	IVM	C34-C36-C37	-2.44	121.02	126.16
4	B	403	IVM	C13-C14-C15	-2.44	109.94	113.21
4	B	403	IVM	C8-C9-C5	2.42	112.06	108.41
4	A	403	IVM	C38-C37-C36	-2.40	118.69	124.53
2	E	401	7C6	O4-C15-C14	2.40	131.06	127.85
4	D	403	IVM	C38-C37-C36	-2.39	118.73	124.53
4	A	403	IVM	O11-C46-C45	-2.38	120.97	125.05
4	C	403	IVM	C34-C19-C17	-2.35	109.21	113.89
2	B	401	7C6	C10-N1-C1	-2.28	107.77	110.68
2	B	401	7C6	O3-S1-N1	2.26	111.09	106.97
4	C	403	IVM	C38-C37-C36	-2.24	119.10	124.53
4	A	403	IVM	C8-C9-C5	2.23	111.78	108.41
7	C	405	NAG	O5-C1-C2	-2.23	107.76	111.29
2	E	401	7C6	C13-S1-N1	2.22	111.31	107.36
4	A	403	IVM	C34-C19-C17	-2.21	109.48	113.89
4	D	403	IVM	C48-C43-C44	-2.20	118.84	123.56
4	E	403	IVM	C48-C43-C44	-2.19	118.87	123.56
4	E	403	IVM	O12-C12-C11	2.18	113.03	107.59
4	E	403	IVM	C8-C9-C5	2.18	111.70	108.41
4	D	403	IVM	C8-C9-C5	2.15	111.66	108.41
2	B	401	7C6	C13-S1-N1	2.15	111.18	107.36
2	C	401	7C6	C10-N1-C1	-2.12	107.97	110.68
4	C	403	IVM	C18-C17-C19	2.11	119.32	115.68
4	E	403	IVM	C38-C37-C36	-2.09	119.46	124.53
4	D	403	IVM	O1-C6-C11	2.08	109.28	106.26
4	C	403	IVM	C7-C6-C11	-2.07	108.97	112.55
2	C	401	7C6	C13-S1-N1	2.07	111.04	107.36
4	B	403	IVM	C18-C17-C19	2.03	119.19	115.68
4	C	403	IVM	O12-C12-C11	2.02	112.63	107.59
4	C	403	IVM	C48-C43-C44	-2.01	119.26	123.56
2	D	401	7C6	C10-N1-C1	-2.01	108.11	110.68

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	403	IVM	C26-C25-O4-C24
4	A	403	IVM	C26-C25-O4-C24
4	B	403	IVM	C1-C2-C3-C5
4	D	403	IVM	C26-C25-O4-C24
4	C	403	IVM	C26-C25-O4-C24
4	E	403	IVM	O7-C25-O4-C24
4	A	403	IVM	O7-C25-O4-C24
4	D	403	IVM	O7-C25-O4-C24
4	C	403	IVM	O7-C25-O4-C24
4	D	403	IVM	C21-C22-O3-C23
4	C	403	IVM	C1-C2-C3-C4
4	B	403	IVM	C1-C2-C3-C4
4	E	403	IVM	C1-C2-C3-C5
4	C	403	IVM	C1-C2-C3-C5
4	A	403	IVM	C21-C22-O3-C23
4	E	403	IVM	C1-C2-C3-C4
4	E	403	IVM	C19-C34-C36-C37
4	A	403	IVM	C19-C34-C36-C37
4	C	403	IVM	C19-C34-C36-C37
7	C	405	NAG	O5-C5-C6-O6

All (2) ring outliers are listed below:

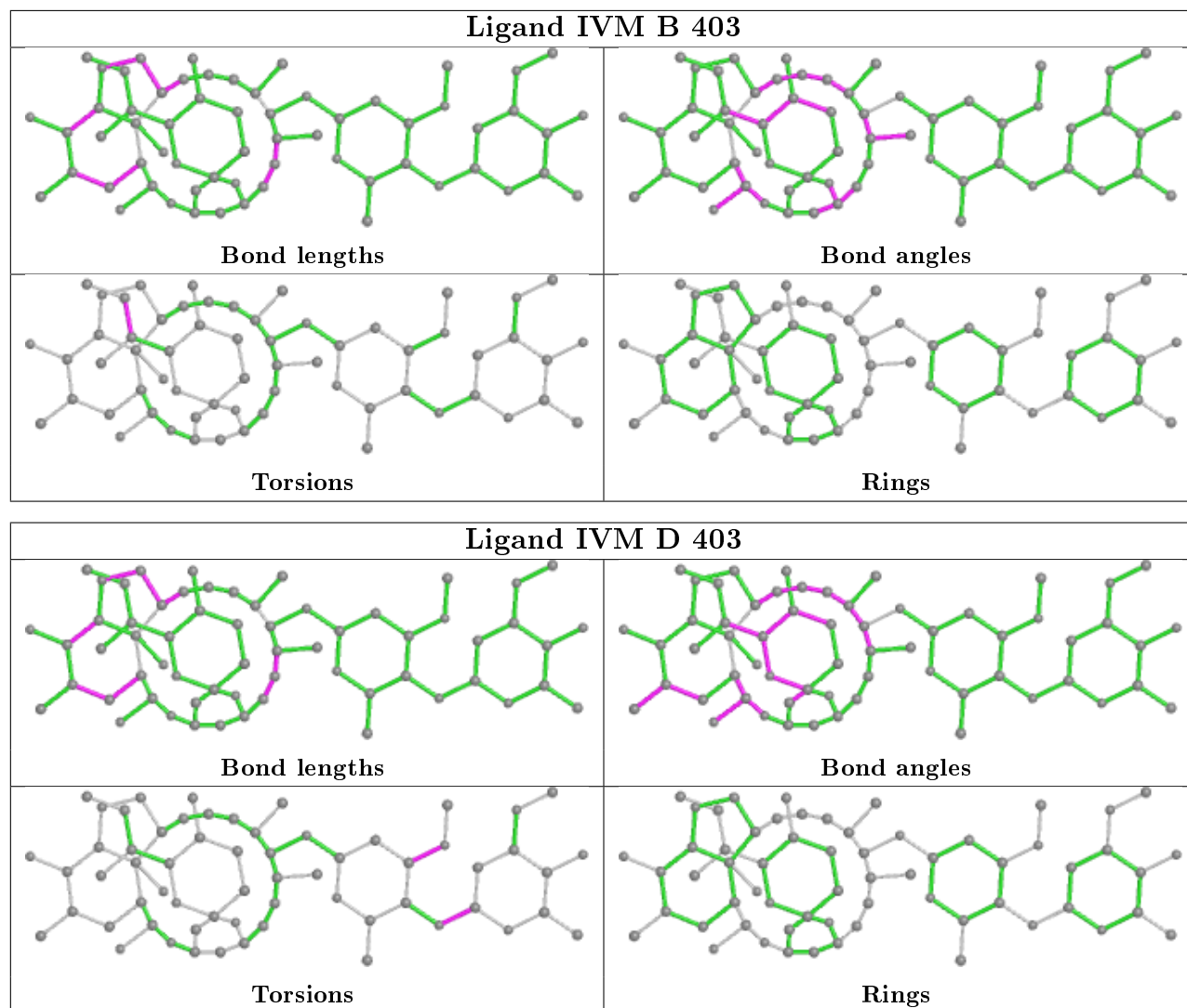
Mol	Chain	Res	Type	Atoms
4	A	403	IVM	C5-C6-C7-C8-C9-O1
4	C	403	IVM	C5-C6-C7-C8-C9-O1

4 monomers are involved in 10 short contacts:

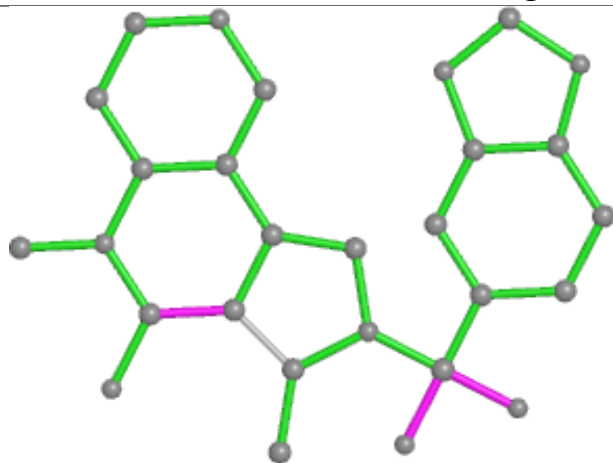
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	IVM	3	0
4	D	403	IVM	2	0
4	A	403	IVM	3	0
4	C	403	IVM	2	0

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

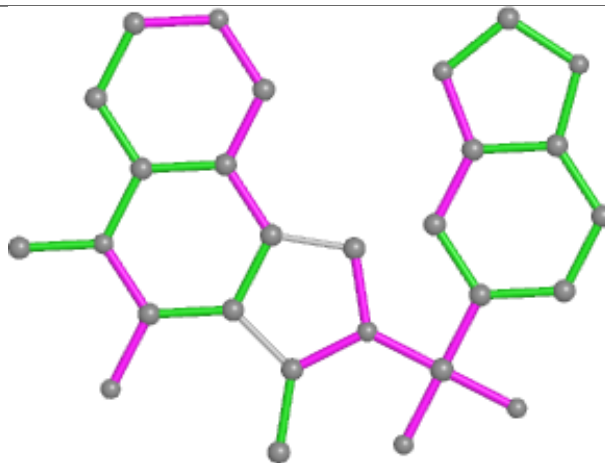
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



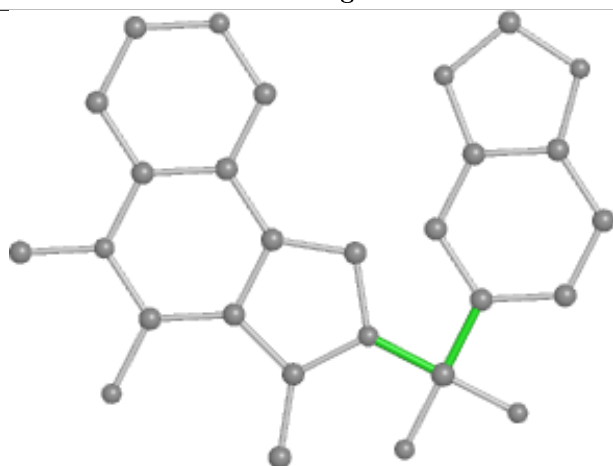
Ligand 7C6 E 401



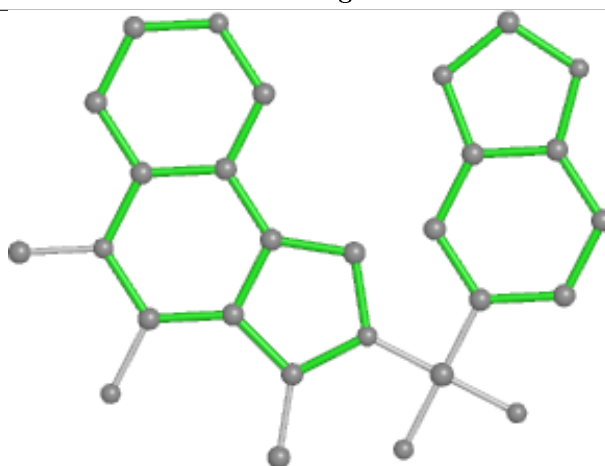
Bond lengths



Bond angles

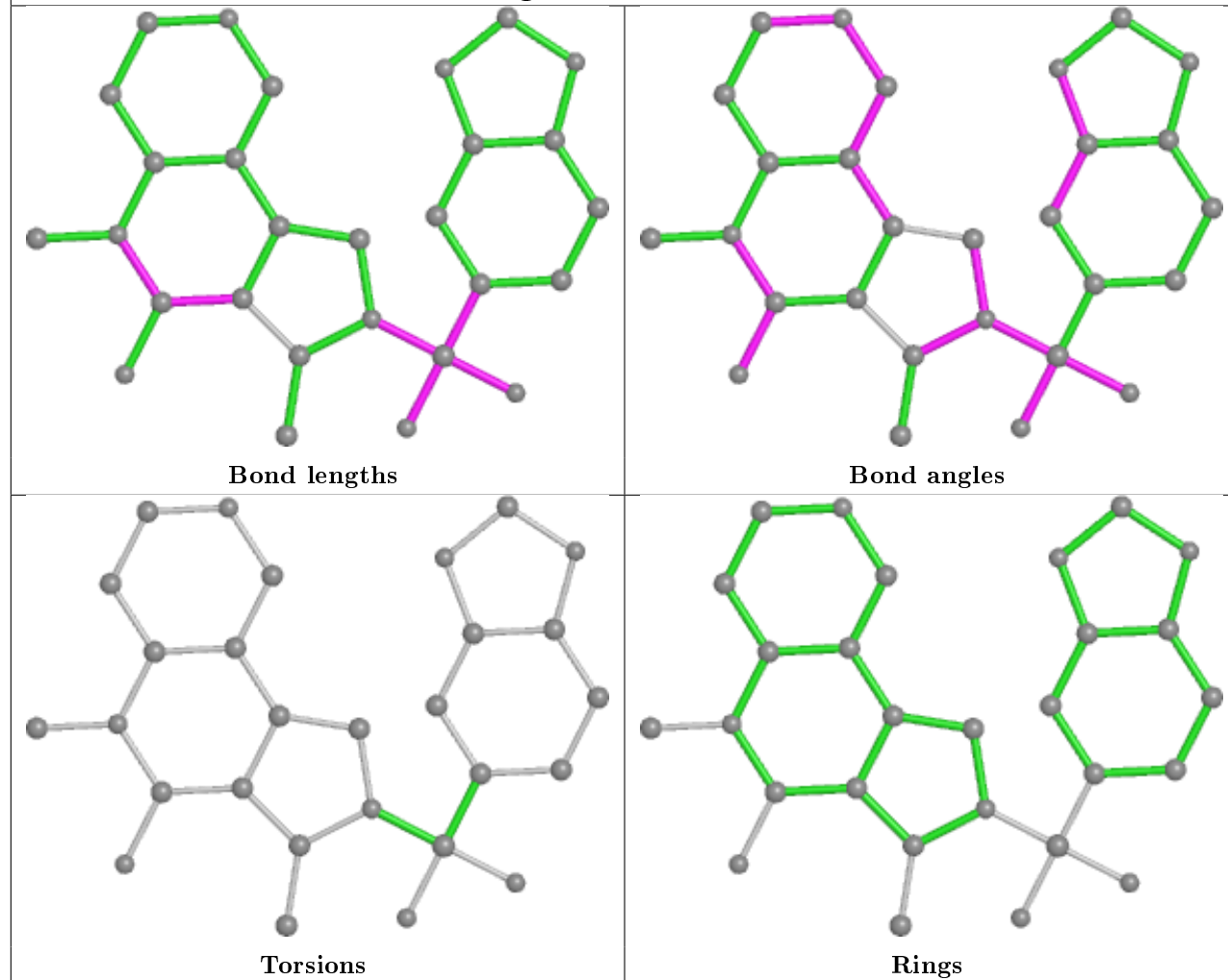


Torsions

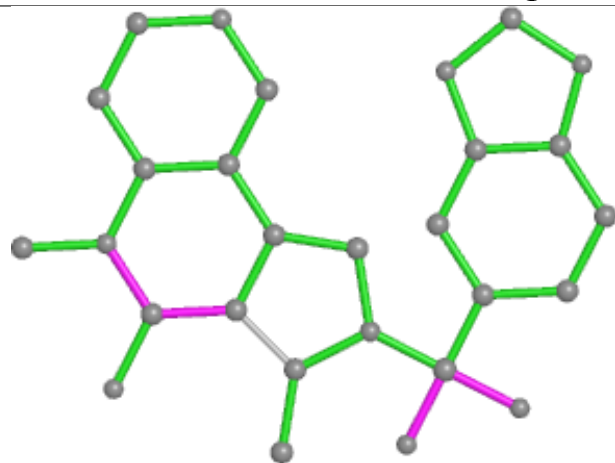


Rings

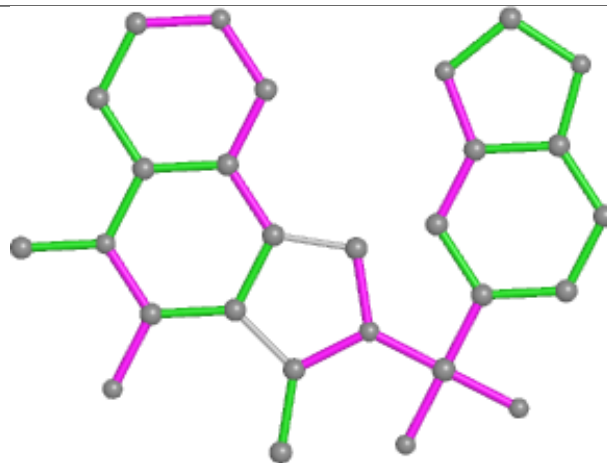
Ligand 7C6 A 401



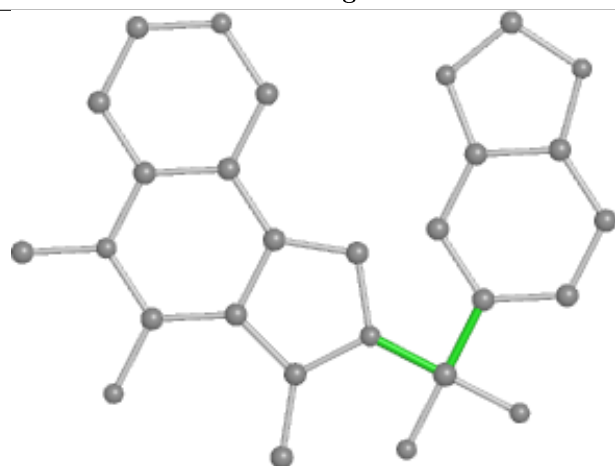
Ligand 7C6 B 401



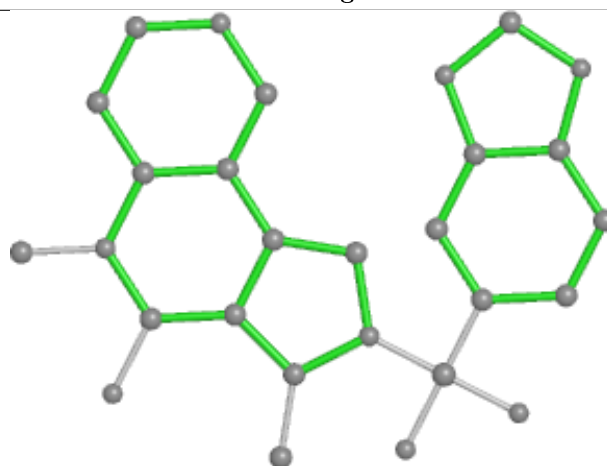
Bond lengths



Bond angles

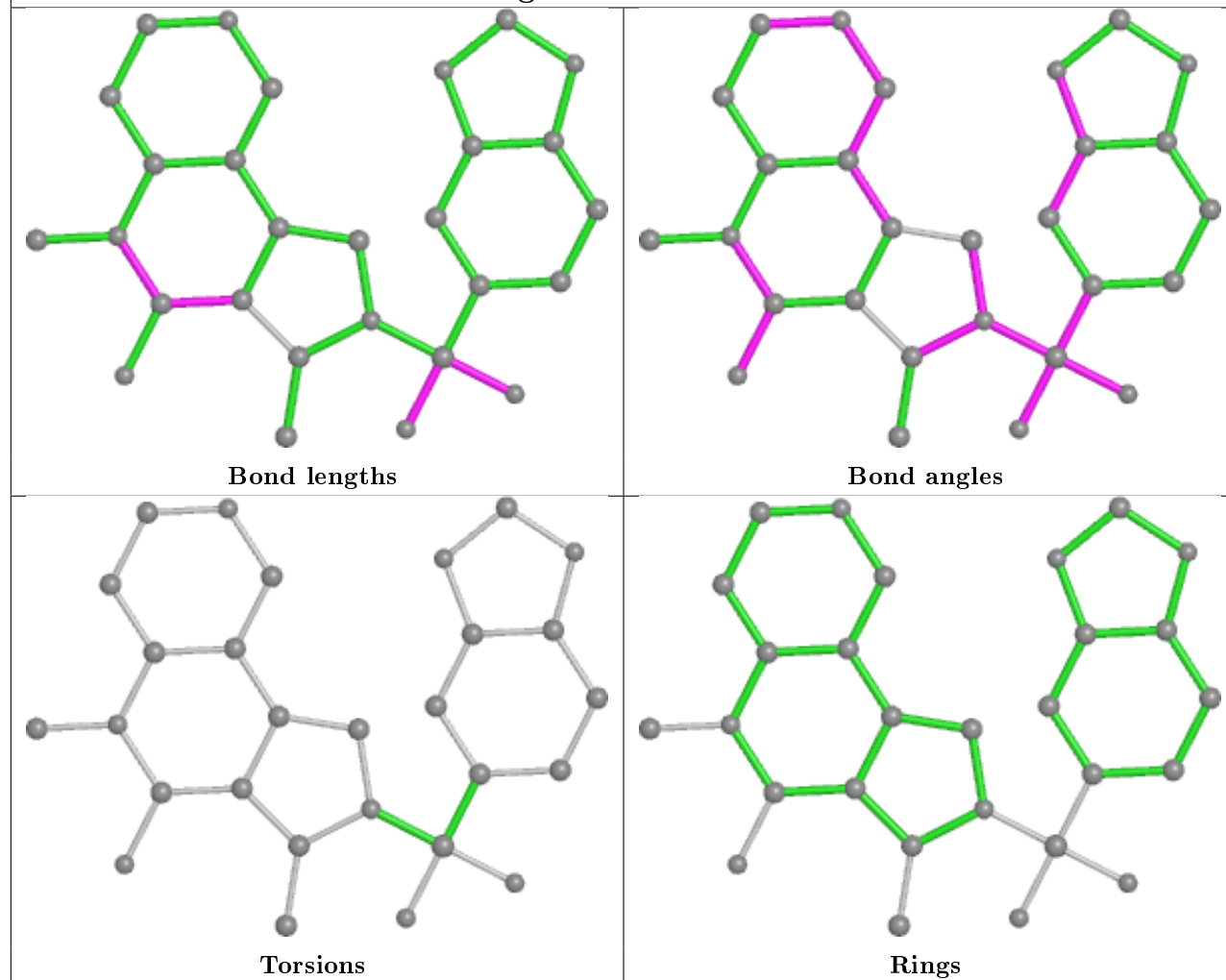


Torsions

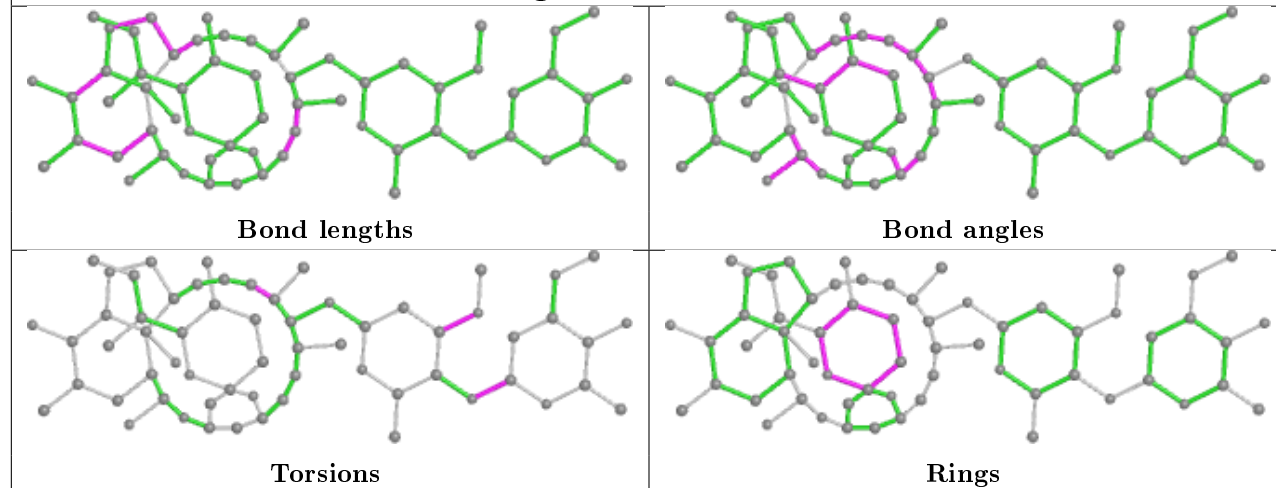


Rings

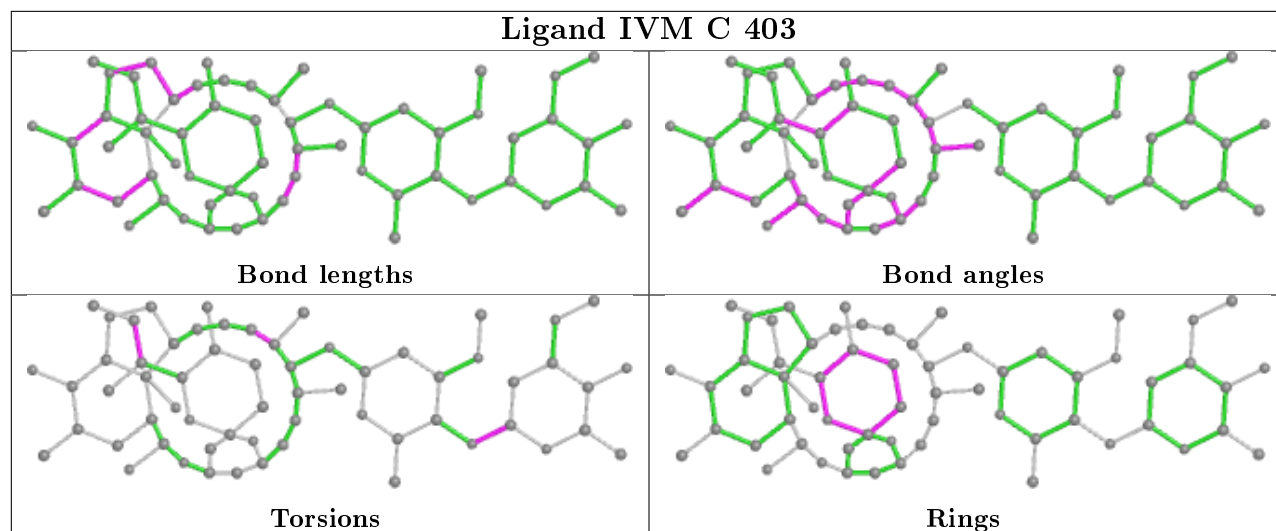
Ligand 7C6 C 401



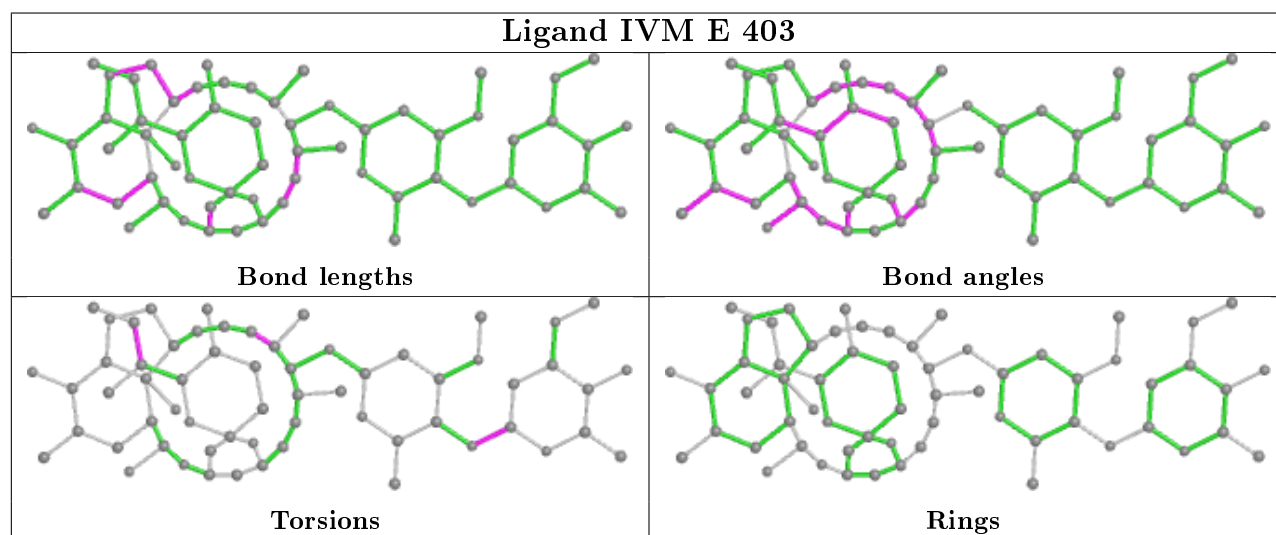
Ligand IVM A 403

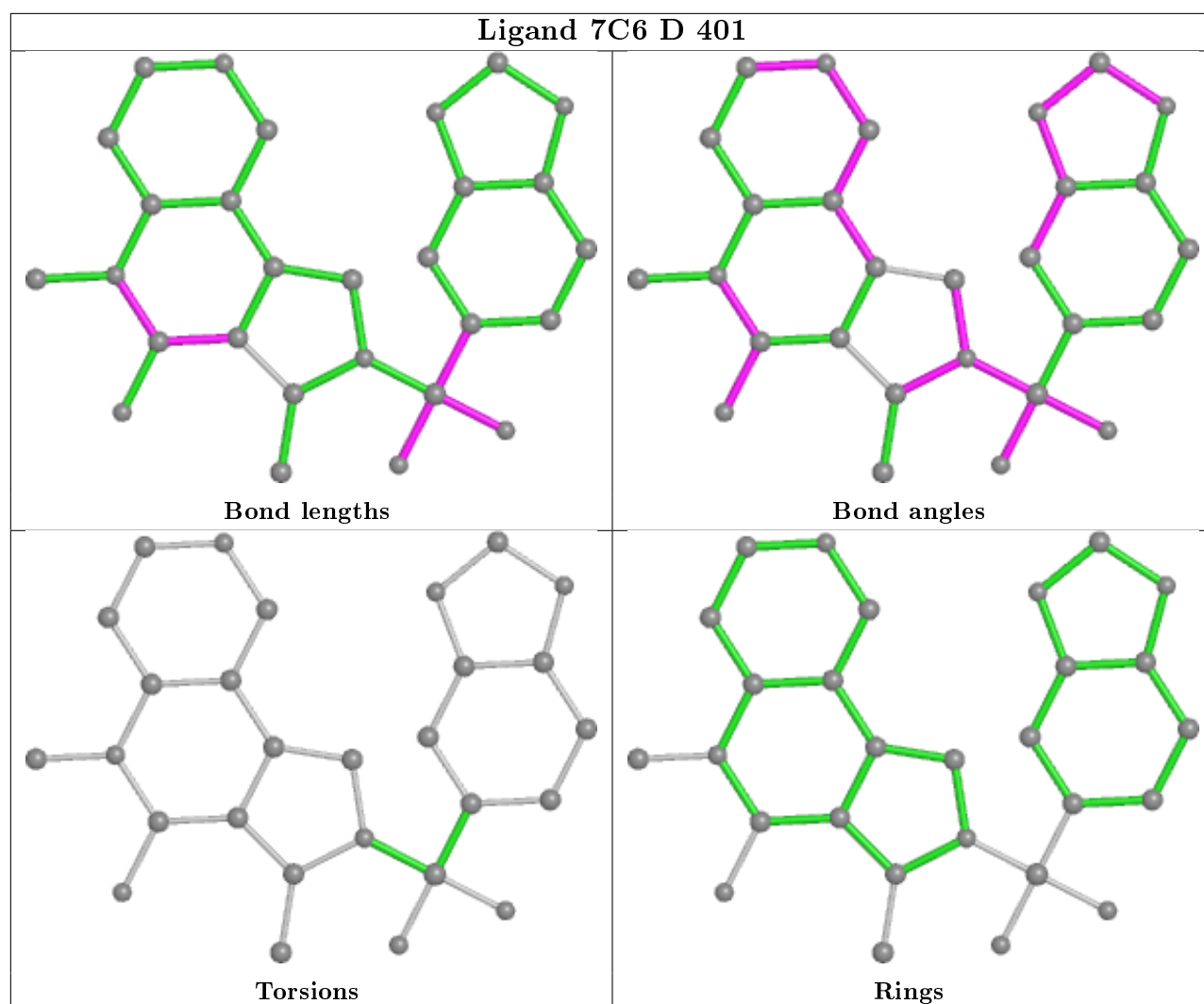


Ligand IVM C 403



Ligand IVM E 403





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%)	0.25	11 (3%) 46 41	41, 75, 136, 173	0
1	B	343/362 (94%)	0.21	10 (2%) 51 47	42, 78, 144, 188	0
1	C	338/362 (93%)	0.56	41 (12%) 4 2	46, 88, 171, 224	0
1	D	343/362 (94%)	0.49	25 (7%) 15 11	50, 94, 173, 217	0
1	E	338/362 (93%)	0.34	20 (5%) 22 17	50, 87, 152, 195	0
All	All	1700/1810 (93%)	0.37	107 (6%) 20 15	41, 85, 162, 224	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	307	VAL	6.2
1	D	325	ILE	5.9
1	C	323	ASP	5.4
1	D	324	THR	5.1
1	C	325	ILE	5.0
1	C	329	CYS	5.0
1	D	3	SER	4.9
1	D	317	ASP	4.7
1	C	324	THR	4.6
1	C	315	PHE	4.6
1	C	322	ILE	4.4
1	C	265	THR	4.3
1	D	341	TYR	4.2
1	B	345	TYR	4.2
1	D	265	THR	4.0
1	A	310	ALA	4.0
1	A	307	VAL	3.9
1	C	316	ILE	3.7
1	C	306	PHE	3.7
1	C	242	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	303	ALA	3.7
1	C	312	THR	3.7
1	E	342	TRP	3.6
1	C	189	LEU	3.6
1	D	345	TYR	3.5
1	C	188	LEU	3.5
1	E	189	LEU	3.4
1	C	310	ALA	3.3
1	A	315	PHE	3.3
1	A	306	PHE	3.2
1	E	265	THR	3.1
1	C	308	SER	3.1
1	C	172	ASP	3.1
1	E	345	TYR	3.1
1	B	310	ALA	3.1
1	C	217	GLU	3.1
1	D	262	THR	3.0
1	E	188	LEU	3.0
1	E	217	GLU	3.0
1	D	269	GLY	3.0
1	D	272	ALA	2.9
1	C	319	ALA	2.9
1	B	309	ARG	2.9
1	D	248	ALA	2.9
1	A	21	THR	2.8
1	D	217	GLU	2.8
1	D	342	TRP	2.8
1	C	326	SER	2.7
1	D	326	SER	2.7
1	D	327	ARG	2.7
1	E	300	GLU	2.7
1	C	314	VAL	2.7
1	B	258	THR	2.6
1	C	268	SER	2.6
1	C	264	THR	2.6
1	C	261	LEU	2.6
1	D	323	ASP	2.6
1	E	183	THR	2.6
1	A	265	THR	2.5
1	A	319	ALA	2.5
1	C	225	ILE	2.5
1	C	327	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	311	GLY	2.4
1	D	310	ALA	2.4
1	E	258	THR	2.4
1	D	175	PRO	2.4
1	B	306	PHE	2.4
1	B	315	PHE	2.4
1	E	214	PHE	2.4
1	C	280	VAL	2.4
1	E	261	LEU	2.4
1	A	342	TRP	2.4
1	D	307	VAL	2.4
1	B	316	ILE	2.3
1	D	214	PHE	2.3
1	E	21	THR	2.3
1	E	12	ASP	2.3
1	C	246	MET	2.3
1	A	8	MET	2.3
1	E	73	LEU	2.3
1	C	243	TRP	2.2
1	A	217	GLU	2.2
1	D	176	VAL	2.2
1	E	325	ILE	2.2
1	C	262	THR	2.2
1	E	341	TYR	2.2
1	C	309	ARG	2.2
1	C	339	ILE	2.2
1	C	220	MET	2.2
1	C	75	TYR	2.2
1	C	258	THR	2.2
1	C	77	GLU	2.1
1	B	312	THR	2.1
1	C	181	GLY	2.1
1	C	332	LEU	2.1
1	D	224	LEU	2.1
1	A	278	SER	2.1
1	E	268	SER	2.1
1	C	197	TYR	2.1
1	E	192	GLU	2.1
1	B	220	MET	2.1
1	B	265	THR	2.1
1	D	32	PHE	2.1
1	D	273	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	262	THR	2.0
1	E	264	THR	2.0
1	D	188	LEU	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(Å ²)	Q<0.9
5	ZN	E	404	1/1	0.63	0.39	104,104,104,104	1
6	CL	A	405	1/1	0.66	1.03	102,102,102,102	0
5	ZN	D	404	1/1	0.70	0.57	122,122,122,122	1
5	ZN	A	404	1/1	0.76	0.10	85,85,85,85	1
5	ZN	C	404	1/1	0.81	0.46	123,123,123,123	1
7	NAG	C	405	14/15	0.82	0.30	115,123,127,127	0
4	IVM	E	403	62/62	0.86	0.21	86,101,121,128	0
4	IVM	C	403	62/62	0.88	0.24	109,135,156,162	0
4	IVM	B	403	62/62	0.89	0.24	91,114,132,134	0
4	IVM	D	403	62/62	0.89	0.21	106,132,149,154	0
4	IVM	A	403	62/62	0.91	0.22	80,99,122,128	0
5	ZN	B	404	1/1	0.92	0.43	110,110,110,110	1
3	GLY	E	402	5/5	0.95	0.21	63,63,64,65	0
3	GLY	C	402	5/5	0.96	0.22	74,75,75,77	0
2	7C6	C	401	28/28	0.96	0.21	64,72,79,81	0
3	GLY	A	402	5/5	0.96	0.24	64,64,65,65	0
3	GLY	D	402	5/5	0.96	0.30	72,73,73,74	0
2	7C6	E	401	28/28	0.96	0.22	69,74,79,81	0
2	7C6	A	401	28/28	0.97	0.18	50,61,67,69	0
2	7C6	B	401	28/28	0.97	0.23	64,71,79,81	0

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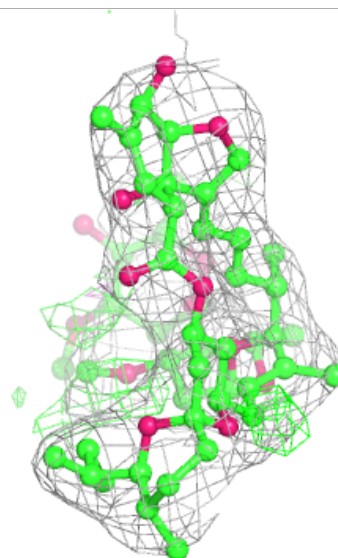
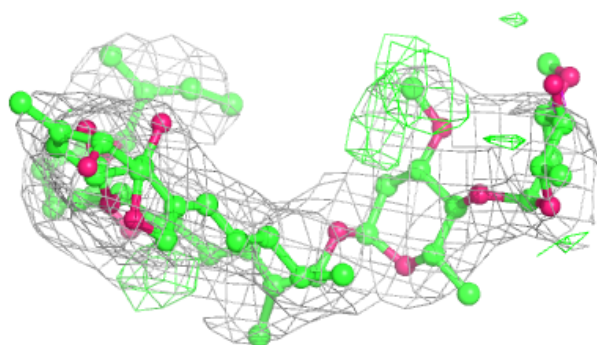
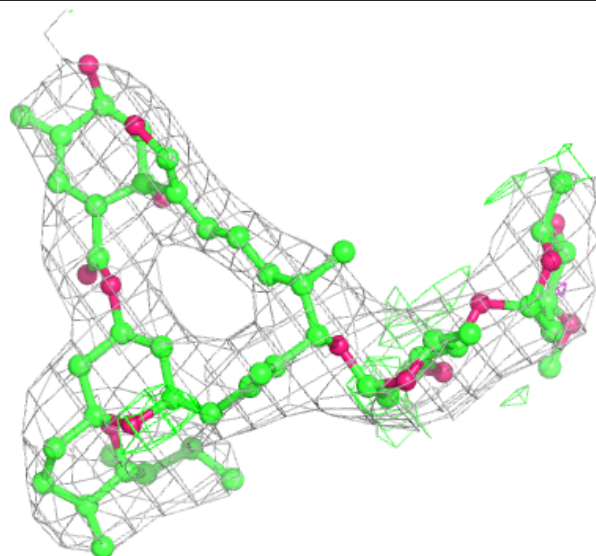
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLY	B	402	5/5	0.98	0.21	71,72,72,73	0
2	7C6	D	401	28/28	0.98	0.20	71,78,85,87	0

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.

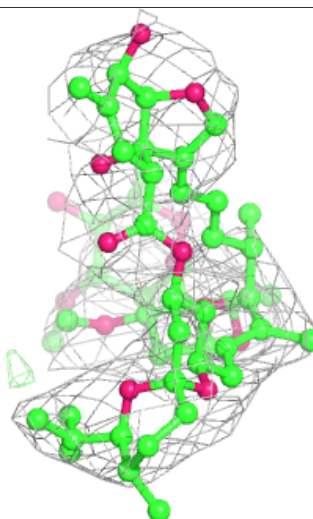
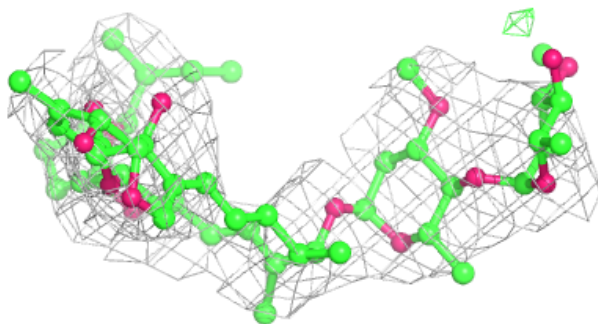
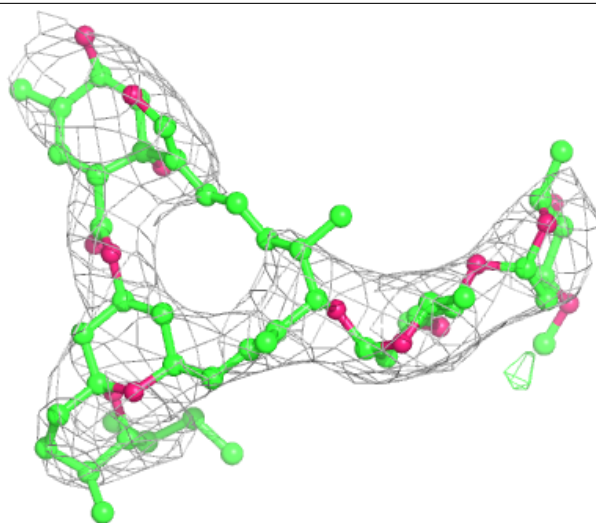
Electron density around IVM E 403:

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



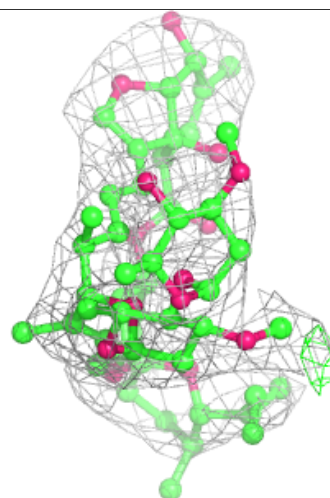
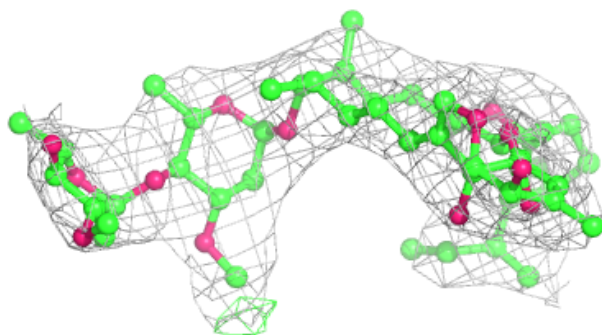
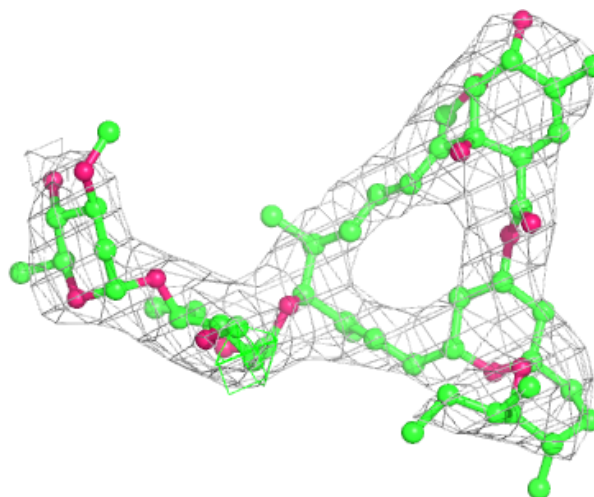
Electron density around IVM C 403:

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



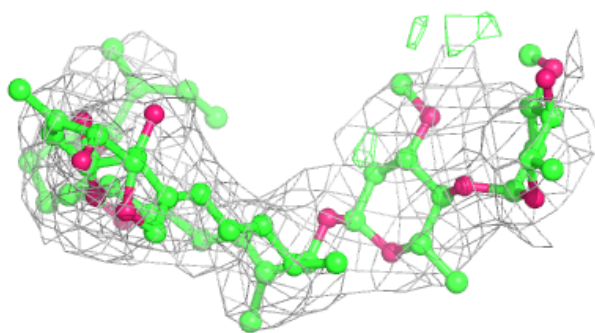
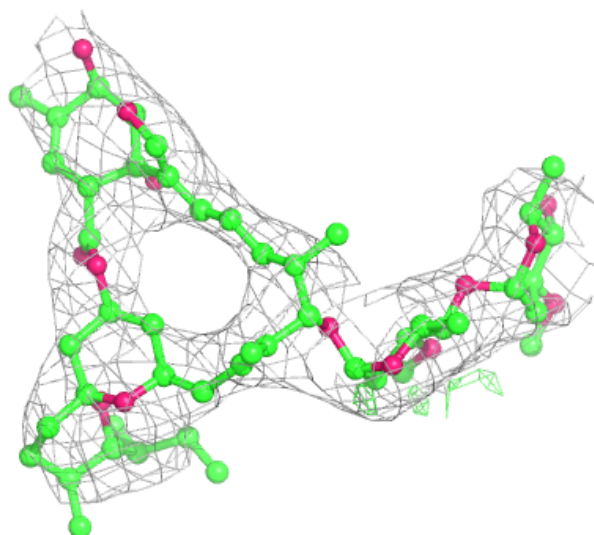
Electron density around IVM B 403:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



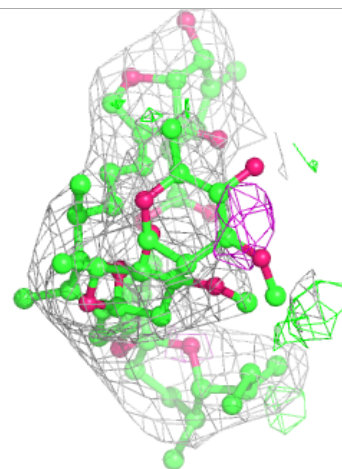
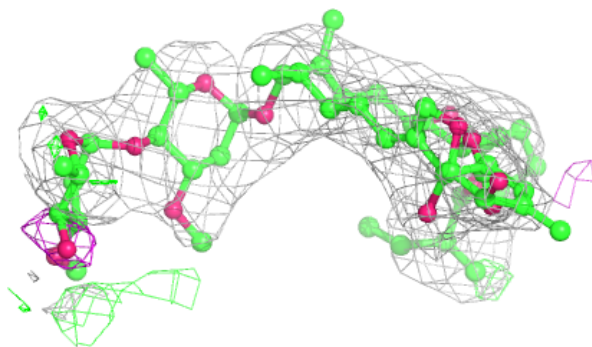
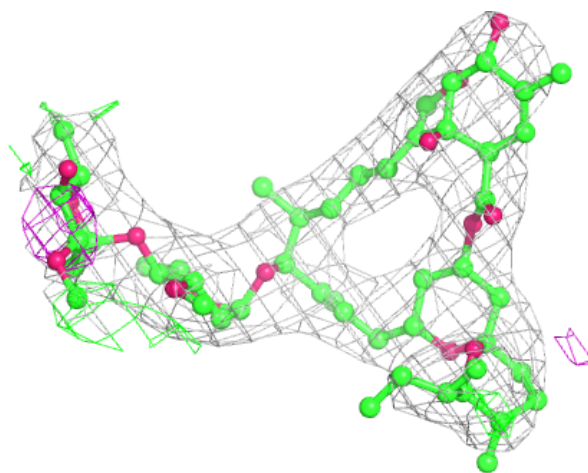
Electron density around IVM D 403:

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and green (positive)



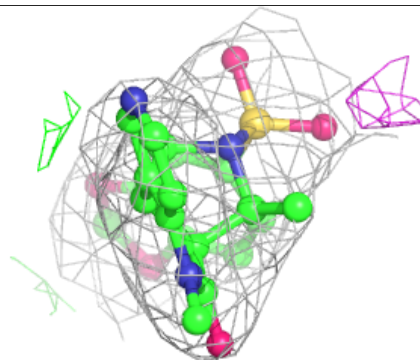
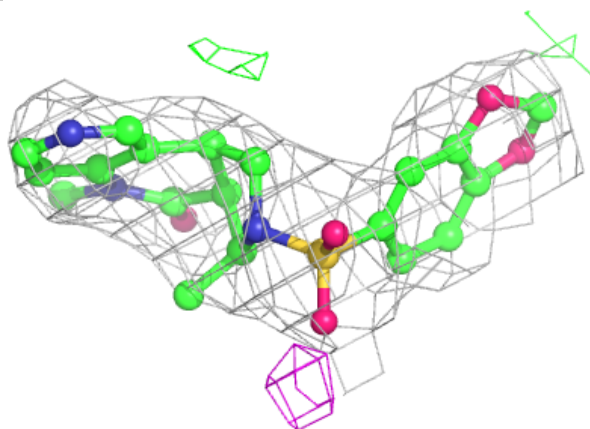
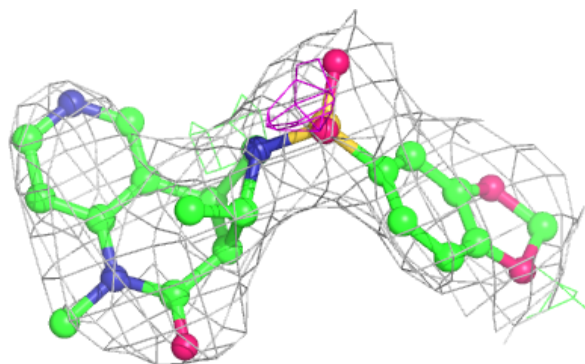
Electron density around IVM A 403:

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and green (positive)

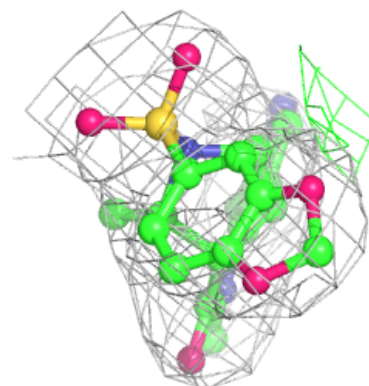
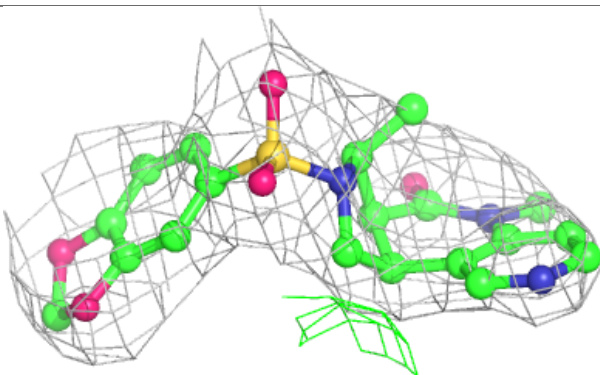
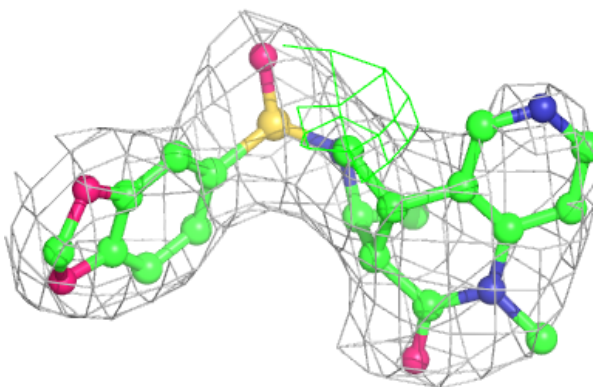


Electron density around 7C6 C 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

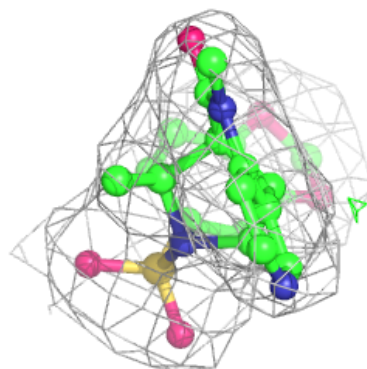
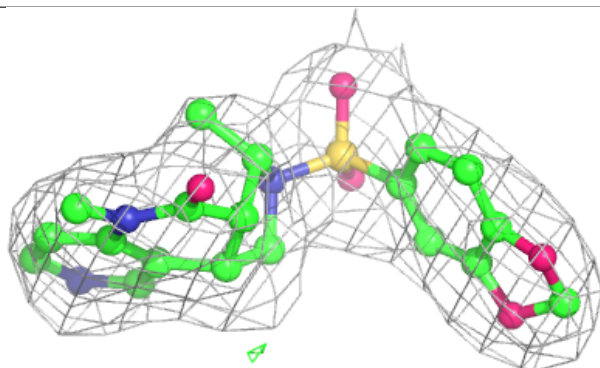
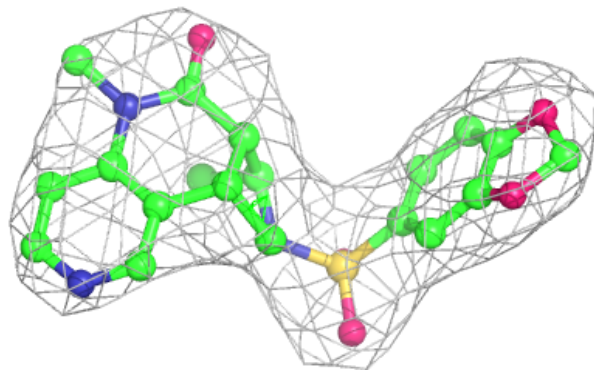
**Electron density around 7C6 E 401:**

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

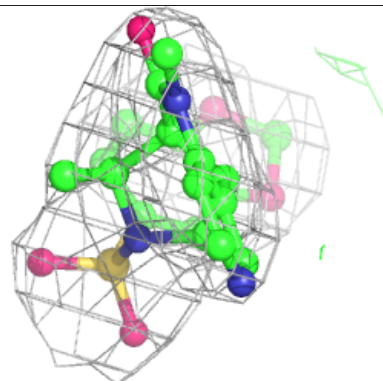
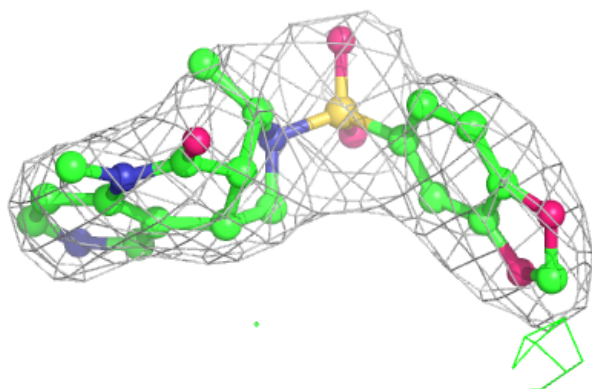
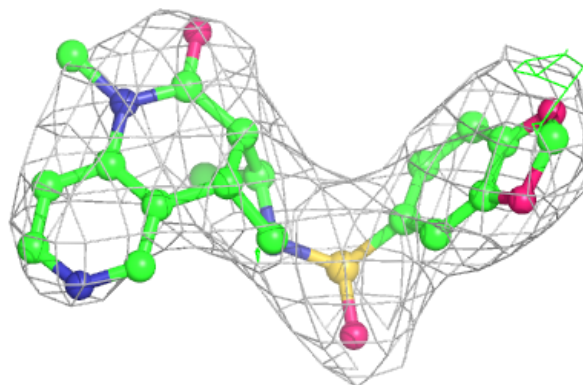


Electron density around 7C6 A 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

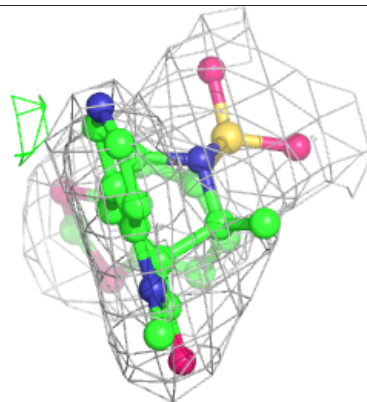
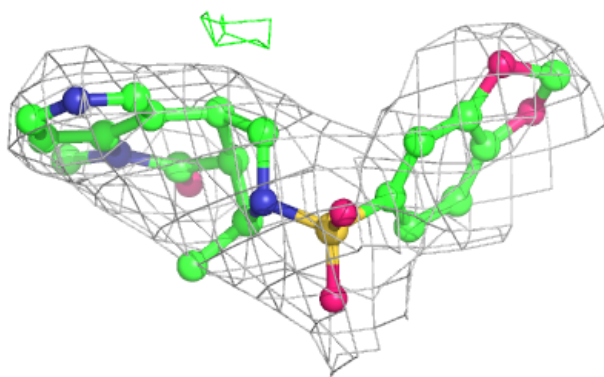
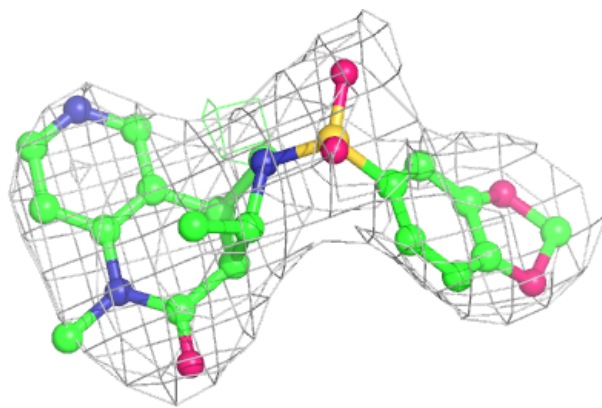
**Electron density around 7C6 B 401:**

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.