



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 04:44 PM UTC

PDB ID : 1XPU / pdb_00001xpu
Title : Structural mechanism of inhibition of the Rho transcription termination factor by the antibiotic 5a-(3-formylphenylsulfanyl)-dihydrobicyclomycin (FPDB)
Authors : Skordalakes, E.; Brogan, A.P.; Park, B.S.; Kohn, H.; Berger, J.M.
Deposited on : 2004-10-09
Resolution : 3.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

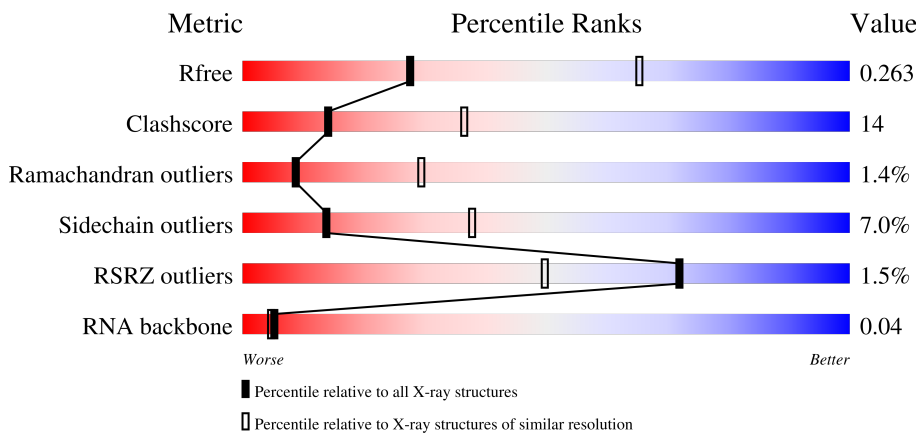
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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.



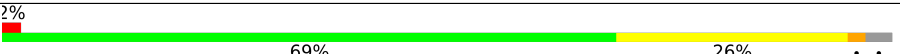
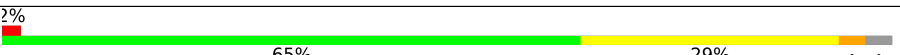
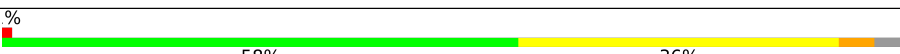
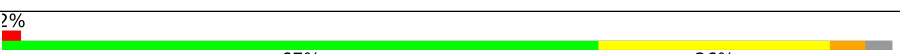
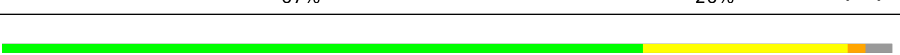
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)
RNA backbone	3983	1079 (3.30-2.82)

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 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	G	8	12% 25% 75%
1	H	8	12% 12% 75%
1	J	8	12% 12% 75%
1	K	8	25% 75%

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Mol	Chain	Length	Quality of chain
1	L	8	
1	M	8	
2	A	419	
2	B	419	
2	C	419	
2	D	419	
2	E	419	
2	F	419	

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
4	AGS	E	5600	-	-	X	-
5	FPD	C	3701	-	-	X	-
5	FPD	E	5701	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19873 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 RNA chain called 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	M	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	H	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	J	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	K	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	L	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			

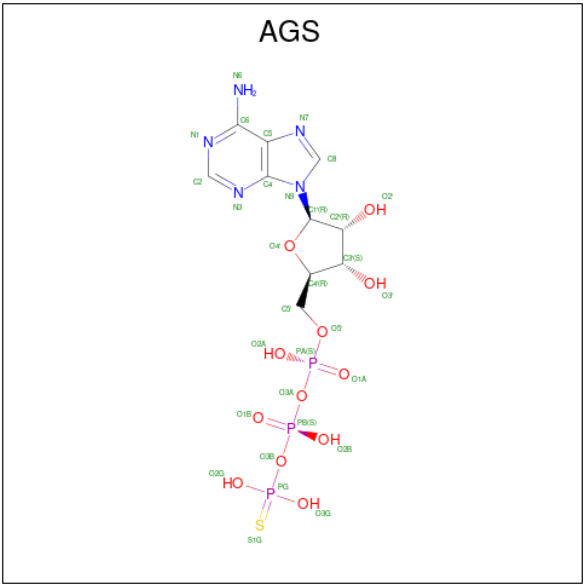
- Molecule 2 is a protein called Rho transcription termination factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	B	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	C	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	D	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	E	407	Total	C	N	O	S	0	0	0
			3206	2023	563	603	17			
2	F	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



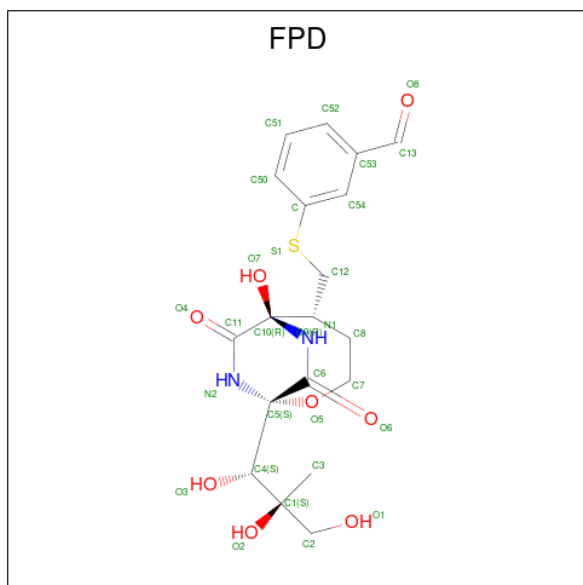
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 5 is 5A-(3-FORMYLPHENYLSULFANYL)-DIHYDROBICYCLOMYCIN (CCD ID: FPD) (formula: $C_{19}H_{24}N_2O_8S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	S		0	0
			30	19	2	8	1			
5	C	1	Total	C	N	O	S		0	0
			30	19	2	8	1			
5	D	1	Total	C	N	O	S		0	0
			30	19	2	8	1			
5	E	1	Total	C	N	O	S		0	0
			30	19	2	8	1			
5	F	1	Total	C	N	O	S		0	0
			30	19	2	8	1			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total 1 O	0	0
6	H	1	Total 1 O	0	0
6	A	2	Total 2 O	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	5	Total 5	O 5	0	0
6	C	3	Total 3	O 3	0	0
6	D	4	Total 4	O 4	0	0
6	E	3	Total 3	O 3	0	0
6	F	1	Total 1	O 1	0	0

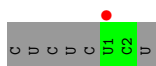
3 Residue-property plots [i](#)

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: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'



Chain A:

Position	Amino Acid	Conservation Level
1	M1	High
4	T4	High
7	K7	High
8	H8	High
9	T9	High
10	P10	High
14	L14	High
19	L39	High
20	K40	High
21	Q41	High
22	H42	High
23	A43	High
24	K44	High
25	S45	High
26	G46	High
27	E47	High
28	D48	High
29	I49	High
36	E56	High
41	F62	High
42	G63	High
43	F64	High
44	L65	High
45	I79	High
46	I86	High
47	F89	High
48	N90	High
49	L91	High
50	R92	High
51	T93	High
52	I101	High
53	R102	High
54	L113	High
55	L114	High
56	K115	High
57	V116	High
58	M117	High
59	E118	High
60	V119	High
61	N120	High
62	R126	High
63	ALA	Non-conserved
64	ARG	Non-conserved
65	N129	High
66	K130	High
67	I131	High
68	L132	High
69	F132	High
70	E134	High
71	N135	High
72	L136	High
73	T137	High
74	P138	High
75	L139	High
76	H140	High
77	R144	High
78	L145	High
79	L146	High
80	M147	High
81	GLU	High
82	ARG	Non-conserved
83	GLY	Non-conserved
84	ASN	High
85	G152	High
86	S153	High
87	R160	High
88	V161	High
89	L162	High
90	D163	High
91	P167	High
92	I168	High
93	G169	High
94	R170	High
95	G171	High
96	Q172	High
97	R173	High
98	G183	High
99	S194	High
100	M198	High
101	L208	High
102	I209	High
103	D210	High
104	E214	High
105	E218	High
106	M219	High
107	F232	High
108	D233	High
109	E234	High
110	P235	High
111	A236	High
112	S237	High
113	R238	High
114	H239	High
115	E244	High
116	I247	High
117	A250	High
118	K251	High
119	R252	High
120	L253	High
121	V254	High
122	E255	High
123	H256	High
124	D265	High
125	S266	High
126	T267	High
127	T268	High
128	R269	High
129	R272	High
130	A280	High
131	SER	Non-conserved
132	GLY	Non-conserved
133	LYS	Non-conserved
134	V284	High
135	V289	High
136	L294	High
137	H295	High
138	R296	High
139	P297	High
140	K298	High
141	R299	High
142	F300	High
143	F301	High
144	A304	High
145	R305	High
146	N306	High
147	V307	High
148	E308	High
149	E309	High
150	T314	High
151	T318	High
152	M327	High
153	L331	High
154	E334	High
155	F336	High
156	G339	High
157	N340	High
158	M341	High
159	E342	High
160	L343	High
161	H344	High
162	L345	High
163	T346	High

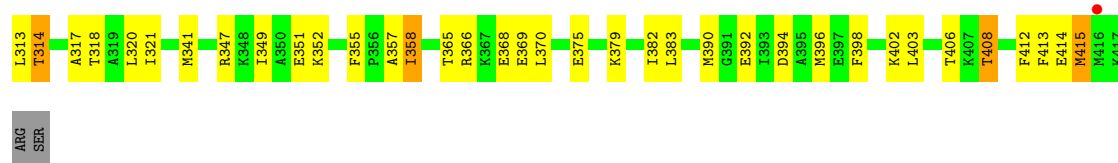
Chain B:

2% 69% 26%

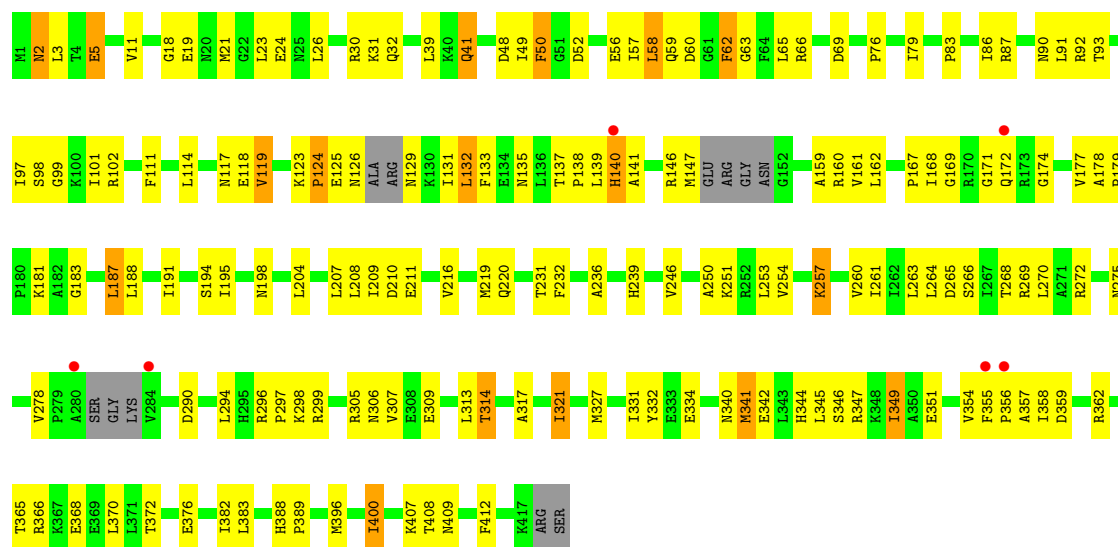
M1 N2 L3 K7 G18 E19 N21 N20 L23 E24 L26 N29 R30 K31 I35 F36 Q41 H42 K44 I49 F50 G51 I57 L58 Q59 L65 S71 D77 D78 I79 I86 R90 T93 S98 P104 E108 R109 Y110 E118 N126 A130 ARG I131 L132 F133 L139 H140 A141 M142 N143 R144 L145 R146 H147 GLU ARG GLY ASN G152 D156 A157 T158 A159 R160 V161 P167 I168 G169 R170 G171 Q172 R173 I176 K181 A182 G183 K184 L187 Q193 L207 L208 E211 R212 V216 Q220 V228 T231 V242 A243 E244 M245 V246 I247 E248 K249 A250 K251 R252 L253 V254 D255 S266 S267 T267 T268 R269 A280 SER GLY LYS V284 R299 F300 A304 E309 L313 T314 T318 A319 L320 I331 G337 M341 E342 L343 H344 L345 S346 T349 A350 E351 F352 P353 V354 F355 P356 A357 I358 R366 L370 Q378 K379 I382 L383 R384 K385 I386 I387 H388 P389 E392 I393 M396 L399 I400 L403 T408 F412 F413 E414 K417 ARG SER

Chain C:

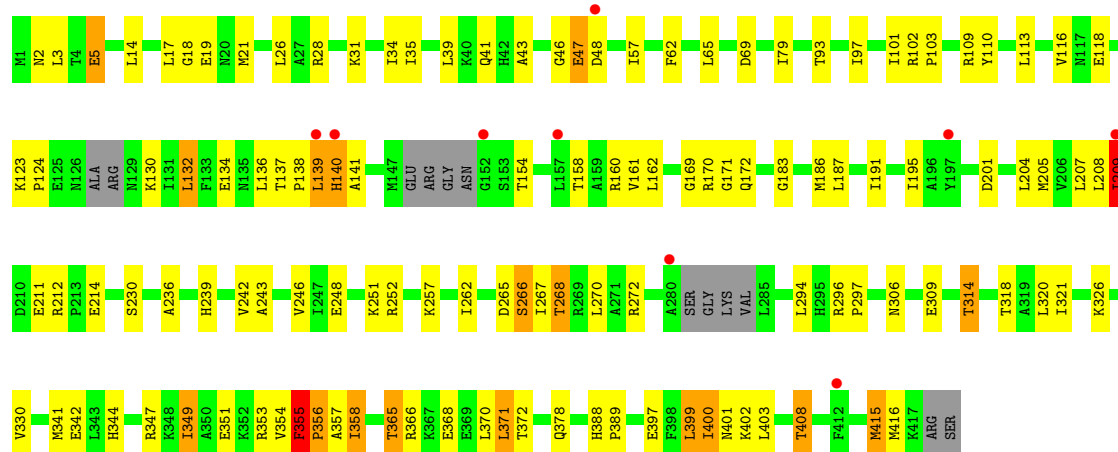
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M1	Green	K115	Green	E211	Green	M2	Green	V116	Green	R212	Green	E214	Red	E218	Green
L3	Green	K123	Green	P213	Green	L4	Green	A125	Green	E219	Green	E220	Green	E224	Green
L14	Green	K126	Green	P124	Green	L23	Green	A126	Green	E225	Green	E226	Green	E230	Green
L26	Green	ALA	Green	E125	Green	L26	Green	ARG	Grey	E227	Green	E228	Green	E232	Green
M29	Green	N129	Green	E126	Green	M29	Green	N130	Green	E229	Green	E231	Green	E235	Green
D33	Green	K130	Green	E129	Green	D33	Green	K131	Green	E233	Green	E236	Green	E240	Green
I34	Green	I131	Green	E130	Green	I34	Green	I132	Green	E237	Green	E241	Green	E245	Green
I38	Green	F133	Green	E131	Green	I38	Green	F133	Green	E238	Green	E242	Green	E249	Green
I39	Green	T137	Green	E132	Green	I39	Green	T137	Green	E239	Green	E243	Green	E253	Green
K40	Green	P138	Green	E133	Green	K40	Green	P138	Green	E240	Green	E244	Green	E257	Green
Q41	Green	L139	Green	E134	Green	Q41	Green	L139	Green	E241	Green	E245	Green	E261	Green
G46	Green	H140	Green	E135	Green	G46	Green	H140	Green	E242	Green	E246	Green	E265	Green
E47	Red	A141	Orange	E136	Green	E47	Red	A141	Orange	E243	Green	E247	Green	E266	Green
D48	Red	S143	Yellow	E137	Green	D48	Red	S143	Yellow	E244	Green	E248	Green	E272	Green
I49	Green	G147	Green	E138	Green	I49	Green	G147	Green	E245	Green	E249	Green	E275	Green
F50	Green	GLU	Green	E139	Green	F50	Green	GLU	Green	E246	Green	E250	Green	E278	Green
G51	Green	ARG	Grey	E140	Green	G51	Green	ARG	Grey	E247	Green	E251	Green	E279	Green
L55	Green	GLY	Grey	E141	Green	L55	Green	GLY	Grey	E248	Green	E252	Green	E280	Green
L58	Orange	ASN	Green	E142	Green	L58	Orange	ASN	Green	E249	Green	E253	Green	E281	Green
Q59	Yellow	G152	Green	E143	Green	Q59	Yellow	G152	Green	E250	Green	E254	Green	E282	Green
P64	Yellow	R160	Green	E144	Green	P64	Yellow	R160	Green	E251	Green	E255	Green	E283	Green
L65	Yellow	V161	Green	E145	Green	L65	Yellow	V161	Green	E252	Green	E256	Green	E284	Green
R66	Yellow	L162	Green	E146	Green	R66	Yellow	L162	Green	E253	Green	E257	Green	E285	Green
D69	Green	P167	Yellow	E147	Green	D69	Green	P167	Yellow	E254	Green	E258	Green	E286	Green
I79	Green	R170	Green	E148	Green	I79	Green	R170	Green	E255	Green	E259	Green	E287	Green
I86	Green	Q171	Green	E149	Green	I86	Green	Q171	Green	E256	Green	E260	Green	E288	Green
L91	Green	L176	Green	E150	Green	L91	Green	L176	Green	E257	Green	E261	Green	E289	Green
R92	Green	V177	Green	E151	Green	R92	Green	V177	Green	E258	Green	E262	Green	E290	Green
T93	Green	A178	Grey	E152	Green	T93	Green	A178	Grey	E259	Green	E263	Green	E291	Green
I97	Green	P179	Green	E153	Green	I97	Green	P179	Green	E260	Green	E264	Green	E292	Green
K100	Green	G183	Green	E154	Green	K100	Green	G183	Green	E261	Green	E265	Green	E293	Green
I101	Green	K184	Green	E155	Green	I101	Green	K184	Green	E262	Green	E266	Green	E294	Green
E106	Red	T185	Yellow	E156	Green	E106	Red	T185	Yellow	E263	Green	E267	Green	E295	Green
G107	Green	M186	Yellow												



• Molecule 2: Rho transcription termination factor

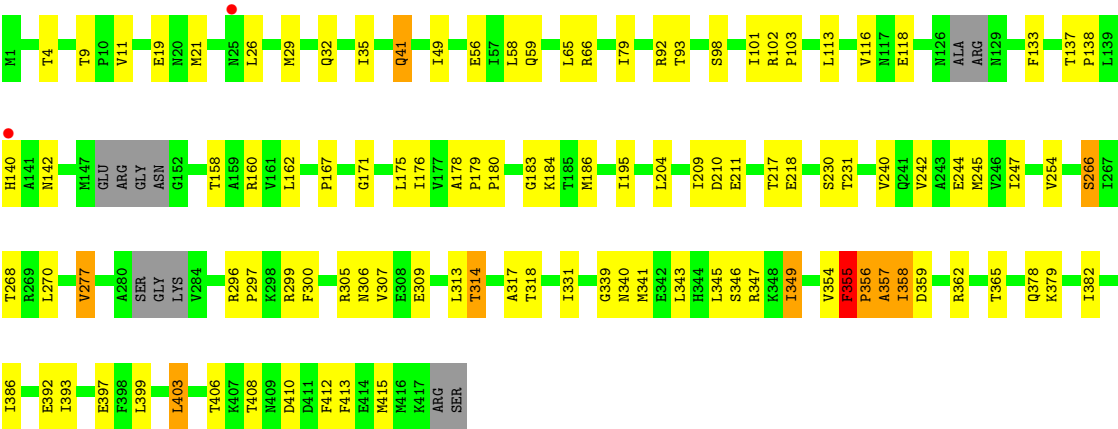


• Molecule 2: Rho transcription termination factor



• Molecule 2: Rho transcription termination factor





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.48Å 206.94Å 148.61Å 90.00° 96.95° 90.00°	Depositor
Resolution (Å)	20.00 – 3.05 20.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	86.5 (20.00-3.05) 82.8 (20.00-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.276 , 0.295 0.268 , 0.263	Depositor DCC
R_{free} test set	3105 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	92.4	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19873	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: AGS, MG, FPD

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	G	0.64	0/43	1.08	0/64
1	H	0.79	0/43	1.32	0/64
1	J	0.60	0/43	0.89	0/64
1	K	0.84	0/43	1.33	0/64
1	L	0.58	0/43	0.85	0/64
1	M	0.73	0/43	0.94	0/64
2	A	0.40	0/3259	0.81	0/4387
2	B	0.42	0/3259	0.84	0/4387
2	C	0.41	0/3259	0.82	0/4387
2	D	0.41	0/3259	0.82	0/4387
2	E	0.40	0/3252	0.84	3/4377 (0.1%)
2	F	0.41	0/3259	0.80	0/4387
All	All	0.41	0/19805	0.83	3/26696 (0.0%)

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
2	A	0	1
2	E	0	1
2	F	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	355	PHE	CB-CA-C	7.38	121.02	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	355	PHE	N-CA-C	5.82	117.29	110.31
2	E	209	ILE	N-CA-C	5.10	116.56	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	355	PHE	Peptide
2	E	355	PHE	Peptide
2	F	355	PHE	Peptide

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	G	40	0	22	0	0
1	H	40	0	22	2	0
1	J	40	0	22	2	0
1	K	40	0	22	3	0
1	L	40	0	22	1	0
1	M	40	0	22	0	0
2	A	3213	0	3289	110	0
2	B	3213	0	3288	81	0
2	C	3213	0	3289	88	0
2	D	3213	0	3289	124	0
2	E	3206	0	3279	92	0
2	F	3213	0	3288	67	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	31	0	12	4	0
4	B	31	0	12	6	0
4	C	31	0	12	7	0
4	D	31	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	62	0	24	16	0
5	B	30	0	24	6	0
5	C	30	0	24	9	0
5	D	30	0	24	8	0
5	E	30	0	24	10	0
5	F	30	0	24	3	0
6	A	2	0	0	0	0
6	B	5	0	0	1	0
6	C	3	0	0	0	0
6	D	4	0	0	1	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
All	All	19873	0	20046	570	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 14.

The worst 5 of 570 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)
2:C:366:ARG:NE	4:D:4600:AGS:S1G	2.12	1.22
2:A:366:ARG:NE	4:B:2600:AGS:S1G	2.13	1.20
2:D:356:PRO:HG3	2:D:400:ILE:HD11	1.26	1.15
2:B:366:ARG:NE	4:C:3600:AGS:S1G	2.23	1.11
2:D:366:ARG:NE	4:E:5600:AGS:S1G	2.24	1.11

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	
2	A	400/419 (96%)	368 (92%)	25 (6%)	7 (2%)	6	24
2	B	400/419 (96%)	366 (92%)	32 (8%)	2 (0%)	24	52
2	C	400/419 (96%)	364 (91%)	29 (7%)	7 (2%)	6	24
2	D	400/419 (96%)	358 (90%)	37 (9%)	5 (1%)	9	31
2	E	399/419 (95%)	368 (92%)	25 (6%)	6 (2%)	8	28
2	F	400/419 (96%)	366 (92%)	28 (7%)	6 (2%)	8	28
All	All	2399/2514 (95%)	2190 (91%)	176 (7%)	33 (1%)	9	29

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	47	GLU
2	C	140	HIS
2	E	356	PRO
2	E	358	ILE
2	F	355	PHE

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	
2	A	351/359 (98%)	327 (93%)	24 (7%)	14	39
2	B	351/359 (98%)	328 (93%)	23 (7%)	15	40
2	C	351/359 (98%)	322 (92%)	29 (8%)	10	32
2	D	351/359 (98%)	328 (93%)	23 (7%)	15	40
2	E	350/359 (98%)	322 (92%)	28 (8%)	11	33
2	F	351/359 (98%)	331 (94%)	20 (6%)	18	45
All	All	2105/2154 (98%)	1958 (93%)	147 (7%)	14	38

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	314	THR

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Mol	Chain	Res	Type
2	F	358	ILE
2	E	371	LEU
2	F	32	GLN
2	C	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	409	ASN
2	D	306	ASN
2	D	41	GLN
2	D	129	ASN
2	E	41	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	G	2/8 (25%)	1 (50%)	1 (50%)
1	H	2/8 (25%)	1 (50%)	1 (50%)
1	J	1/8 (12%)	1 (100%)	0
1	K	2/8 (25%)	1 (50%)	1 (50%)
1	L	1/8 (12%)	1 (100%)	0
1	M	1/8 (12%)	0	0
All	All	9/48 (18%)	5 (55%)	3 (33%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	G	2	C
1	H	2	C
1	J	2	C
1	K	2	C
1	L	2	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	G	1	U
1	H	1	U
1	K	1	U

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 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FPD	E	5701	-	26,32,32	1.16	3 (11%)	26,49,49	0.97	1 (3%)
4	AGS	B	2600	3	32,33,33	1.96	10 (31%)	45,52,52	1.75	14 (31%)
4	AGS	A	1600	3	32,33,33	2.04	10 (31%)	45,52,52	1.73	13 (28%)
5	FPD	D	4701	-	26,32,32	1.14	3 (11%)	26,49,49	0.97	2 (7%)
4	AGS	E	6600	3	32,33,33	2.06	10 (31%)	45,52,52	1.79	11 (24%)
5	FPD	B	2701	3	26,32,32	1.25	3 (11%)	26,49,49	0.98	1 (3%)
4	AGS	D	4600	3	32,33,33	1.94	10 (31%)	45,52,52	1.73	12 (26%)
5	FPD	C	3701	-	26,32,32	1.19	3 (11%)	26,49,49	1.04	1 (3%)
5	FPD	F	6701	3	26,32,32	1.20	4 (15%)	26,49,49	0.94	1 (3%)
4	AGS	C	3600	-	32,33,33	2.00	10 (31%)	45,52,52	1.75	12 (26%)
4	AGS	E	5600	-	32,33,33	1.93	10 (31%)	45,52,52	1.74	13 (28%)

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
5	FPD	E	5701	-	-	14/15/57/57	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	B	2600	3	-	2/21/38/38	0/3/3/3
4	AGS	A	1600	3	-	2/21/38/38	0/3/3/3
5	FPD	D	4701	-	-	14/15/57/57	0/2/3/3
4	AGS	E	6600	3	-	2/21/38/38	0/3/3/3
5	FPD	B	2701	3	-	12/15/57/57	0/2/3/3
4	AGS	D	4600	3	-	2/21/38/38	0/3/3/3
5	FPD	C	3701	-	-	14/15/57/57	0/2/3/3
5	FPD	F	6701	3	-	12/15/57/57	0/2/3/3
4	AGS	C	3600	-	-	2/21/38/38	0/3/3/3
4	AGS	E	5600	-	-	3/21/38/38	0/3/3/3

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1600	AGS	PG-S1G	6.51	2.04	1.90
4	E	6600	AGS	PG-S1G	6.47	2.04	1.90
4	C	3600	AGS	PG-S1G	5.99	2.03	1.90
4	B	2600	AGS	PG-S1G	5.65	2.02	1.90
4	D	4600	AGS	PG-S1G	5.61	2.02	1.90

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	6600	AGS	PB-O3B-PG	-4.16	117.94	133.17
4	E	6600	AGS	C5-C4-N9	3.77	109.92	105.81
4	D	4600	AGS	C5-C4-N9	3.73	109.88	105.81
4	C	3600	AGS	C5-C4-N9	3.67	109.81	105.81
4	A	1600	AGS	C5-C4-N9	3.67	109.81	105.81

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

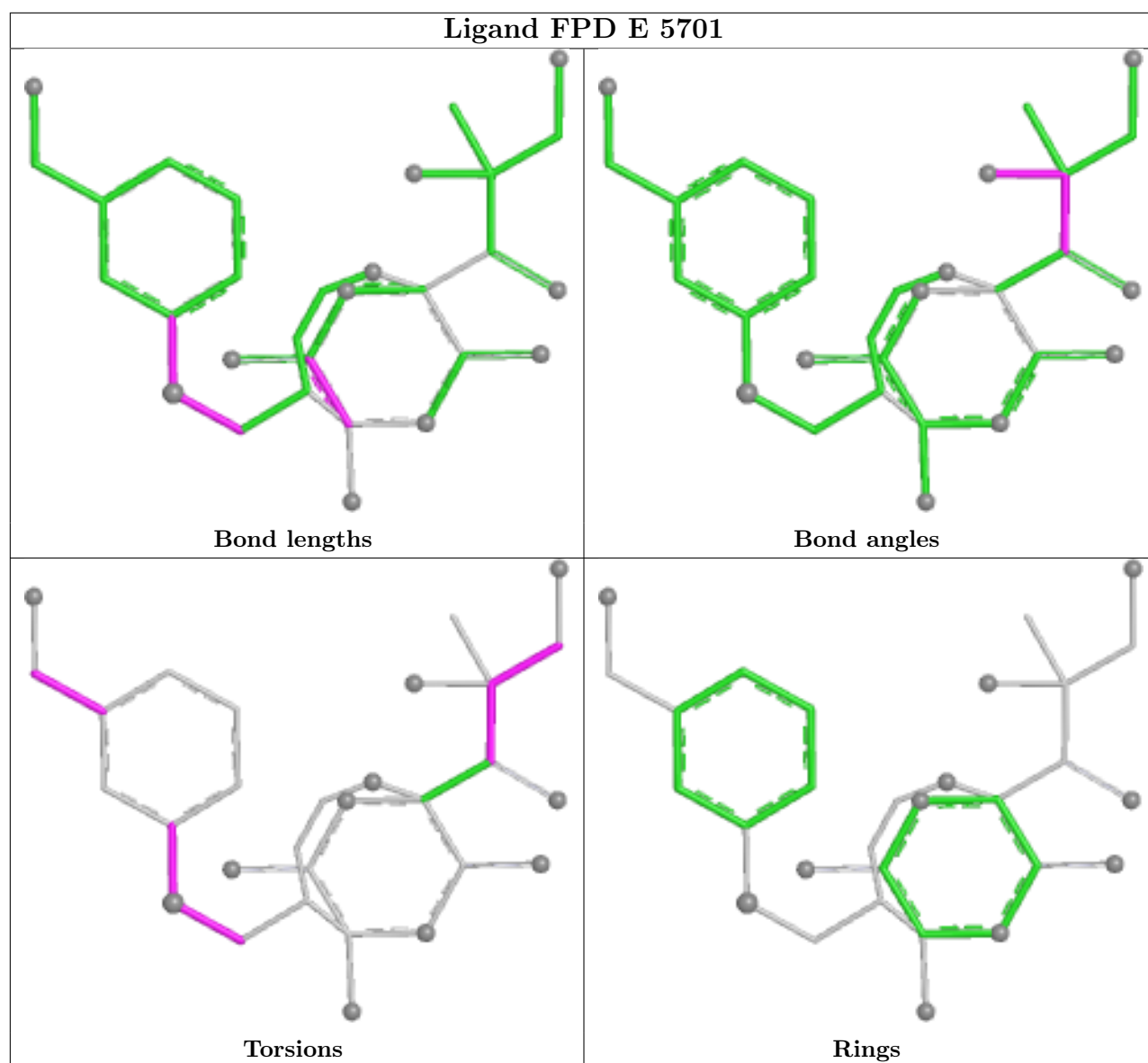
Mol	Chain	Res	Type	Atoms
5	B	2701	FPD	C3-C1-C4-C5
5	B	2701	FPD	O2-C1-C4-C5
5	B	2701	FPD	C2-C1-C4-C5
5	B	2701	FPD	C3-C1-C4-O3
5	B	2701	FPD	O2-C1-C4-O3

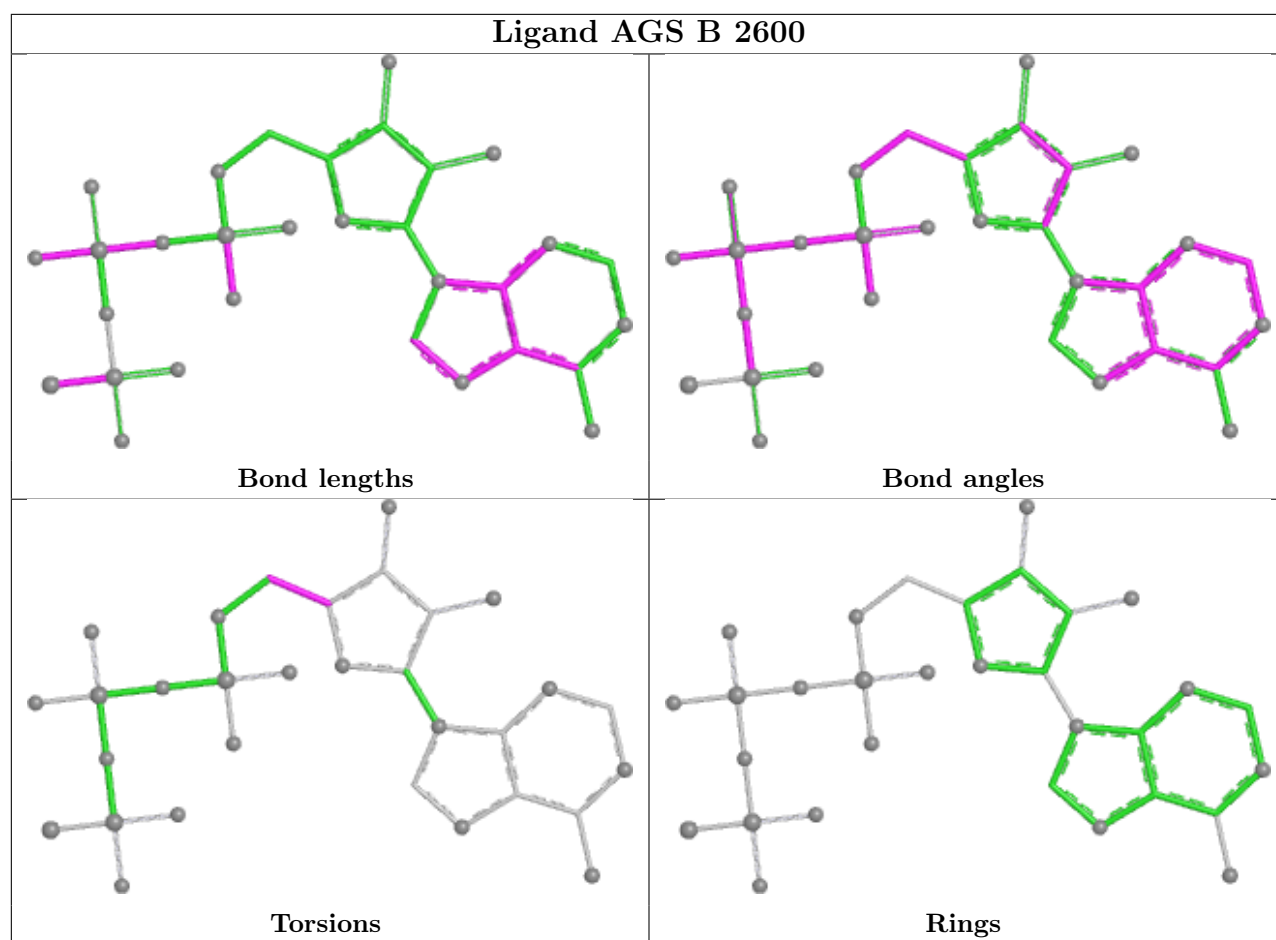
There are no ring outliers.

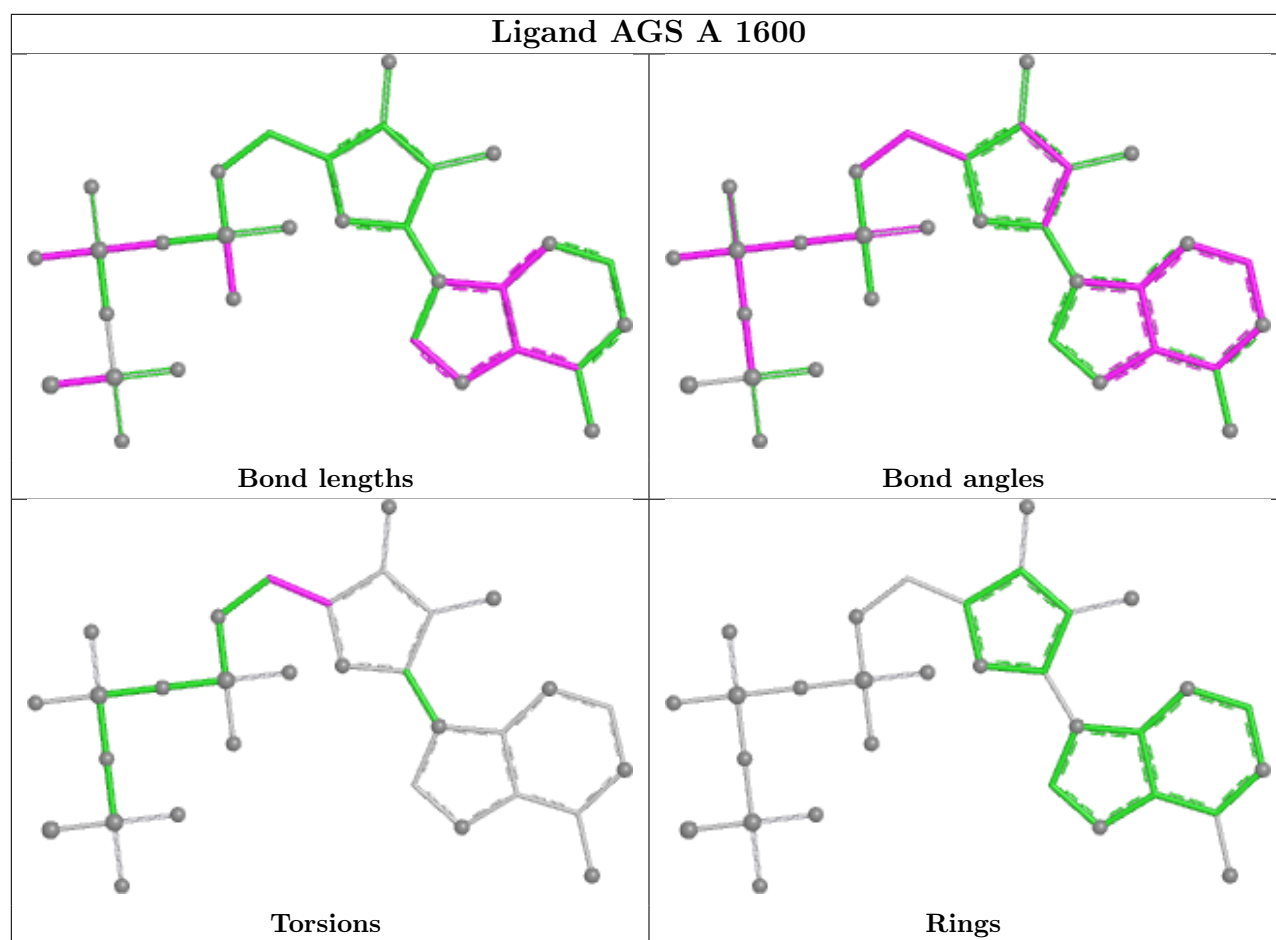
11 monomers are involved in 74 short contacts:

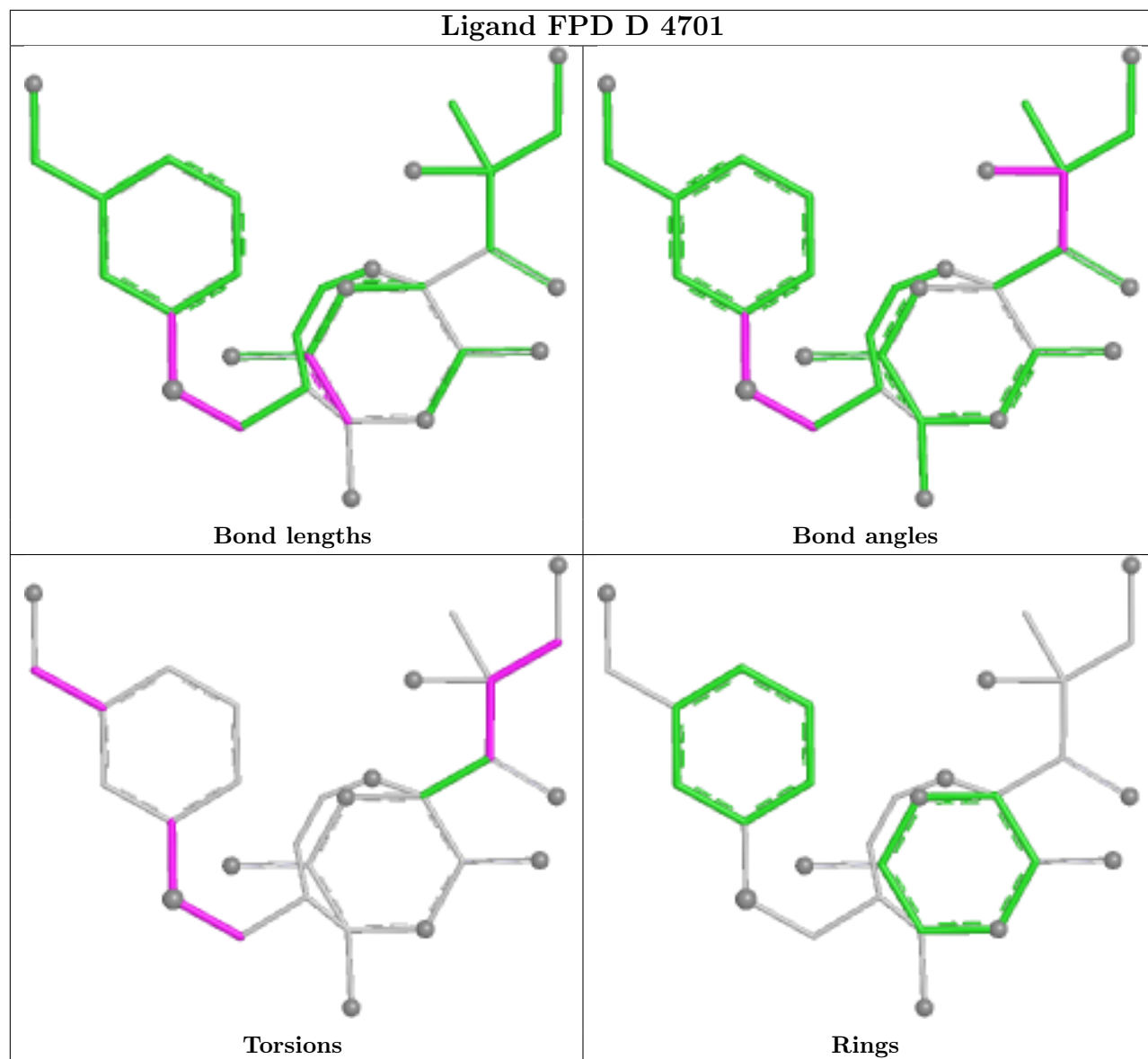
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	5701	FPD	10	0
4	B	2600	AGS	6	0
4	A	1600	AGS	4	0
5	D	4701	FPD	8	0
4	E	6600	AGS	6	0
5	B	2701	FPD	6	0
4	D	4600	AGS	5	0
5	C	3701	FPD	9	0
5	F	6701	FPD	3	0
4	C	3600	AGS	7	0
4	E	5600	AGS	10	0

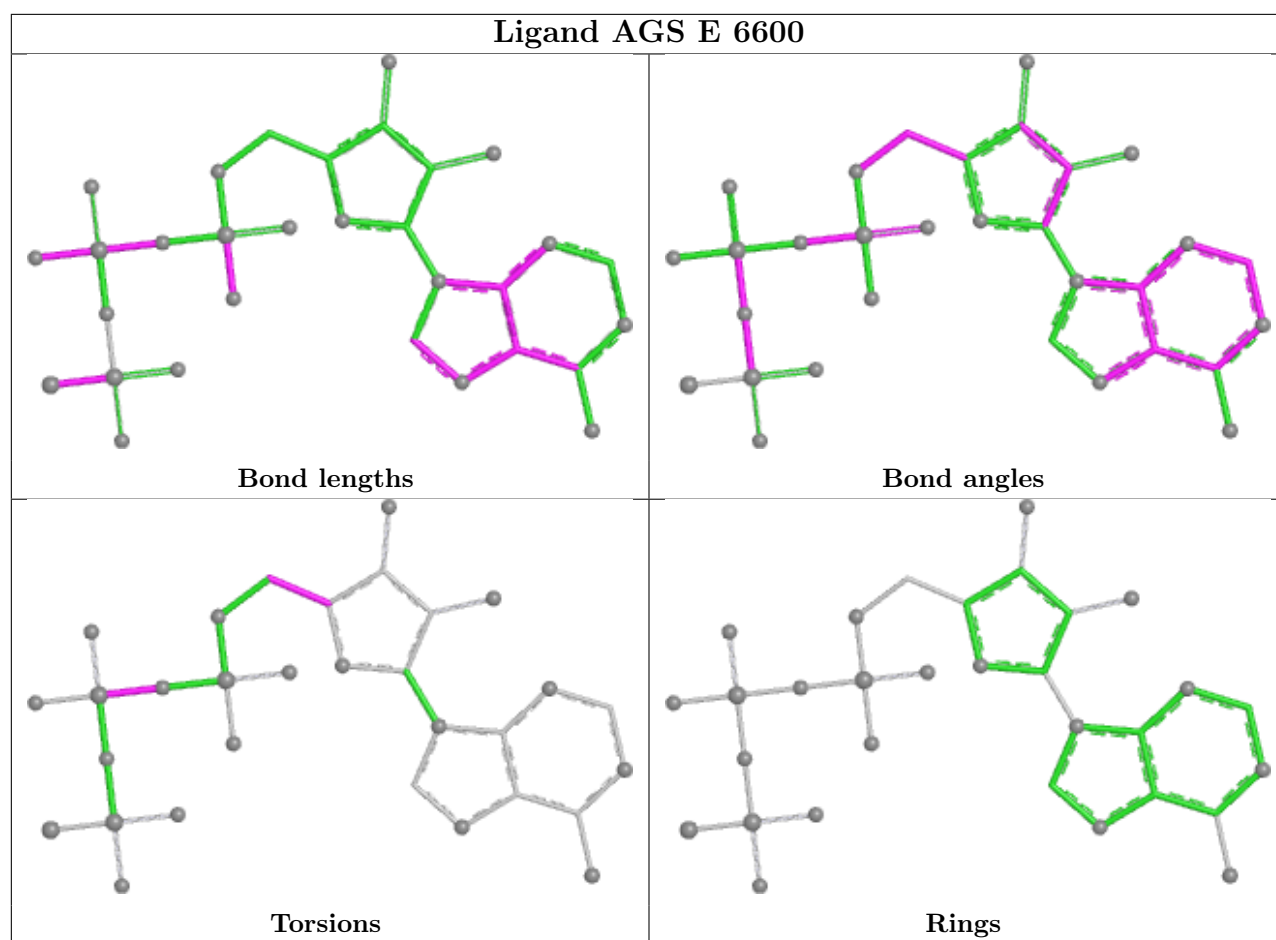
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

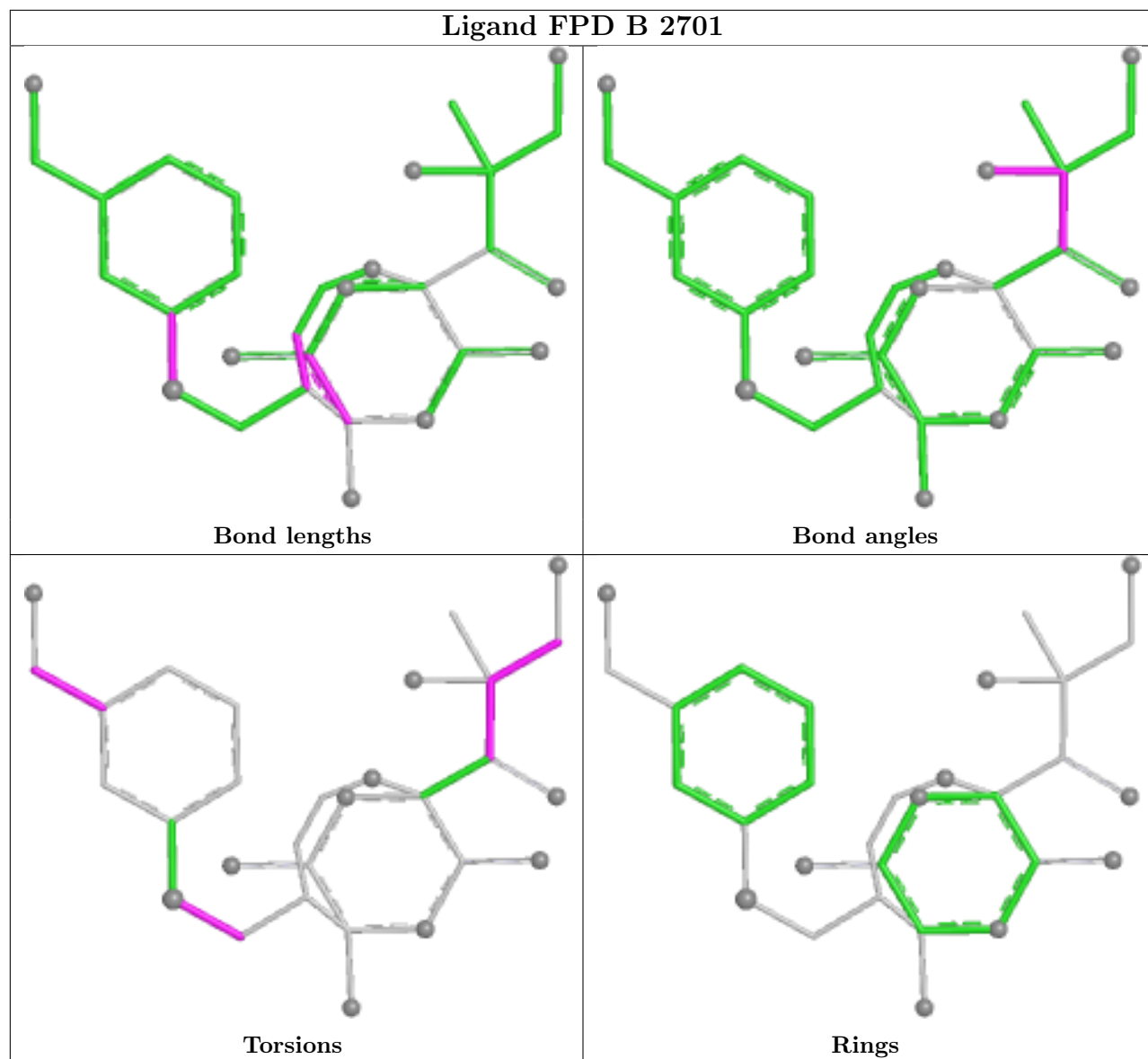


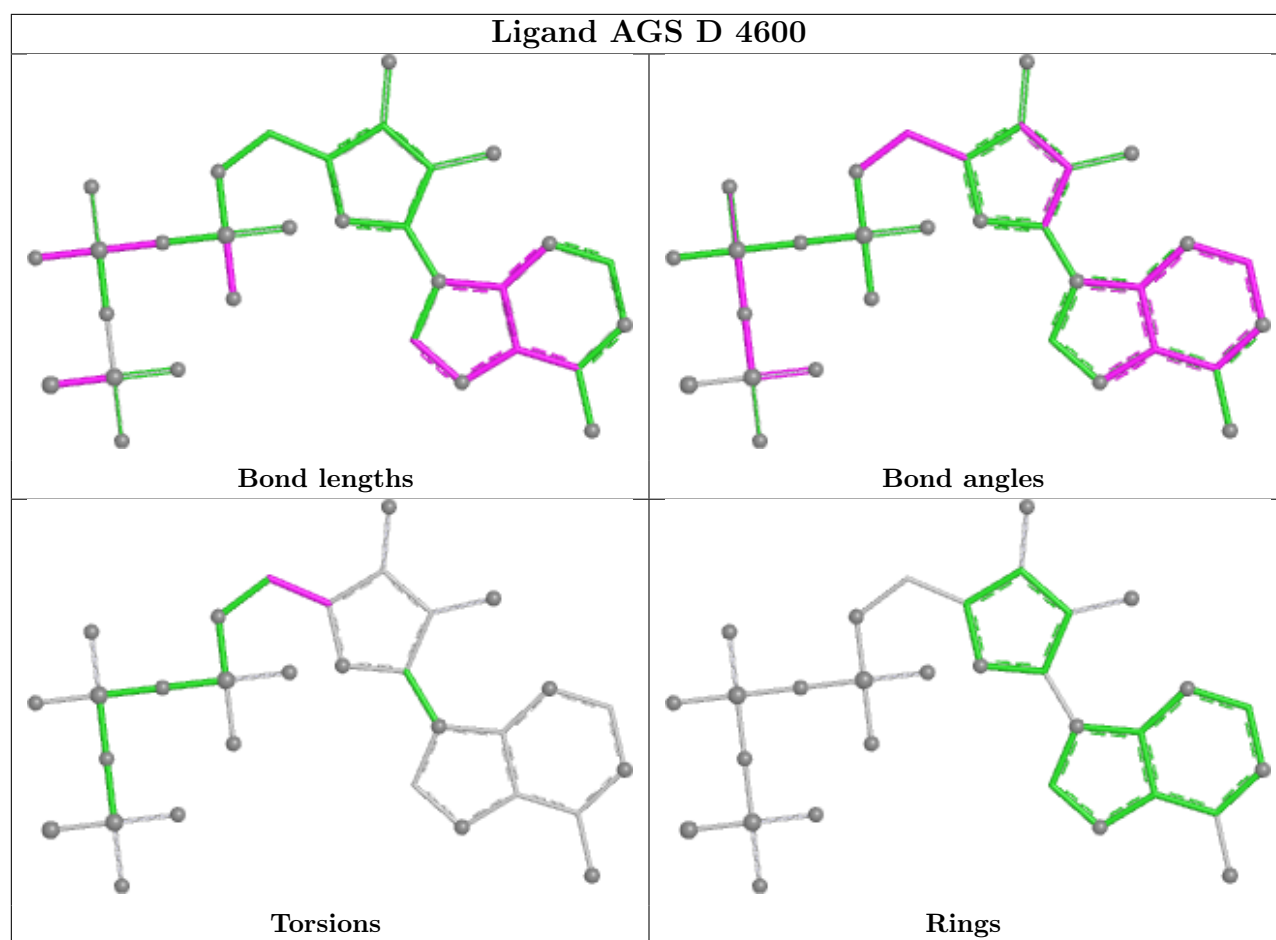


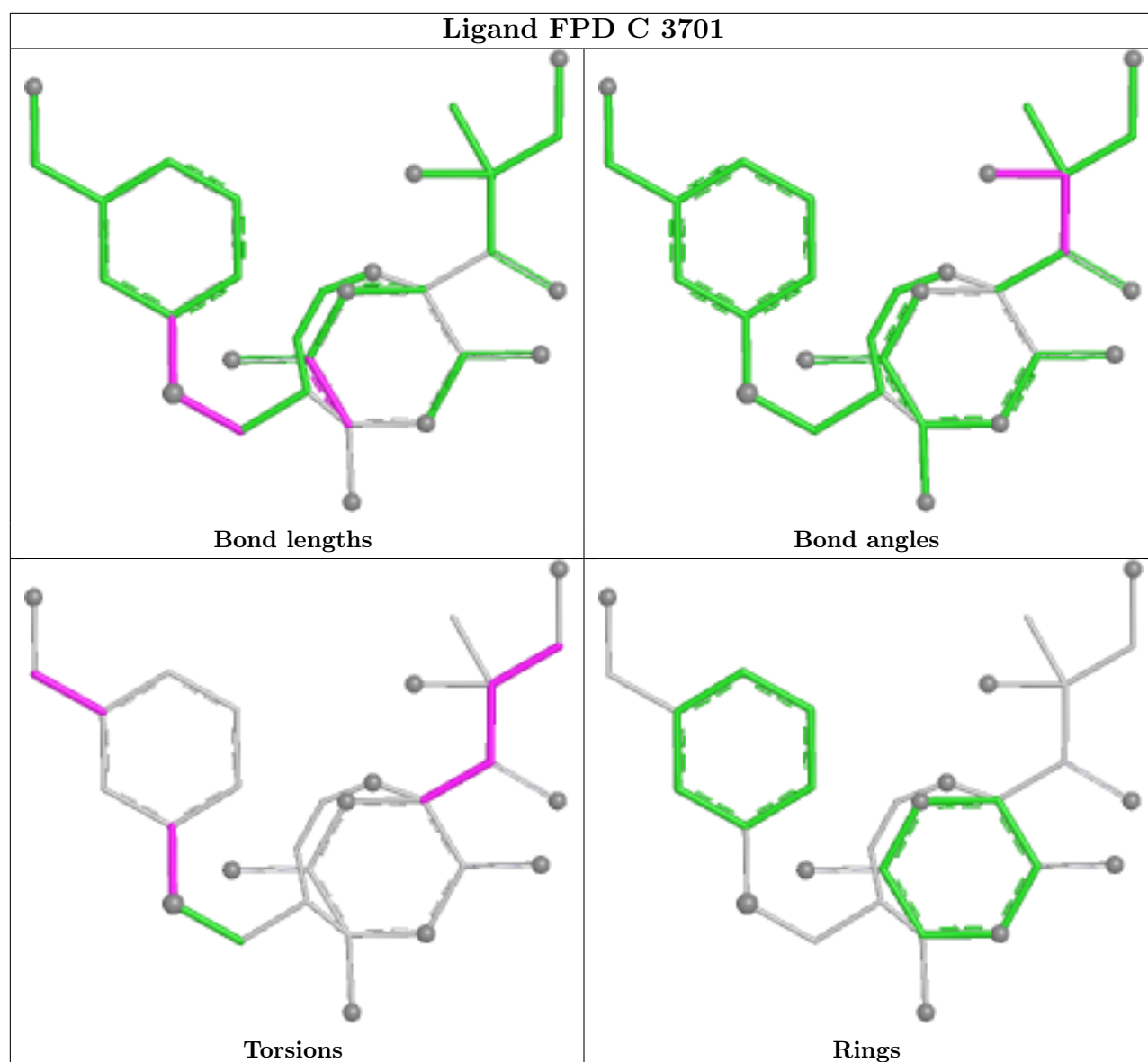


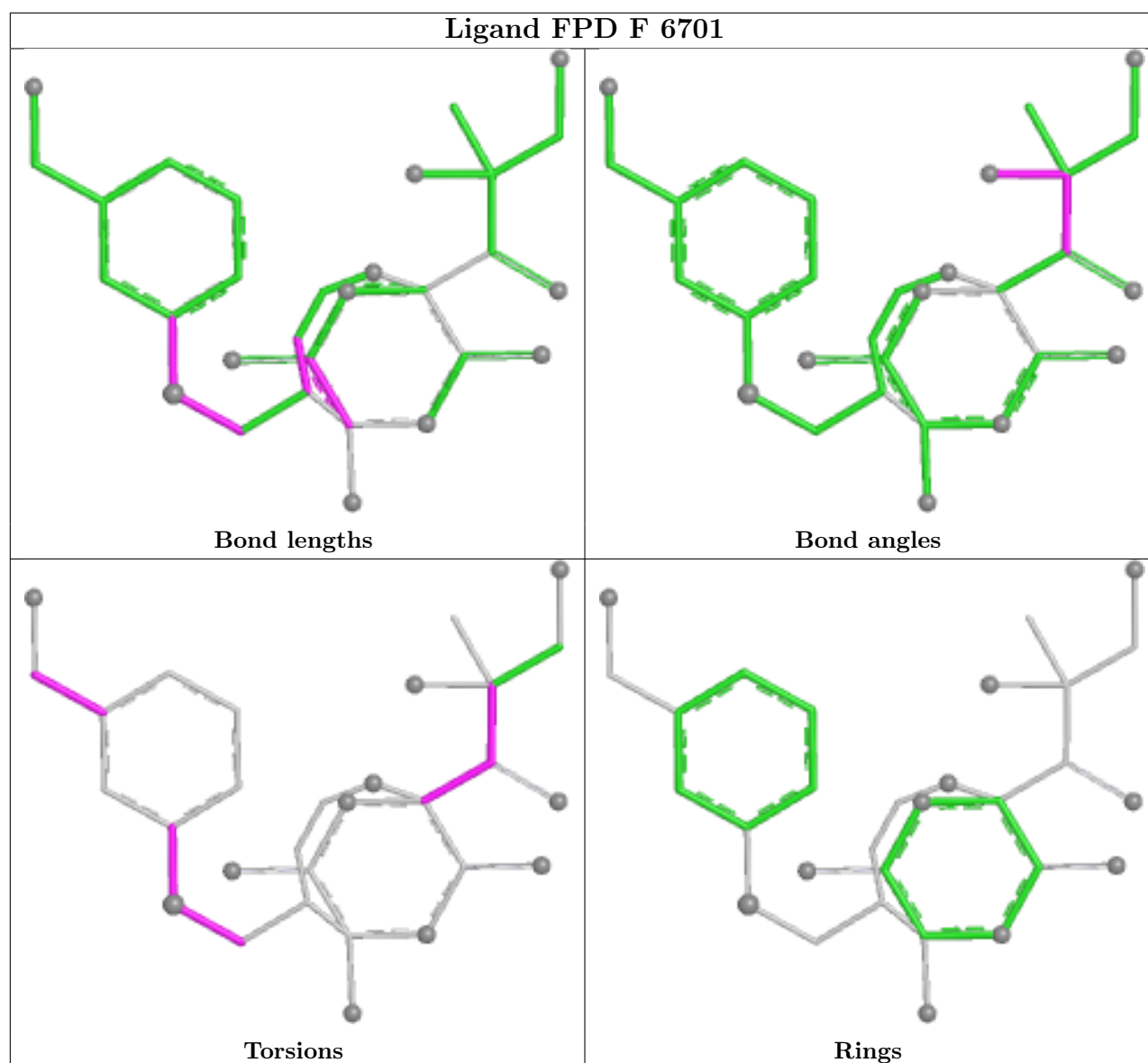


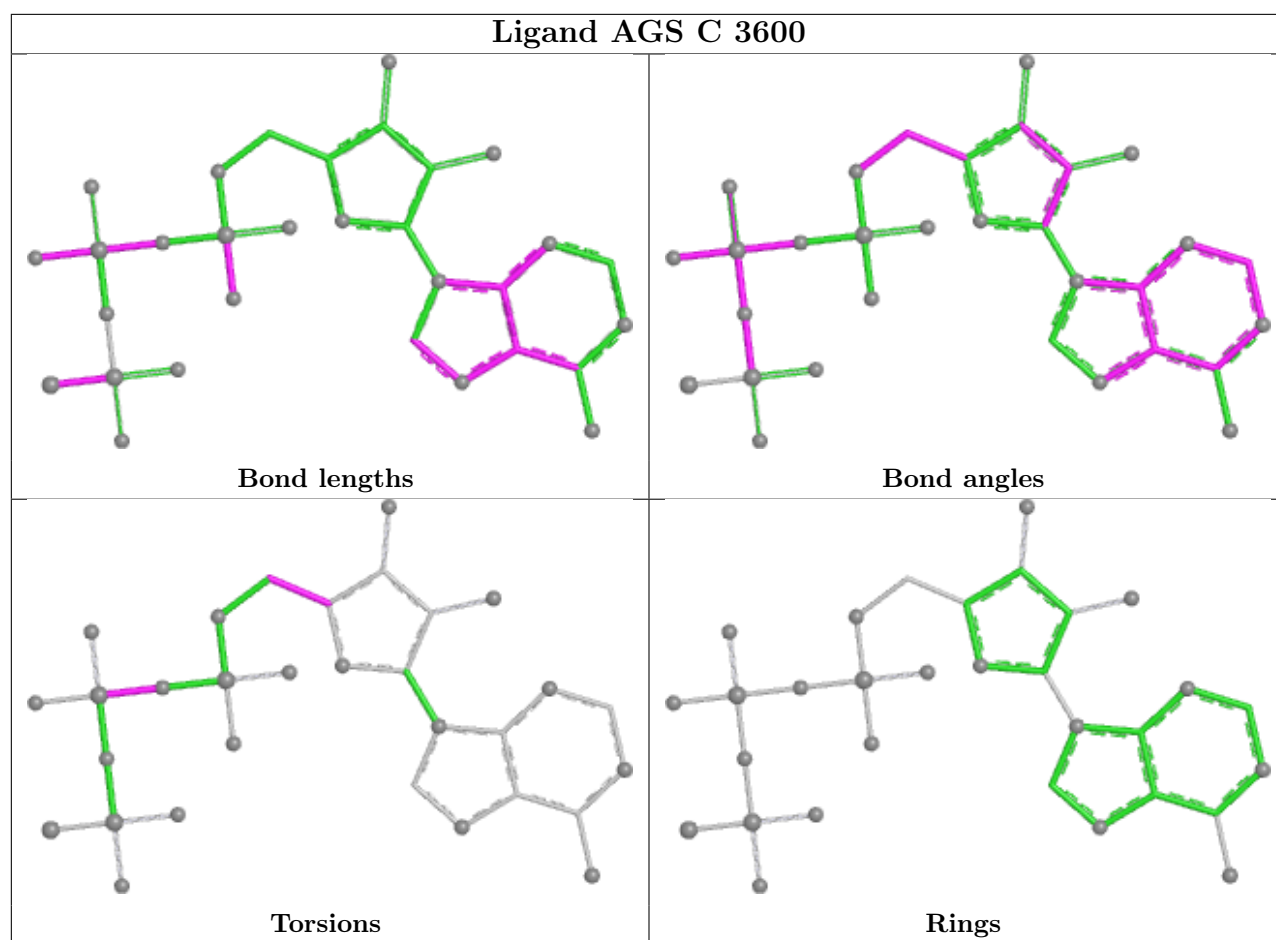


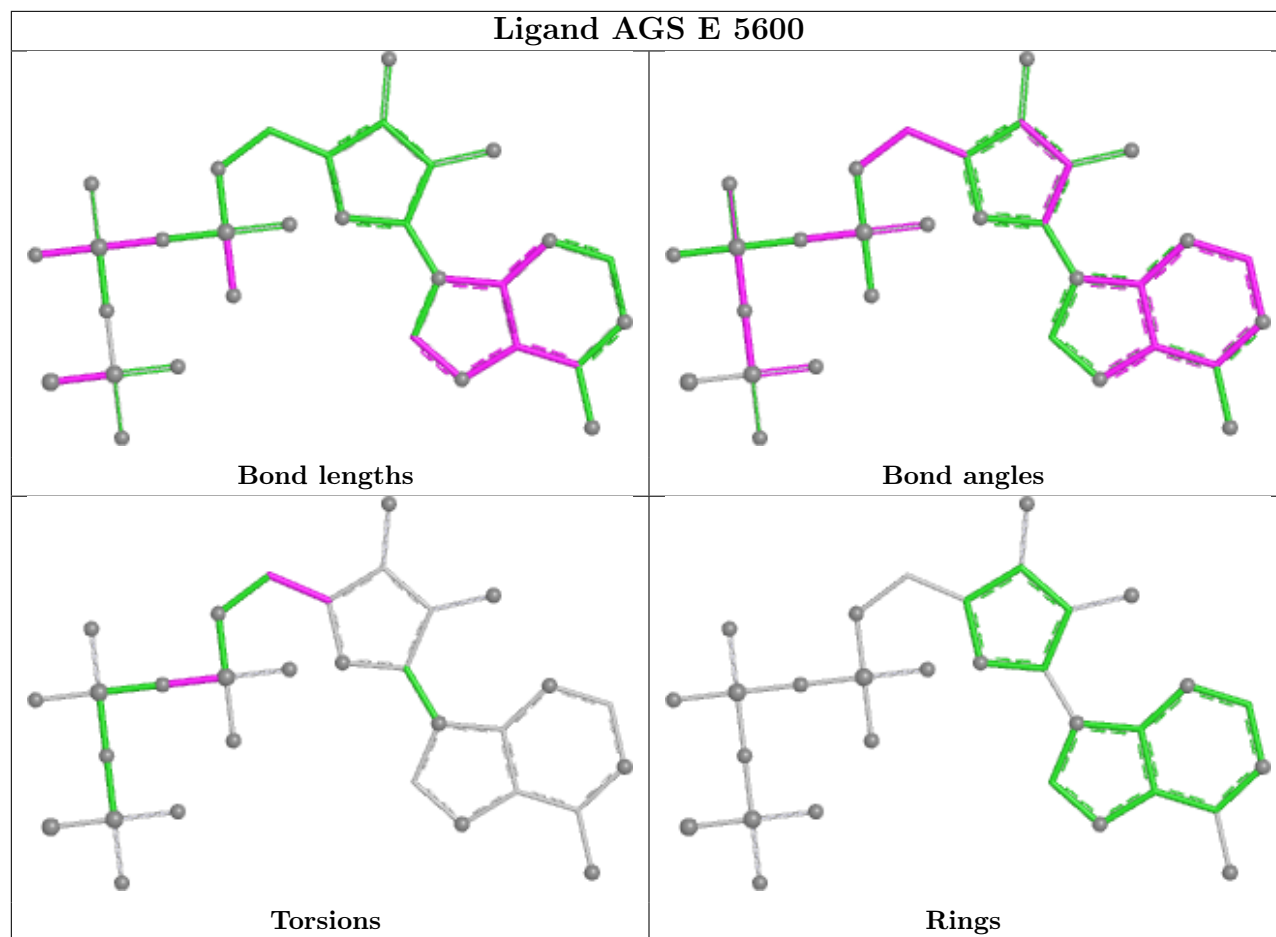












5.7 Other polymers [i](#)

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	G	2/8 (25%)	1.78	1 (50%) 0 0	53, 53, 53, 53	0
1	H	2/8 (25%)	1.68	0 100 100	53, 53, 53, 53	0
1	J	2/8 (25%)	0.42	0 100 100	53, 53, 53, 53	0
1	K	2/8 (25%)	1.13	0 100 100	55, 55, 55, 56	0
1	L	2/8 (25%)	0.04	0 100 100	53, 53, 53, 53	0
1	M	2/8 (25%)	2.39	1 (50%) 0 0	53, 53, 53, 53	0
2	A	408/419 (97%)	-0.10	5 (1%) 76 55	53, 53, 53, 53	0
2	B	408/419 (97%)	0.05	7 (1%) 69 46	53, 53, 53, 53	0
2	C	408/419 (97%)	-0.00	7 (1%) 69 46	53, 53, 53, 53	0
2	D	408/419 (97%)	0.19	6 (1%) 72 50	53, 53, 53, 53	0
2	E	407/419 (97%)	0.08	9 (2%) 62 39	53, 53, 53, 53	0
2	F	408/419 (97%)	-0.13	2 (0%) 87 72	53, 53, 53, 53	0
All	All	2459/2562 (95%)	0.02	38 (1%) 72 50	53, 53, 53, 56	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	140	HIS	5.5
2	B	139	LEU	5.5
2	C	140	HIS	5.3
2	B	140	HIS	5.2
2	D	140	HIS	5.2

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

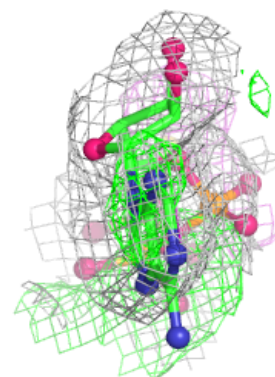
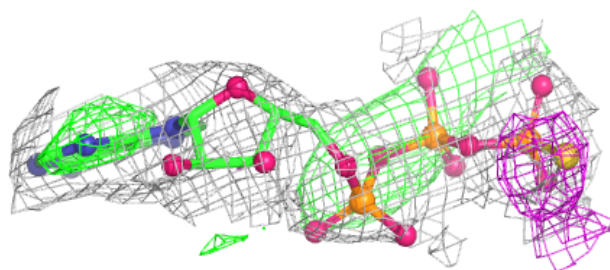
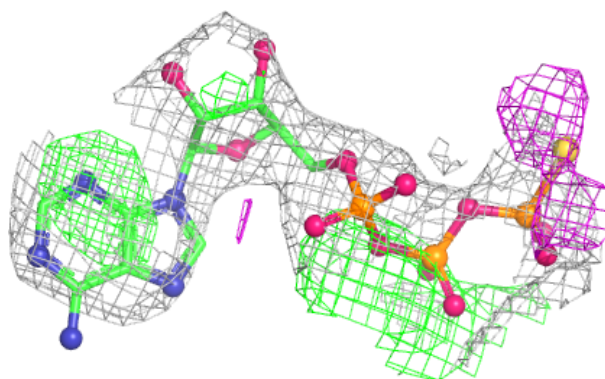
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	3601	1/1	0.50	0.18	53,53,53,53	0
4	AGS	E	6600	31/31	0.52	0.20	53,53,53,53	0
5	FPD	C	3701	30/30	0.54	0.24	53,53,53,53	0
5	FPD	E	5701	30/30	0.58	0.23	53,53,53,53	0
3	MG	A	1601	1/1	0.63	0.13	54,54,54,54	0
5	FPD	F	6701	30/30	0.64	0.19	53,53,53,53	0
4	AGS	C	3600	31/31	0.67	0.15	53,53,53,53	0
5	FPD	B	2701	30/30	0.68	0.15	53,53,53,53	0
5	FPD	D	4701	30/30	0.69	0.22	53,53,53,53	0
4	AGS	D	4600	31/31	0.75	0.12	53,53,53,53	0
3	MG	D	4601	1/1	0.76	0.09	53,53,53,53	0
4	AGS	A	1600	31/31	0.76	0.12	53,53,53,53	0
4	AGS	B	2600	31/31	0.81	0.12	53,53,53,53	0
4	AGS	E	5600	31/31	0.82	0.12	53,53,53,53	0
3	MG	E	5601	1/1	0.87	0.17	53,53,53,53	0
3	MG	F	6601	1/1	0.90	0.19	53,53,53,53	0
3	MG	B	2601	1/1	0.94	0.06	54,54,54,54	0

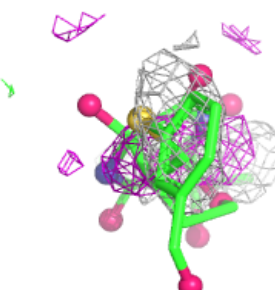
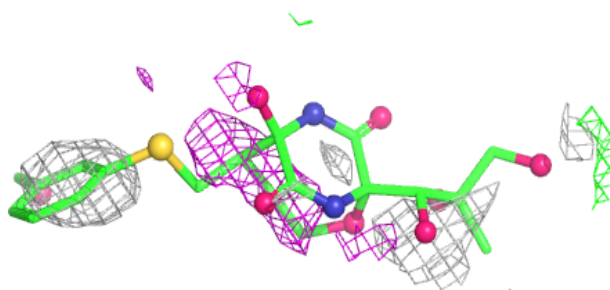
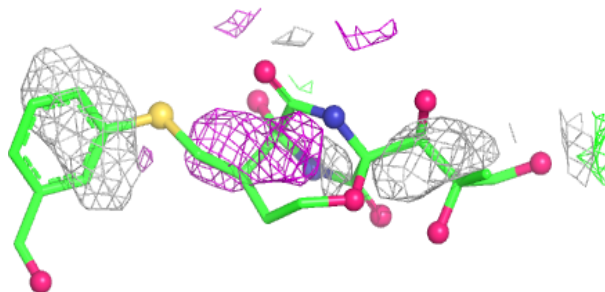
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS E 6600:

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

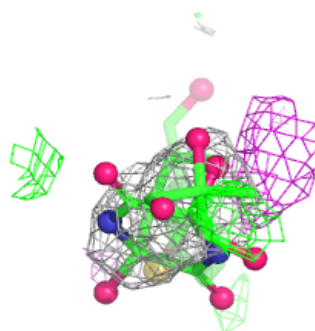
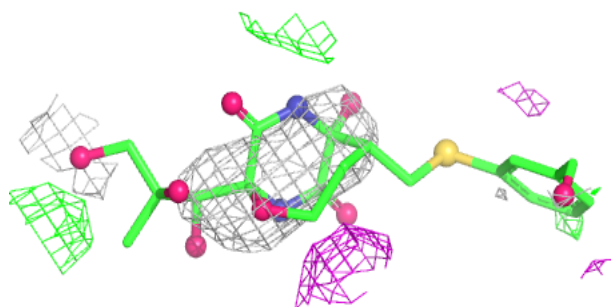
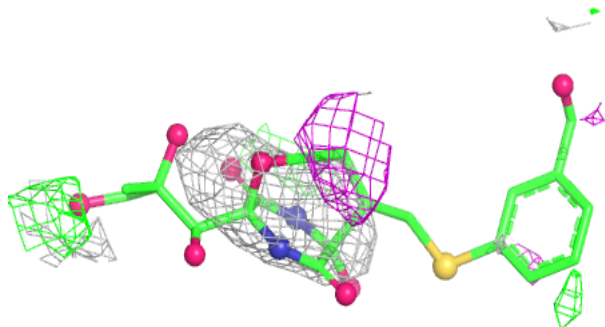
**Electron density around FPD C 3701:**

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

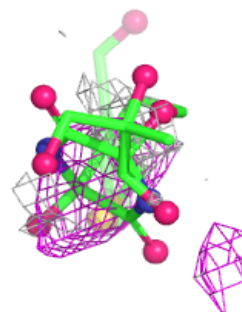
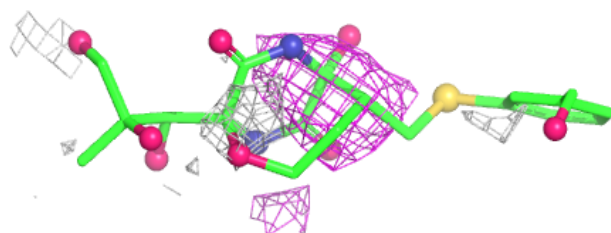
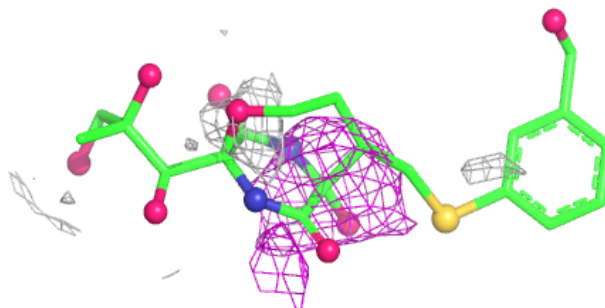


Electron density around FPD E 5701:

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

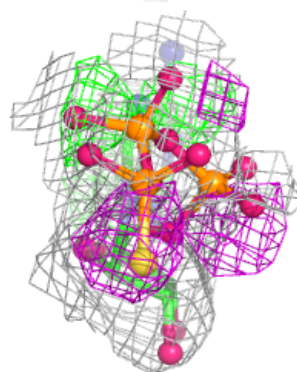
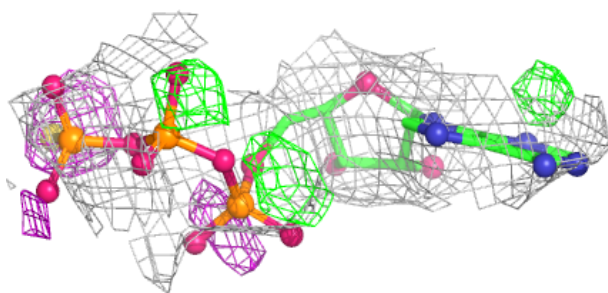
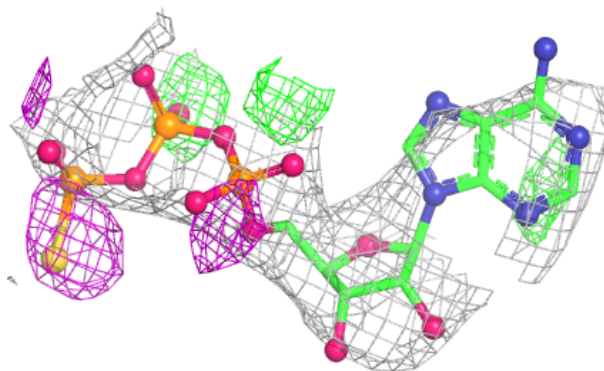
**Electron density around FPD F 6701:**

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

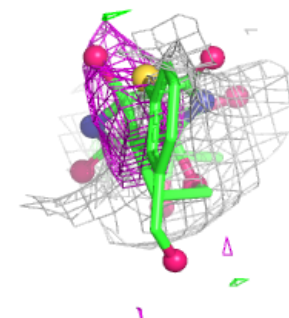
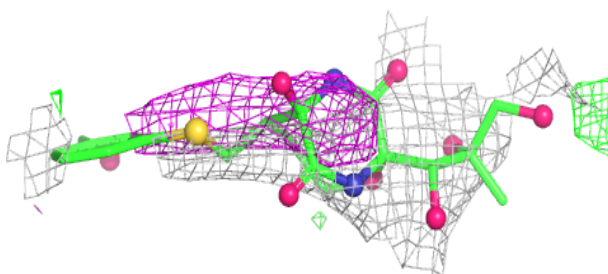
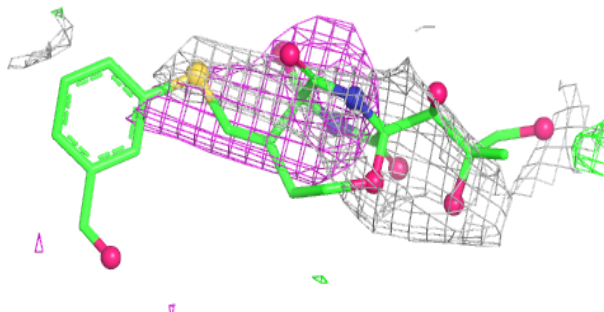


Electron density around AGS C 3600:

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

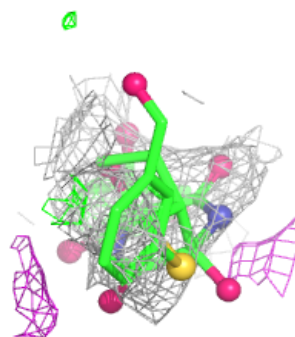
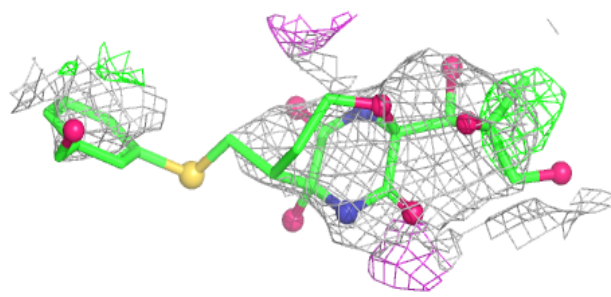
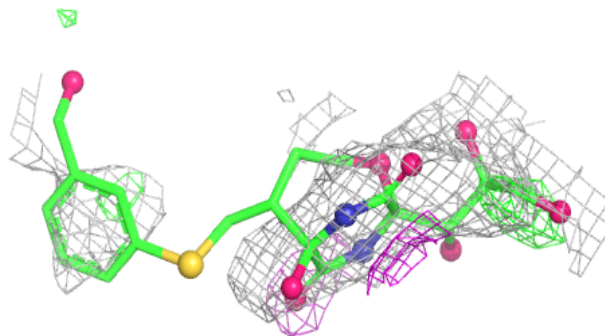
**Electron density around FPD B 2701:**

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

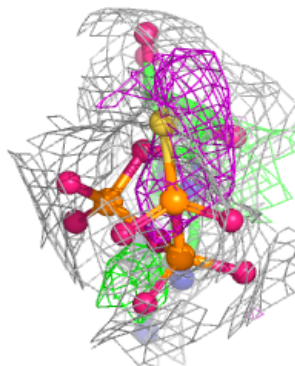
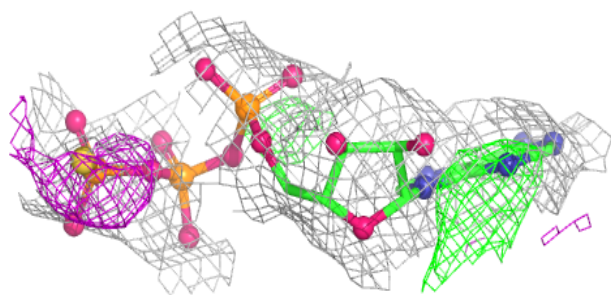
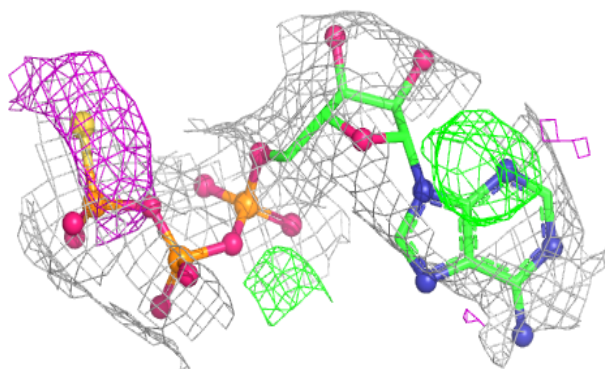


Electron density around FPD D 4701:

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

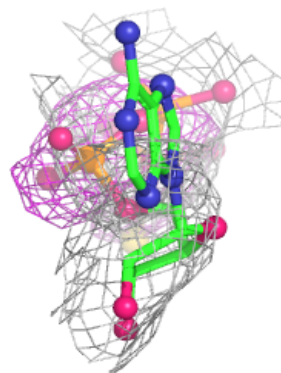
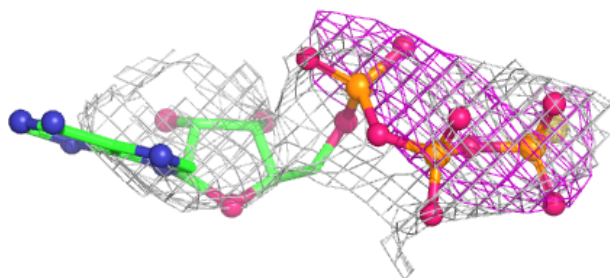
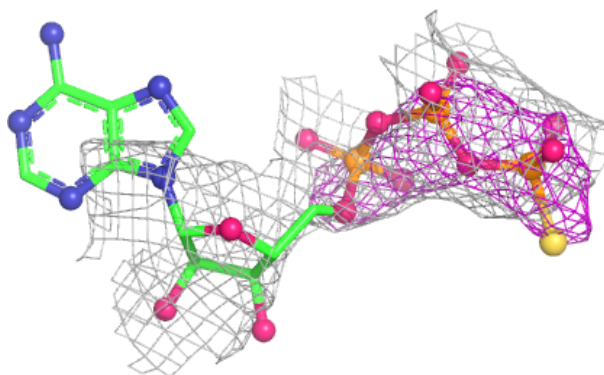
**Electron density around AGS D 4600:**

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

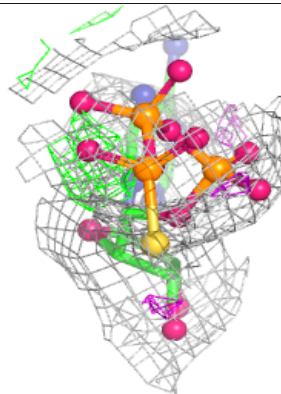
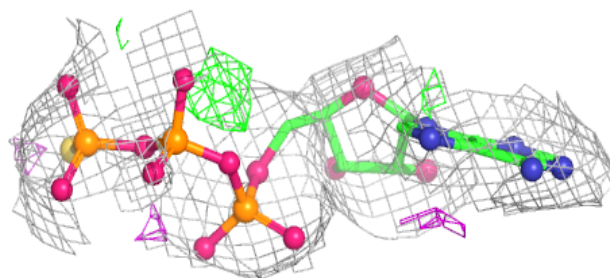
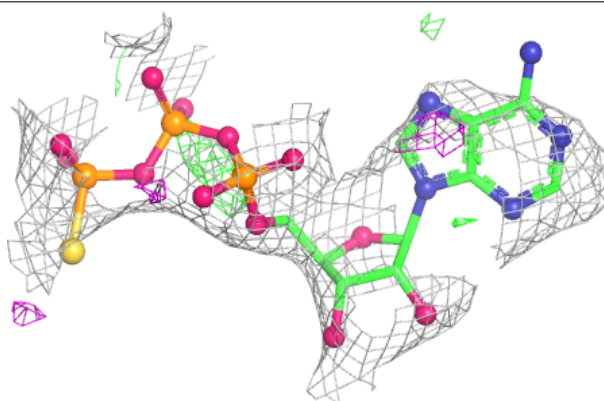


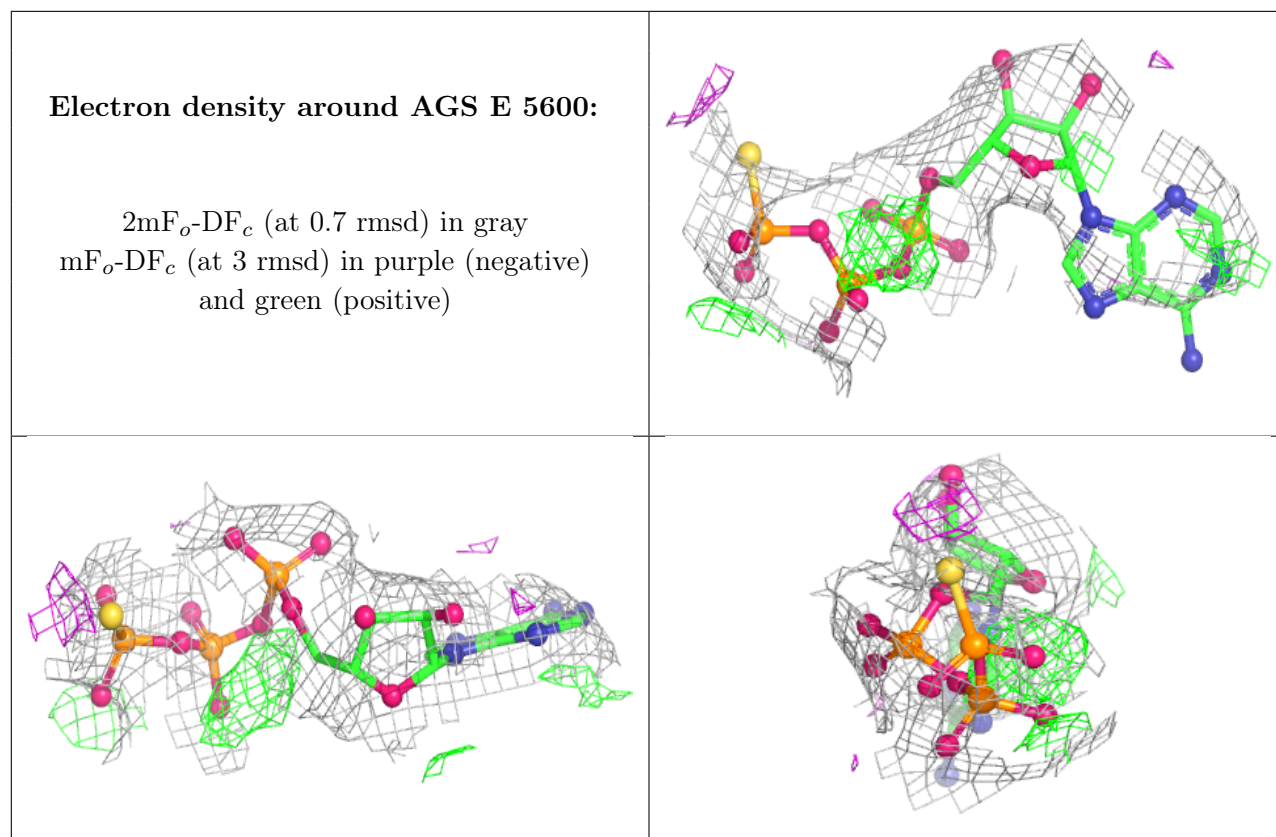
Electron density around AGS A 1600:

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

**Electron density around AGS B 2600:**

$2mF_o-DF_c$ (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.