WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 12:46 am BST

PDB ID	:	3QS1
Title	:	Crystal structure of KNI-10006 complex of Plasmepsin I (PMI) from Plasmodium falciparum
Authors	:	Bhaumik, P.; Gustchina, A.; Wlodawer, A.
Deposited on	:	2011-02-19
Resolution	:	3.10 Å(reported)

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

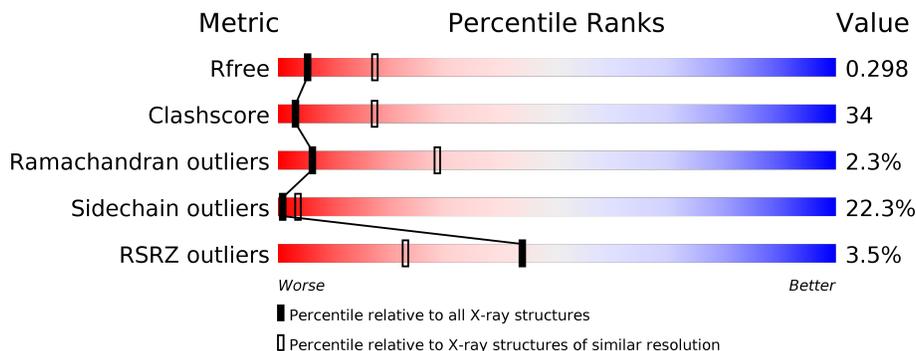|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.298
Clashscore		34
Ramachandran outliers		2.3%
Sidechain outliers		22.3%
RSRZ outliers		3.5%

Worse　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 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 <=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	336	2% — 45% 39% 13% • •
1	B	336	% — 46% 36% 13% • •
1	C	336	2% — 36% 49% 12% • •
1	D	336	9% — 35% 49% 11% • •

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 crite-

ria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	331	-	-	X	-
3	GOL	C	331	-	-	X	X
3	GOL	C	333	-	-	X	-
3	GOL	D	331	-	-	X	-
3	GOL	D	332	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10646 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 Plasmepsin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2604	1693	403	500	8			
1	B	327	Total	C	N	O	S	0	0	0
			2604	1693	403	500	8			
1	C	326	Total	C	N	O	S	0	0	0
			2599	1690	402	499	8			
1	D	326	Total	C	N	O	S	0	0	0
			2599	1690	402	499	8			

- Molecule 2 is (4R)-3-[(2S,3S)-3-{[(2,6-dimethylphenoxy)acetyl]amino}-2-hydroxy-4-phenylb utanoyl]-N-[(1S,2R)-2-hydroxy-2,3-dihydro-1H-inden-1-yl]-5,5-dimethyl-1,3-thiazolidine-4-c arboxamide (three-letter code: 006) (formula: $C_{35}H_{41}N_3O_6S$).
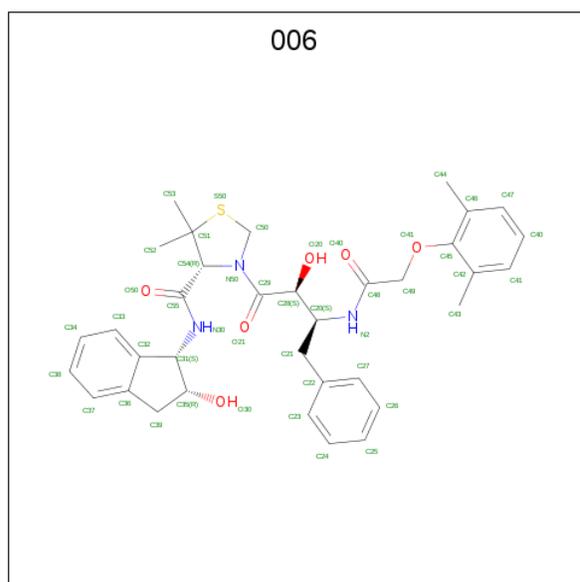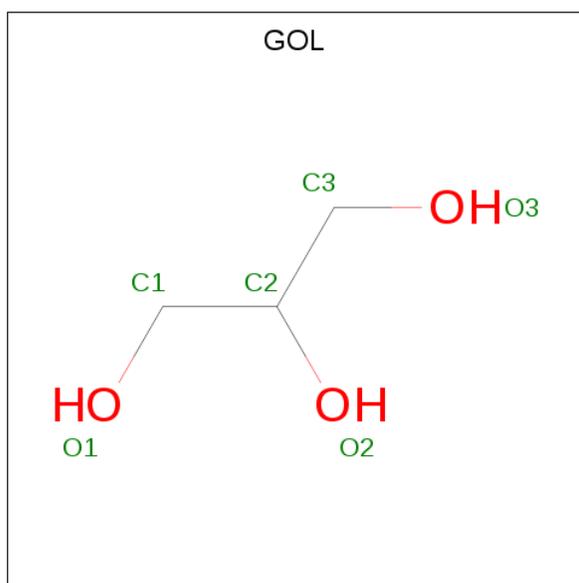

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			45	35	3	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			45	35	3	6	1		
2	C	1	Total	C	N	O	S	0	0
			45	35	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			45	35	3	6	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Plasmepsin-1

- Molecule 1: Plasmepsin-1

L291 N292 K296 F299 T311 V312 F313 N317 H318 K327 K328 LEU

• Molecule 1: Plasmepsin-1

Chain C:

2%
36%   49%   12%

THR GLN LYS PRO HIS LEU GLY ASN ALA G1 D2 S3 V4 T5 L6 N7 D8 V9 A10 N11 V12 M13 Y14 Y15 G16 E17 A18 Q19 I20 G21 D22 N23 K24 Q25 K26 F27 I30 F31 D32 T33 G34 S35 A36 W39 V40 P41 S42 C45 N46 T47 I48 G49 C50 K51 T52 K53 N54

L55 Y56 K60 T63 Y64 E65 K66 D67 V71 E72 M73 N74 Y75 V76 S77 G78 T79 V80 S81 G82 F83 F84 S85 K86 D87 I88 V89 T90 I91 A92 N93 L94 S95 K100 E103 V104 T105 D106 A111 Y112 T113 L114 G115 Q116 V121 G122 L123 D127 S132 V133

V136 E139 L140 K141 N144 K145 I146 E147 Q148 A149 V150 F151 L152 F153 P156 F157 D158 D159 K160 H161 K162 G163 Y164 L165 T166 I167 G168 G169 I170 E171 Y175 Q178 L179 T180 K183 L184 N185 H186 D187 L188 W190 Q191 V192 D193 L197 H198 F199 G201 N203 L205 T206 V207

E208 K209 A210 T211 A212 D215 S216 G217 T218 S219 S220 I221 T222 A223 P224 T225 E226 F227 L228 N229 K230 F231 F232 L235 D236 V237 V238 K239 I240 P241 F242 L243 P243A L244 Y245 I246 C249 N250 N251 P253 K254 L255 L258 E259 F260 R261 T264 N265 V266 Y267 T268 L269 E270 P271 E272

Y273 Y274 Q276 Q277 I278 F278A D279 F279A S280 L281 C282 M283 V284 S285 I286 I287 P288 V289 D290 L291 N292 K296 N297 T298 L301 G302 R307 K308 Y309 F310 T311 V312 N317 H318 T319 F322 A323 L324 K327 K328 LEU

• Molecule 1: Plasmepsin-1

Chain D:

9%
35%   49%   11%

THR GLN LYS PRO HIS LEU GLY ASN ALA G1 D2 S3 V4 T5 L6 N7 D8 V9 A10 N11 V12 M13 Y14 E17 A18 Q19 I20 G21 D22 N23 K24 Q25 K26 F27 I30 F31 D32 T33 G34 S35 A36 N37 L38 W39 V40 P41 S42 A43 Q44 C45 N46 T47 I48 G49 C50 N54 L55

Y56 D57 S58 N59 K60 S61 K62 T63 Y64 K66 D67 V71 E72 M73 V76 S77 G78 T79 V80 S81 G82 F83 F84 S85 K86 D87 I88 V89 T90 I91 L94 S95 F96 P98 Y99 K100 F101 I102 E103 V104 T105 D106 T107 N108 E109B Y112 T113 L114 G115 Q116 F117 I120 V121

G122 L123 G124 W125 K126 D127 S132 V133 V136 L140 K141 N144 K145 I146 E147 Q148 A149 V150 F151 T152 F153 Y154 L155 P156 F157 D158 D159 K160 H161 K162 G163 Y164 L165 T166 I167 G168 G169 E171 D172 R173 F174 Y175 Q178 L179 T180 K183 L184 N185 H186 D187 L188 Q191

V192 D193 L194 D195 L197 H198 F199 G201 N203 L205 T206 V207 E208 K209 A210 T211 A212 D215 S216 G217 T218 S219 S220 I221 T222 A223 P224 T225 E226 F227 L228 N229 K230 F231 V238 K239 I240 P241 F242 L243 P243A L244 Y245 N250 N251 L258 E259 F260 R261 S262 N265 V266 Y267 T268 L269

E270 P271 E272 Y273 Y274 Q277 I278 F278A D279 I279C S280 L281 V284 I287 P288 V289 D290 L291 N292 K296 N297 T298 F299 I300 L301 G302 D303 P304 H305 M306 R307 K308 Y309 F310 T311 V312 F313 N317 H318 T319 F322 A323 L324 A325 K326 K327 K328 LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	93.69Å 93.69Å 160.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 29.63 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.10) 99.1 (29.63-3.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.5.0104	Depositor
R, R_{free}	0.211 , 0.300 0.210 , 0.298	Depositor DCC
R_{free} test set	1240 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	78.9	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10646	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 006

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	1.03	3/2670 (0.1%)	1.06	4/3627 (0.1%)
1	B	0.97	2/2670 (0.1%)	1.01	2/3627 (0.1%)
1	C	0.97	2/2665 (0.1%)	0.99	2/3620 (0.1%)
1	D	0.97	0/2665	0.98	3/3620 (0.1%)
All	All	0.98	7/10670 (0.1%)	1.01	11/14494 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	4
1	C	0	2
1	D	0	1
All	All	0	8

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	GLU	CB-CG	6.42	1.64	1.52
1	A	226	GLU	CG-CD	6.05	1.61	1.51
1	C	72	GLU	CG-CD	5.36	1.59	1.51
1	B	9	VAL	CB-CG1	-5.12	1.42	1.52
1	B	158	ASP	CB-CG	5.12	1.62	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	LEU	CB-CG-CD2	-12.98	88.94	111.00
1	A	205	LEU	CB-CG-CD2	-10.89	92.49	111.00
1	A	283	MET	CG-SD-CE	-9.83	84.47	100.20
1	A	205	LEU	CB-CG-CD1	8.76	125.89	111.00
1	D	209	LYS	CD-CE-NZ	-7.20	95.14	111.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	LYS	Peptide
1	B	157	PHE	Peptide
1	B	158	ASP	Peptide
1	B	160	LYS	Peptide
1	B	296	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2604	0	2535	161	0
1	B	2604	0	2535	149	0
1	C	2599	0	2530	196	0
1	D	2599	0	2530	234	0
2	A	45	0	41	6	0
2	B	45	0	41	3	0
2	C	45	0	41	5	0
2	D	45	0	41	1	0
3	A	18	0	24	7	0
3	B	12	0	16	1	0
3	C	18	0	24	23	0
3	D	12	0	16	20	0
All	All	10646	0	10374	711	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 34.

The worst 5 of 711 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ASN:CB	3:A:331:GOL:H32	1.72	1.17
1:A:292:ASN:HB3	3:A:331:GOL:H32	1.16	1.14
1:D:20:ILE:HD11	1:D:87:ASP:HB3	1.32	1.11
3:C:331:GOL:C1	1:D:242:PHE:HA	1.80	1.10
1:B:240:ILE:HD11	1:B:243:LEU:HD12	1.28	1.09

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	325/336 (97%)	286 (88%)	31 (10%)	8 (2%)	5	27
1	B	325/336 (97%)	286 (88%)	31 (10%)	8 (2%)	5	27
1	C	324/336 (96%)	273 (84%)	45 (14%)	6 (2%)	8	33
1	D	324/336 (96%)	261 (81%)	55 (17%)	8 (2%)	5	27
All	All	1298/1344 (97%)	1106 (85%)	162 (12%)	30 (2%)	6	28

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	201	GLY
1	B	158	ASP
1	C	2	ASP
1	C	161	HIS

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	288/296 (97%)	218 (76%)	70 (24%)	0	2
1	B	288/296 (97%)	221 (77%)	67 (23%)	1	3
1	C	288/296 (97%)	226 (78%)	62 (22%)	1	4
1	D	288/296 (97%)	230 (80%)	58 (20%)	1	5
All	All	1152/1184 (97%)	895 (78%)	257 (22%)	1	3

5 of 257 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	236	ASP
1	C	46	ASN
1	D	229	ASN
1	B	244	LEU
1	B	285	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	292	ASN
1	C	116	GLN
1	D	203	ASN
1	C	11	ASN
1	C	148	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	GOL	A	332	-	5,5,5	0.49	0	5,5,5	0.77	0
2	006	D	330	-	49,49,49	1.54	5 (10%)	64,71,71	1.55	10 (15%)
2	006	A	330	-	49,49,49	1.74	9 (18%)	64,71,71	2.37	24 (37%)
2	006	C	330	-	49,49,49	1.55	6 (12%)	64,71,71	2.17	21 (32%)
3	GOL	B	332	-	5,5,5	0.45	0	5,5,5	0.40	0
3	GOL	B	331	-	5,5,5	0.37	0	5,5,5	0.89	0
3	GOL	C	333	-	5,5,5	0.32	0	5,5,5	0.70	0
3	GOL	D	331	-	5,5,5	0.51	0	5,5,5	0.62	0
3	GOL	A	333	-	5,5,5	0.38	0	5,5,5	0.85	0
3	GOL	A	331	-	5,5,5	0.53	0	5,5,5	0.76	0
3	GOL	C	331	-	5,5,5	0.45	0	5,5,5	0.77	0
3	GOL	D	332	-	5,5,5	0.54	0	5,5,5	0.52	0
3	GOL	C	332	-	5,5,5	0.50	0	5,5,5	1.01	0
2	006	B	330	-	49,49,49	1.52	7 (14%)	64,71,71	1.76	19 (29%)

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
3	GOL	A	332	-	-	3/4/4/4	-
2	006	D	330	-	-	3/33/61/61	0/5/5/5
2	006	A	330	-	-	4/33/61/61	0/5/5/5
2	006	C	330	-	-	4/33/61/61	0/5/5/5
3	GOL	B	332	-	-	3/4/4/4	-
3	GOL	B	331	-	-	4/4/4/4	-
3	GOL	C	333	-	-	0/4/4/4	-
3	GOL	D	331	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	333	-	-	4/4/4/4	-
3	GOL	A	331	-	-	0/4/4/4	-
3	GOL	C	331	-	-	4/4/4/4	-
3	GOL	D	332	-	-	4/4/4/4	-
3	GOL	C	332	-	-	2/4/4/4	-
2	006	B	330	-	-	7/33/61/61	0/5/5/5

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	330	006	C28-C29	-5.89	1.47	1.53
2	B	330	006	C51-S50	-5.39	1.74	1.85
2	A	330	006	C28-C29	-5.34	1.48	1.53
2	D	330	006	C51-S50	-5.05	1.75	1.85
2	D	330	006	C28-C29	-4.65	1.49	1.53

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	330	006	C39-C35-C31	7.59	110.27	103.78
2	B	330	006	C36-C39-C35	-6.35	97.40	103.50
2	C	330	006	C39-C35-C31	6.29	109.16	103.78
2	A	330	006	C21-C20-N2	-6.09	101.19	110.07
2	C	330	006	C20-N2-C48	-6.07	113.26	123.48

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	332	GOL	C1-C2-C3-O3
2	A	330	006	N2-C20-C28-O20
2	A	330	006	C21-C20-C28-O20
2	A	330	006	C21-C20-C28-C29
2	C	330	006	C21-C20-C28-O20

There are no ring outliers.

10 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	330	006	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	330	006	6	0
2	C	330	006	5	0
3	B	331	GOL	1	0
3	C	333	GOL	4	0
3	D	331	GOL	19	0
3	A	331	GOL	7	0
3	C	331	GOL	19	0
3	D	332	GOL	1	0
2	B	330	006	3	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 then 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 006 D 330

Bond lengths

Bond angles

Torsions

Rings

Ligand 006 A 330

Bond lengths

Bond angles

Torsions

Rings

Ligand 006 C 330

Bond lengths

Bond angles

Torsions

Rings

Ligand 006 B 330

Bond lengths

Bond angles

Torsions

Rings
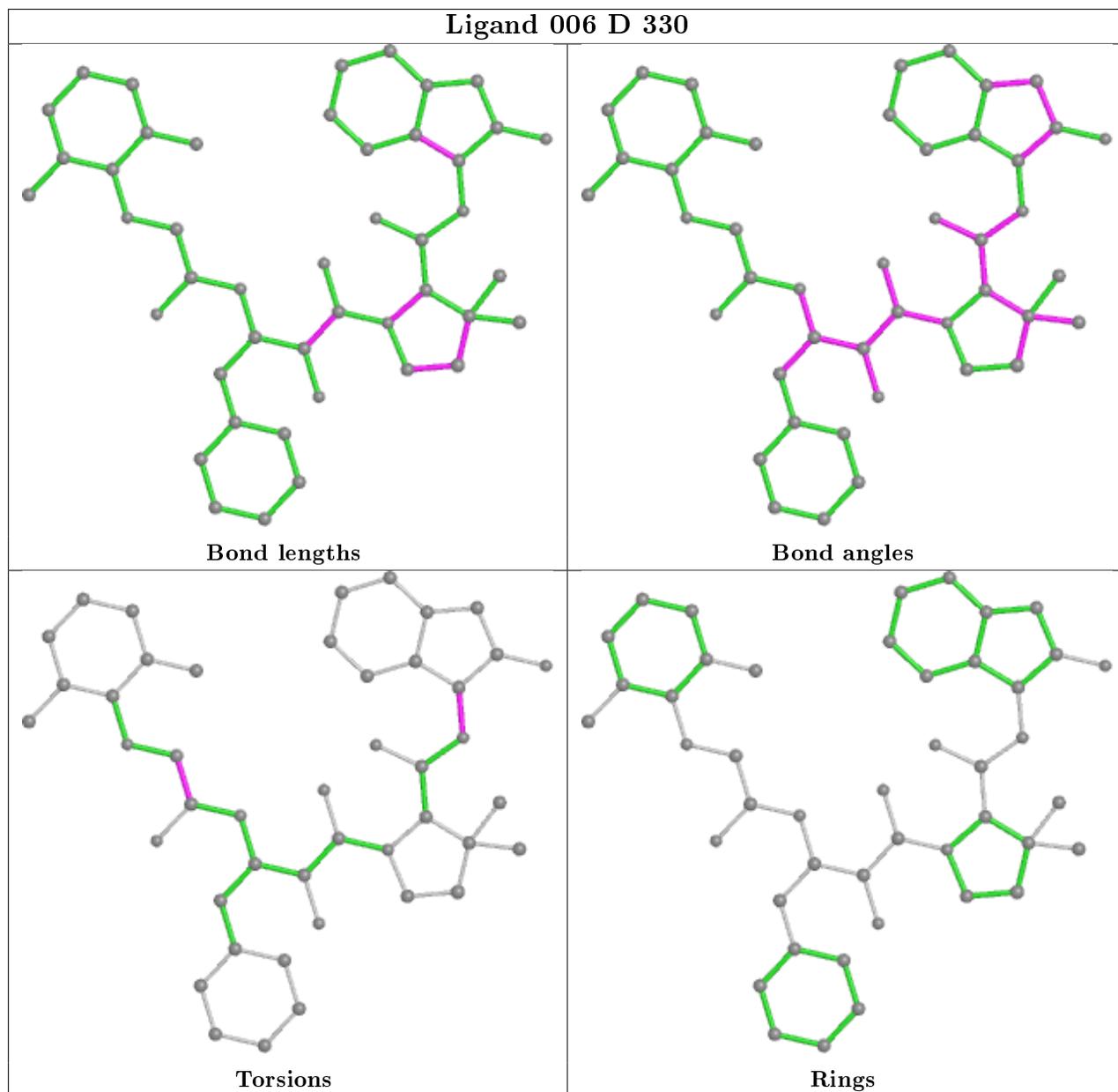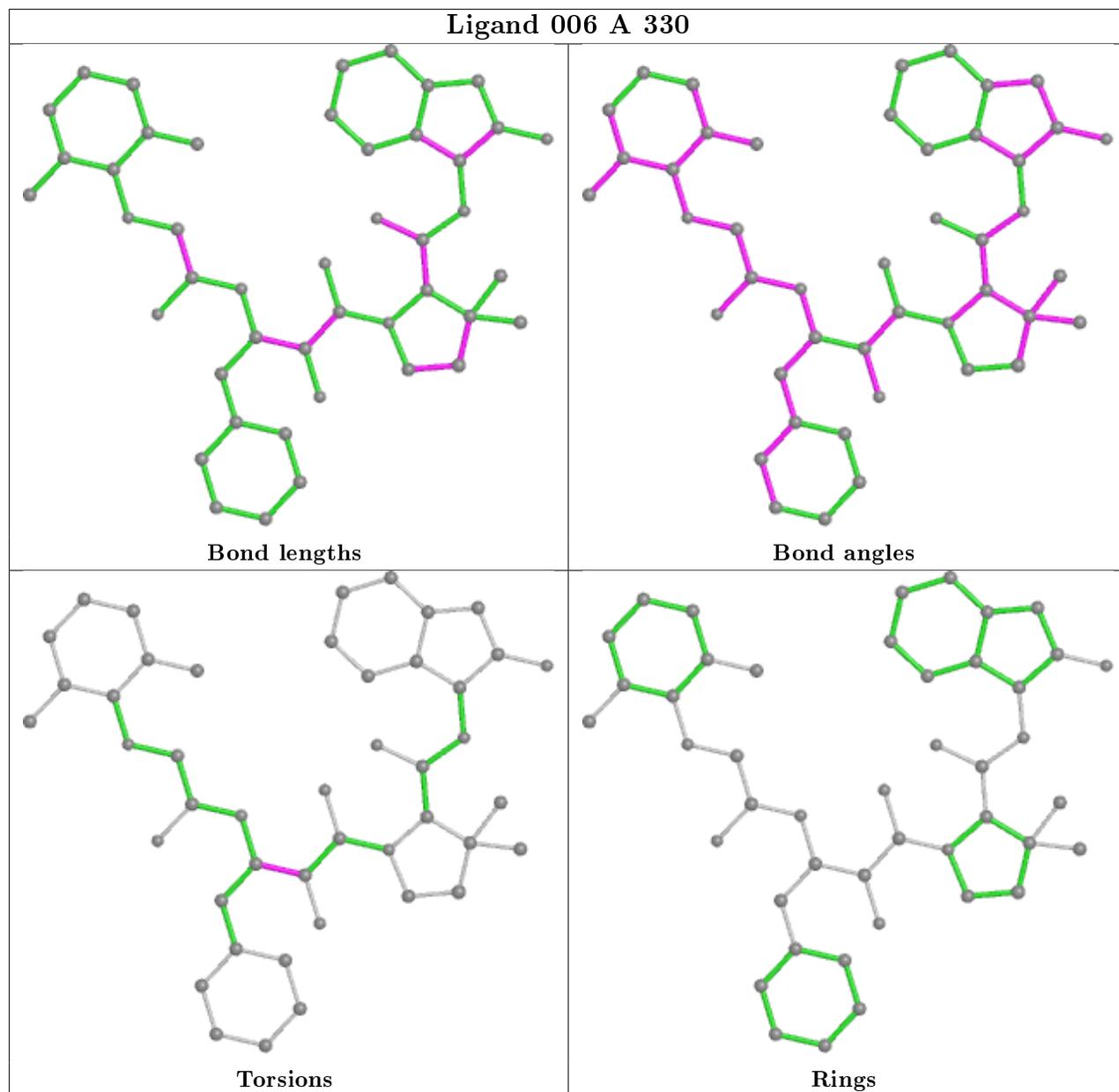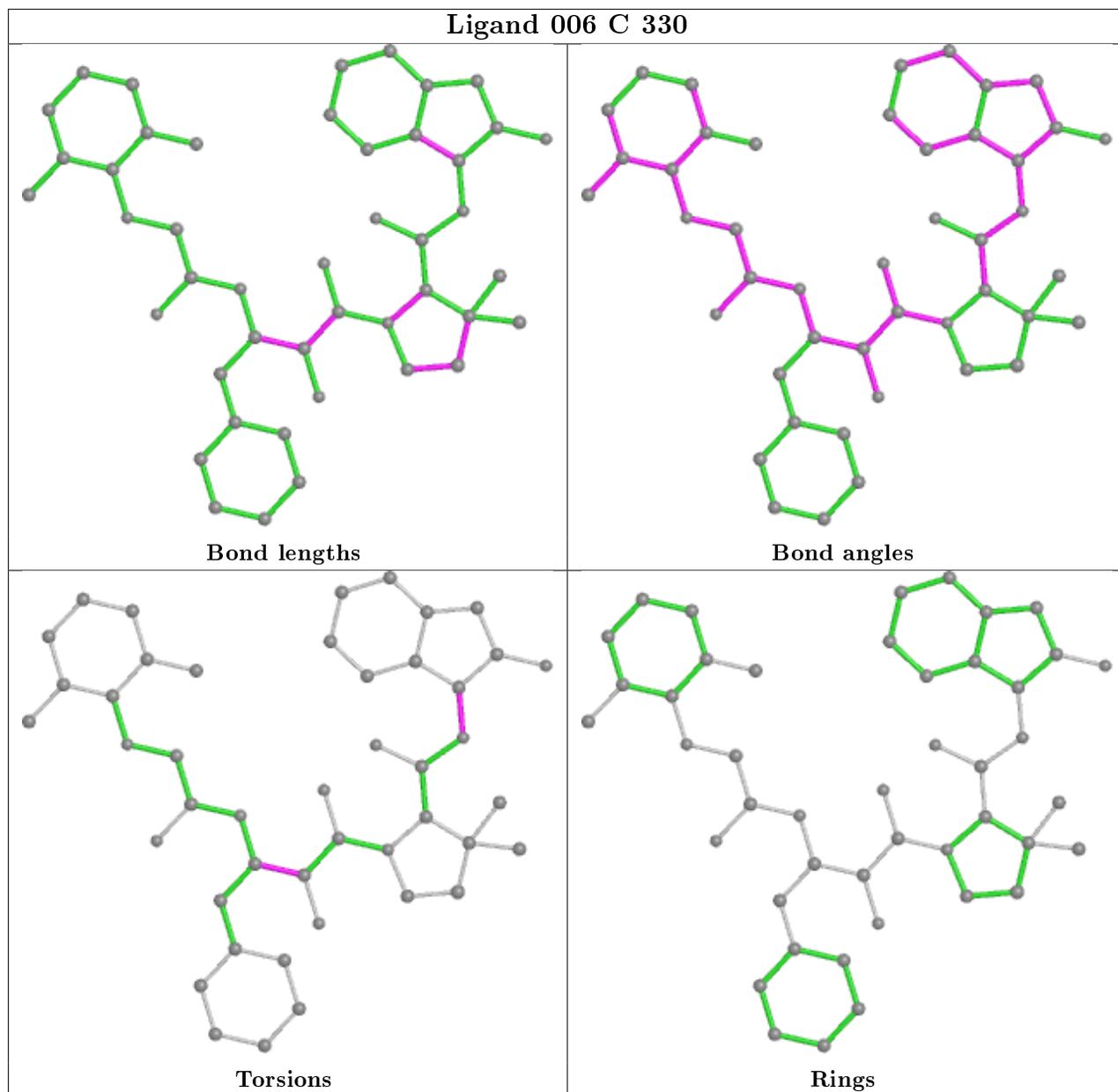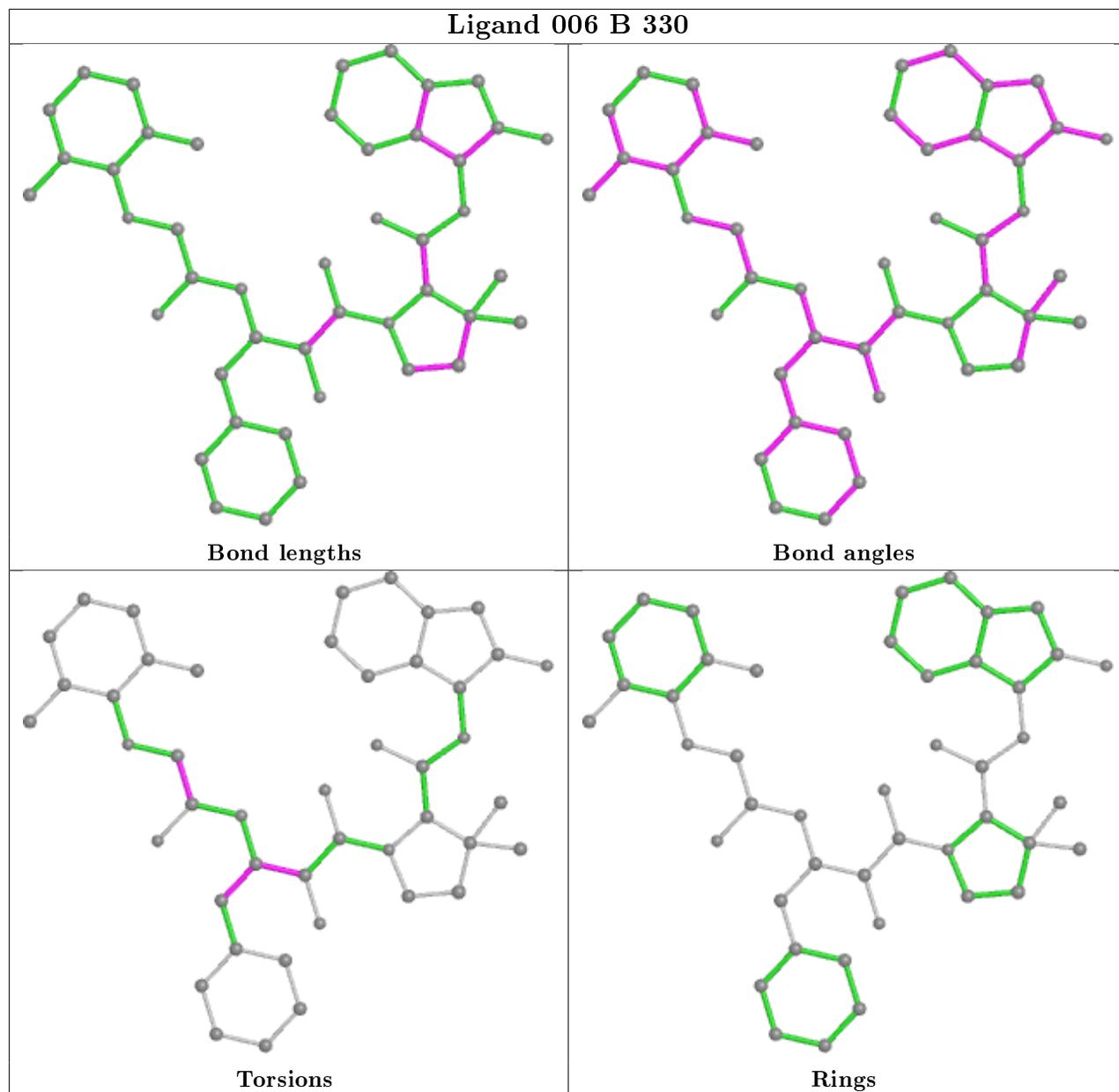
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	327/336 (97%)	-0.22	6 (1%)	68	47	57, 72, 96, 163	0
1	B	327/336 (97%)	-0.20	4 (1%)	79	61	56, 78, 102, 158	0
1	C	326/336 (97%)	-0.06	7 (2%)	63	43	63, 85, 109, 154	0
1	D	326/336 (97%)	0.36	29 (8%)	9	3	56, 101, 121, 307	0
All	All	1306/1344 (97%)	-0.03	46 (3%)	44	23	56, 83, 115, 307	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	46	ASN	4.9
1	D	169	GLY	4.4
1	D	57	ASP	4.2
1	B	216	SER	4.1
1	D	58	SER	3.4

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 carbohydrates 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(Å²)	Q<0.9
3	GOL	A	332	6/6	0.75	0.34	77,85,88,91	0
3	GOL	D	332	6/6	0.78	0.62	86,89,90,91	0
3	GOL	C	331	6/6	0.80	0.74	94,96,100,103	0
3	GOL	A	331	6/6	0.81	0.27	86,92,92,92	0
3	GOL	C	332	6/6	0.82	0.26	83,85,86,86	0
3	GOL	D	331	6/6	0.85	0.21	87,90,90,90	0
3	GOL	B	331	6/6	0.86	0.28	81,82,84,84	0
2	006	D	330	45/45	0.86	0.26	102,107,125,126	0
3	GOL	C	333	6/6	0.87	0.43	97,97,98,98	0
3	GOL	B	332	6/6	0.87	0.41	88,89,91,93	0
3	GOL	A	333	6/6	0.88	0.19	88,88,90,90	0
2	006	C	330	45/45	0.92	0.25	64,69,84,87	0
2	006	A	330	45/45	0.93	0.24	58,64,88,92	0
2	006	B	330	45/45	0.93	0.23	61,74,90,91	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
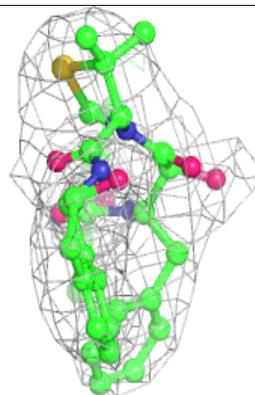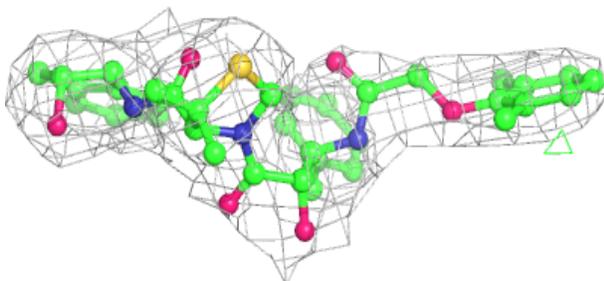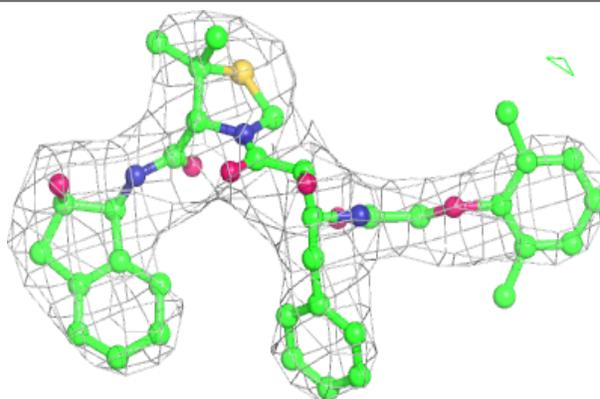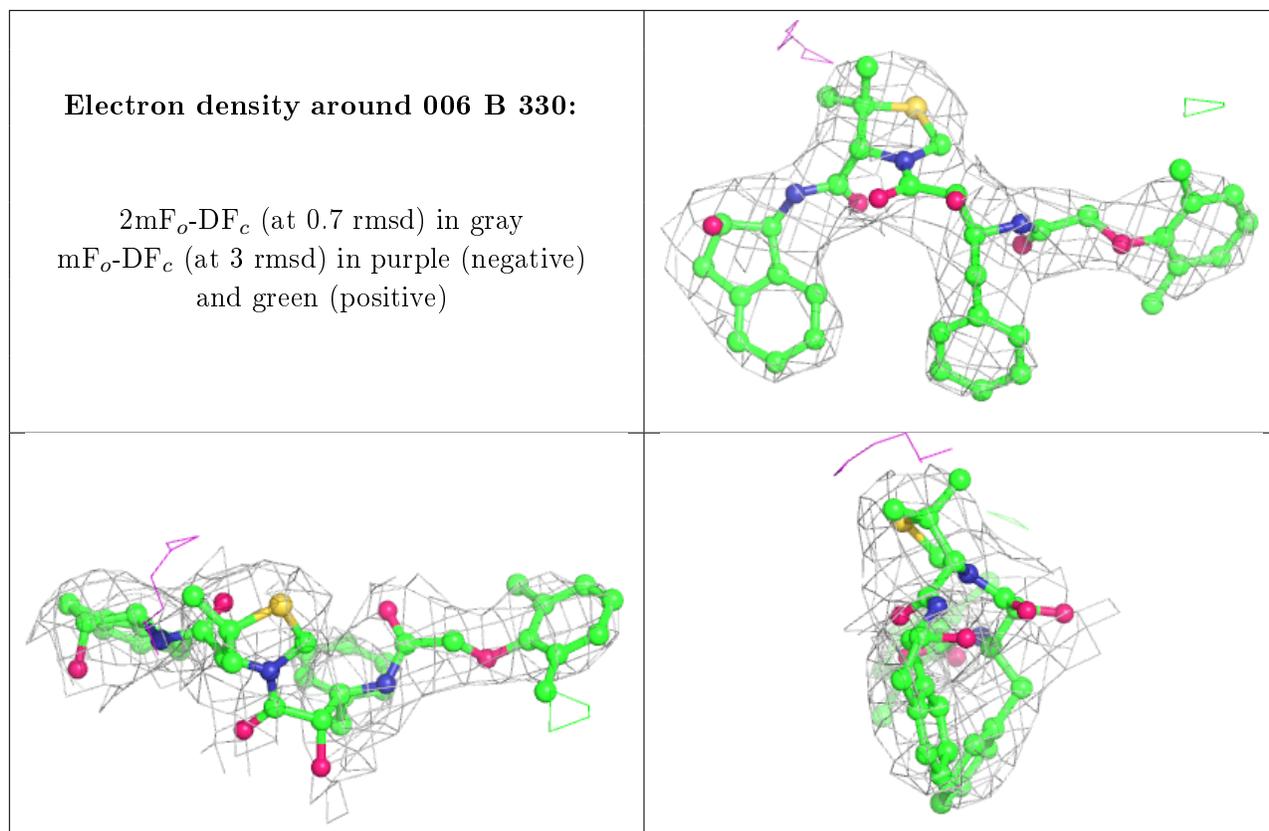
Electron density around 006 D 330:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
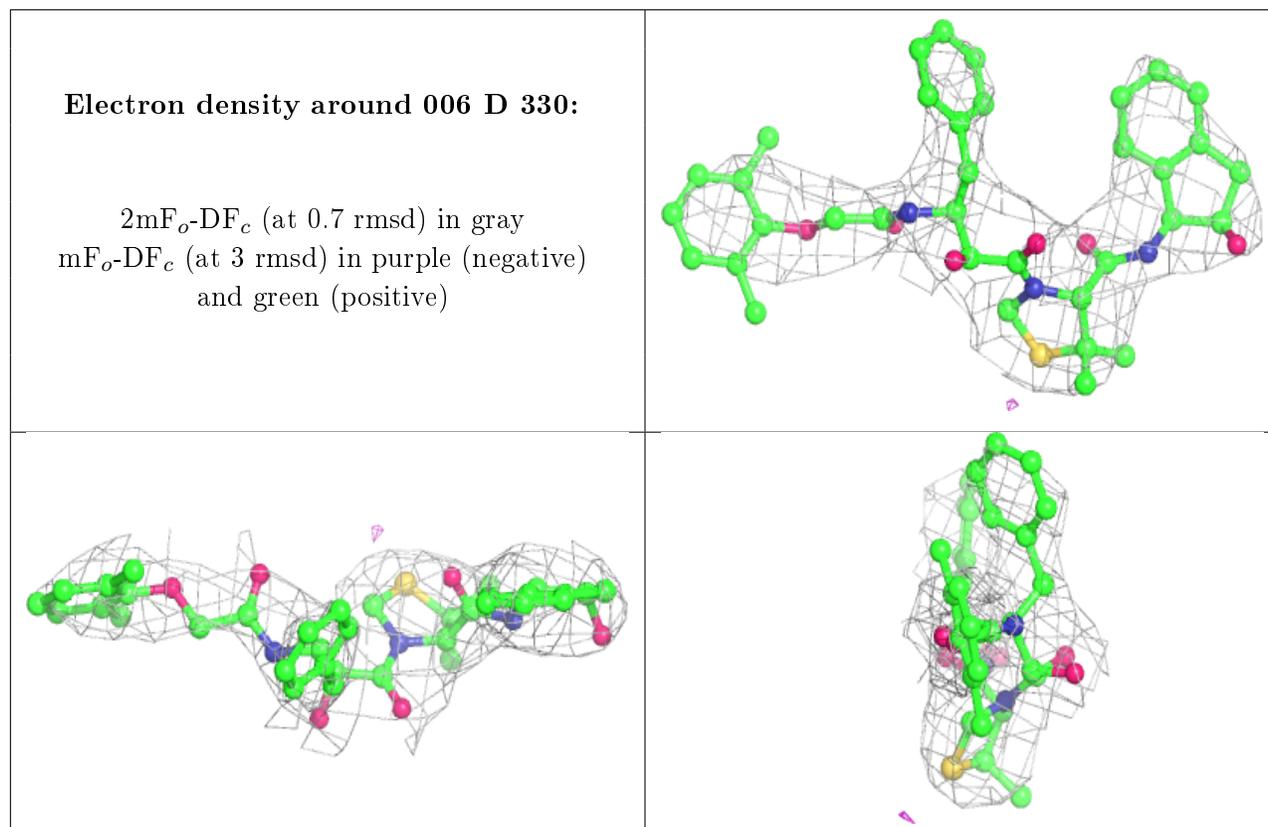
Electron density around 006 C 330:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
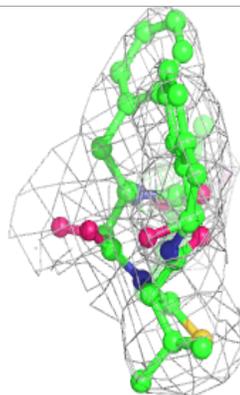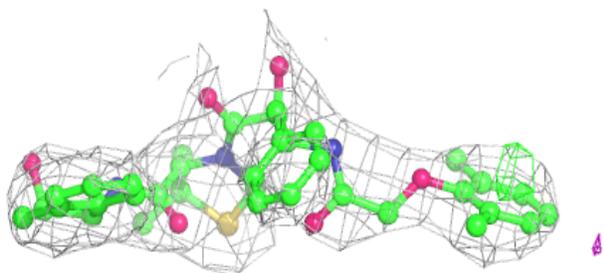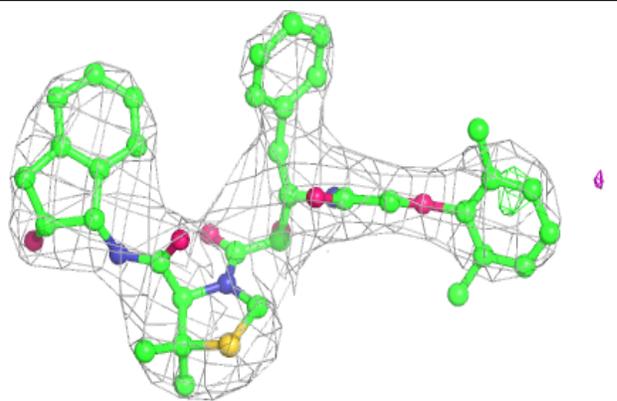
Electron density around 006 A 330:

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

Electron density around 006 B 330:

$2mF_o$-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.