WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 11:36 AM EDT

PDB ID	:	5NWK
Title	:	14-3-3c in complex with CPP and fusicoccin
Authors	:	Saponaro, A.; Porro, A.; Chaves-Sanjuan, A.; Nardini, M.; Thiel, G.; Moroni, A.
Deposited on	:	2017-05-06
Resolution	:	3.30 Å(reported)

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

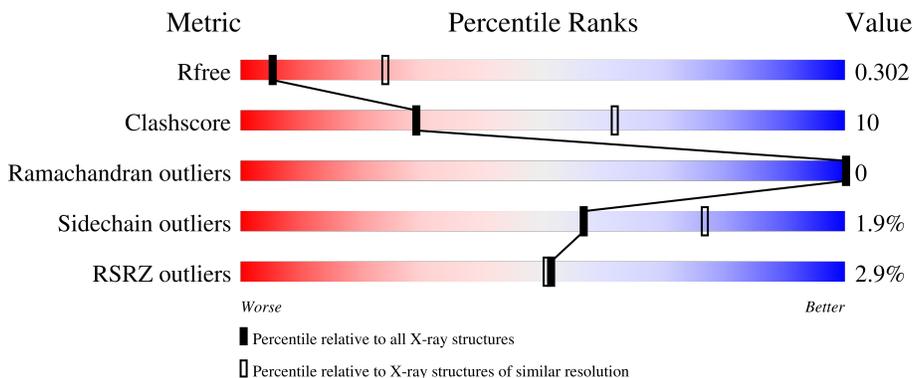|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.30 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.
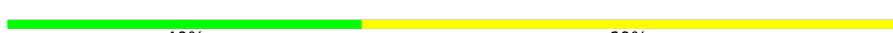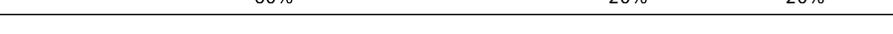
Metric	Percentile Ranks	Value
Rfree		0.302
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		1.9%
RSRZ outliers		2.9%

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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	262	79% 12% 9%
1	B	262	.% 80% 13% 6%
1	C	262	78% 11% 11%
1	D	262	77% 13% 10%
1	E	262	76% 15% 9%

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Mol	Chain	Length	Quality of chain
1	F	262	74% 16% 10%
1	G	262	% 75% 14% 11%
1	H	262	18% 78% · 19%
2	P	5	80% 20%
2	Q	5	40% 60%
2	R	5	60% 20% 20%
2	S	5	100%
2	T	5	60% 20% 20%
2	U	5	60% 20% 20%
2	V	5	40% 40% 20%
2	W	5	20% 80%

2   Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 15163 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 14-3-3 c-1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total 1905	C 1192	N 322	O 383	S 8	0	0	0
1	B	245	Total 1942	C 1214	N 328	O 391	S 9	0	0	0
1	C	234	Total 1866	C 1169	N 316	O 374	S 7	0	0	0
1	D	236	Total 1885	C 1181	N 319	O 378	S 7	0	1	0
1	E	238	Total 1897	C 1189	N 321	O 380	S 7	0	1	0
1	F	237	Total 1888	C 1183	N 319	O 378	S 8	0	0	0
1	G	234	Total 1869	C 1171	N 317	O 373	S 8	0	0	0
1	H	213	Total 1171	C 707	N 230	O 234		0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	PRO	-	expression tag	UNP Q5KTN5
A	0	GLY	-	expression tag	UNP Q5KTN5
B	-1	PRO	-	expression tag	UNP Q5KTN5
B	0	GLY	-	expression tag	UNP Q5KTN5
C	-1	PRO	-	expression tag	UNP Q5KTN5
C	0	GLY	-	expression tag	UNP Q5KTN5
D	-1	PRO	-	expression tag	UNP Q5KTN5
D	0	GLY	-	expression tag	UNP Q5KTN5
E	-1	PRO	-	expression tag	UNP Q5KTN5
E	0	GLY	-	expression tag	UNP Q5KTN5
F	-1	PRO	-	expression tag	UNP Q5KTN5
F	0	GLY	-	expression tag	UNP Q5KTN5
G	-1	PRO	-	expression tag	UNP Q5KTN5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLY	-	expression tag	UNP Q5KTN5
H	-1	PRO	-	expression tag	UNP Q5KTN5
H	0	GLY	-	expression tag	UNP Q5KTN5

- Molecule 2 is a protein called Potassium channel KAT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	4	Total 36	C 19	N 5	O 11	P 1	0	0	0
2	Q	5	Total 48	C 28	N 6	O 13	P 1	0	0	0
2	R	4	Total 36	C 19	N 5	O 11	P 1	0	0	0
2	S	5	Total 48	C 28	N 6	O 13	P 1	0	0	0
2	T	4	Total 36	C 19	N 5	O 11	P 1	0	0	0
2	U	4	Total 36	C 19	N 5	O 11	P 1	0	0	0
2	V	5	Total 48	C 28	N 6	O 13	P 1	0	0	0
2	W	1	Total 5	C 3	N 1	O 1		0	0	0

- Molecule 3 is FUSICOCCIN (three-letter code: FSC) (formula: $C_{36}H_{56}O_{12}$).

FSC
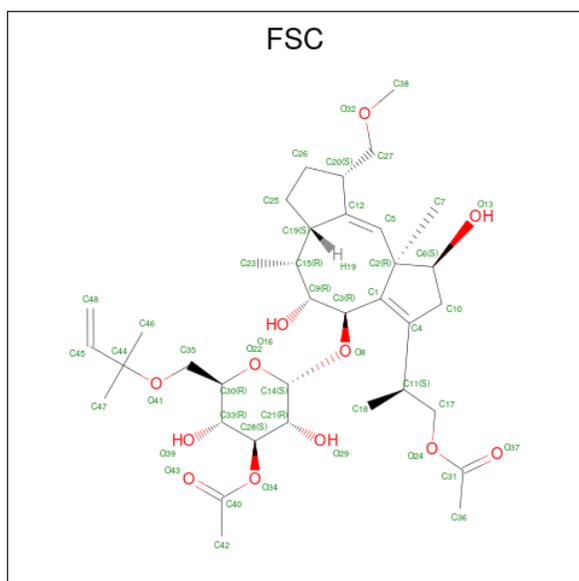
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			48	36	12		
3	B	1	Total	C	O	0	0
			48	36	12		
3	C	1	Total	C	O	0	0
			48	36	12		
3	D	1	Total	C	O	0	0
			48	36	12		
3	E	1	Total	C	O	0	0
			48	36	12		
3	F	1	Total	C	O	0	0
			48	36	12		
3	G	1	Total	C	O	0	0
			48	36	12		

- Molecule 4 is PHOSPHOSERINE (three-letter code: SEP) (formula: $C_3H_8NO_6P$).
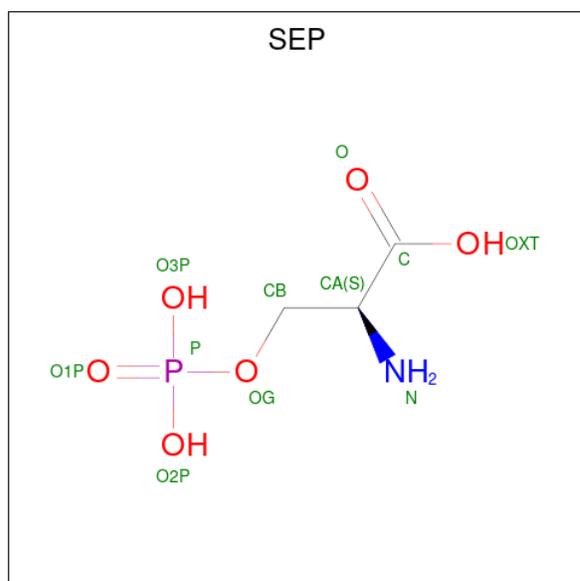
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	W	1	Total	C	N	O	P	0	0
			10	3	1	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total	O	0	0
			14	14		
5	B	11	Total	O	0	0
			11	11		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Q	1	Total 1	O 1	0	0
5	C	15	Total 15	O 15	0	0
5	R	1	Total 1	O 1	0	0
5	D	13	Total 13	O 13	0	0
5	E	21	Total 21	O 21	0	0
5	T	2	Total 2	O 2	0	0
5	F	14	Total 14	O 14	0	0
5	G	7	Total 7	O 7	0	0
5	V	1	Total 1	O 1	0	0
5	H	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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: 14-3-3 c-1 protein

Chain A:

- Molecule 1: 14-3-3 c-1 protein

Chain B:

- Molecule 1: 14-3-3 c-1 protein

Chain C:

- Molecule 1: 14-3-3 c-1 protein

Chain D:

R196 A197 Y220 K221 M227 L236 W237 D240 MET GLN ASP ASP GLY ALA ASP GLU ILE LYS GLU ASP PRO LYS PRO ASP GLU ALA LYS ASN

- Molecule 1: 14-3-3 c-1 protein

Chain E:

| 76% | 15% | 9% |

PRO GLY MET ALA V3 R8 Q20 A21 E22 R23 R48 S52 V53 R63 A64 S65 K75 R79 G80 N81 E82 E83 H84 Y91 L107 S123 F126 Y134 H135 R136 Y137 T154 Y158 P171 P174 I175 R176 F183 I190 Q203

E207 T214 Y220 K221 D222 S223 I226 R231 D232 N233 W237 D240 MET GLN ASP ASP GLY ALA ASP GLU ILE LYS GLU ASP PRO LYS PRO ASP GLU ALA LYS ASN

- Molecule 1: 14-3-3 c-1 protein

Chain F:

| 74% | 16% | 10% |

PRO GLY MET ALA VAL ALA P5 A21 E32 L38 E41 T44 V45 E46 E47 R48 N49 L50 K56 N57 V58 R62 S65 I69 S70 S71 I72 E73 Q74 K75 N81 E82 E83 H84 I88 E96 N97 E98 L99 I102 L109 L110 F126 M130

R136 T154 P174 L177 L181 N182 F183 F186 N192 K202 D206 K221 D222 I226 M227 L230 M241 GLN ASP ASP GLY ALA ASP GLU ILE LYS GLU ASP PRO LYS PRO ASP GLU ALA LYS ASN

- Molecule 1: 14-3-3 c-1 protein

Chain G:

%

| 75% | 14% | 11% |

PRO GLY MET ALA VAL ALA P5 E19 Q20 A21 R48 K56 R62 R63 S71 Q74 K75 E83 H84 I88 Y91 L99 L110 K113 S123 K124 V125 F126 Y127 L128 K129 M130 K131 H135 K142 E146 K159 D163 H173 P174 I175

L181 N182 F183 S184 V185 A201 L212 ASP THR LEU GLY GLU E218 D222 L230 L234 D240 M241 Q242 D243 ASP GLY ALA ASP GLU ILE LYS GLU ASP PRO LYS PRO ASP GLU ALA LYS ASN

- Molecule 1: 14-3-3 c-1 protein

Chain H:

18%

| 78% | . | 19% |

PRO GLY MET ALA VAL ALA P5 Y13 R23 V34 S37 LEU GLY SER GLU GLU LEU T44 V45 E46 S52 Y55 S65 S70 K75 R79 G80 N81 H84 R92 D111 I115 P116 A119 F126 Y137 L138 A139 E140 F141 LYS THR GLY

ALA E146 I164 ALA THR THR E168 P171 T172 H173 P174 I175 R176 L177 A180 L181 S184 V185 F186 Y187 Y188 E189 I190 L191 N192 S193 P194 D195 R196 A197 A201 A204 F205 D206 E207 A208 I209 A210 E211 L212 ASP THR LEU GLY GLU GLU SER Y220 K221 D222 L225 I226

R231 D232 N233 L234 T235 L236 W237 THR SER ASP MET GLN ASP ASP GLY ALA ASP GLU ILE LYS GLU ASP PRO LYS PRO ASP GLU ALA LYS ASN

- Molecule 2: Potassium channel KAT1

Chain P: 80% 20%

TYR F674 N677

• Molecule 2: Potassium channel KAT1

Chain Q: 40% 60%

Y673 S676 N677

• Molecule 2: Potassium channel KAT1

Chain R: 60% 20% 20%

TYR F674 N677

• Molecule 2: Potassium channel KAT1

Chain S: 100%

There are no outlier residues recorded for this chain.

• Molecule 2: Potassium channel KAT1

Chain T: 60% 20% 20%

TYR F674 N677

• Molecule 2: Potassium channel KAT1

Chain U: 60% 20% 20%

TYR F674 N677

• Molecule 2: Potassium channel KAT1

Chain V: 40% 40% 20%

Y673 F674 S675 S676 N677

• Molecule 2: Potassium channel KAT1

Chain W: 20% 80%

TYR PHE S675 SEP ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.81Å 165.66Å 170.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.32 – 3.30 48.32 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.32-3.30) 92.0 (48.32-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.229 , 0.286 0.245 , 0.302	Depositor DCC
R_{free} test set	2934 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 1.7	EDS
L-test for twinning [2]	$< |L| > = 0.38, < L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.084 for -h,l,k	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	15163	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: SEP, FSC

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	0.23	0/1933	0.36	0/2604
1	B	0.23	0/1970	0.37	0/2655
1	C	0.23	0/1893	0.37	0/2550
1	D	0.23	0/1916	0.37	0/2582
1	E	0.23	0/1928	0.38	0/2600
1	F	0.24	0/1916	0.39	1/2581 (0.0%)
1	G	0.23	0/1896	0.38	0/2552
1	H	0.22	0/1174	0.32	0/1620
2	P	0.29	0/25	0.39	0/29
2	Q	0.35	0/38	0.45	0/47
2	R	0.27	0/25	0.35	0/29
2	S	0.38	0/38	0.52	0/47
2	T	0.34	0/25	0.45	0/29
2	U	0.27	0/25	0.32	0/29
2	V	0.31	0/38	0.34	0/47
2	W	0.16	0/4	0.18	0/4
All	All	0.23	0/14844	0.37	1/20005 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	222	ASP	CB-CA-C	-5.79	98.81	110.40

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	1905	0	1882	32	0
1	B	1942	0	1919	33	0
1	C	1866	0	1846	35	0
1	D	1885	0	1867	18	0
1	E	1897	0	1880	45	0
1	F	1888	0	1870	31	0
1	G	1869	0	1850	39	0
1	H	1171	0	662	6	0
2	P	36	0	22	0	0
2	Q	48	0	31	2	0
2	R	36	0	22	1	0
2	S	48	0	31	0	0
2	T	36	0	22	0	0
2	U	36	0	22	1	0
2	V	48	0	31	2	0
2	W	5	0	1	0	0
3	A	48	0	56	14	0
3	B	48	0	56	14	0
3	C	48	0	56	11	0
3	D	48	0	56	13	0
3	E	48	0	56	15	0
3	F	48	0	56	15	0
3	G	48	0	56	20	0
4	W	10	0	5	0	0
5	A	14	0	0	0	0
5	B	11	0	0	0	0
5	C	15	0	0	1	0
5	D	13	0	0	0	0
5	E	21	0	0	0	0
5	F	14	0	0	0	0
5	G	7	0	0	0	0
5	H	1	0	0	0	0
5	Q	1	0	0	0	0
5	R	1	0	0	0	0
5	T	2	0	0	0	0
5	V	1	0	0	0	0
All	All	15163	0	14355	283	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 10.

The worst 5 of 283 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:G:110:LEU:HD21	1:G:130:MET:CE	1.13	1.59
1:C:79:ARG:NH1	1:E:207:GLU:HG2	1.20	1.45
1:G:110:LEU:CD2	1:G:130:MET:CE	2.07	1.31
1:C:55:TYR:HB3	1:C:134:TYR:OH	1.52	1.09
1:B:38:LEU:HD22	1:B:41:GLU:HG3	1.25	1.08

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/262 (90%)	232 (98%)	5 (2%)	0	100	100
1	B	243/262 (93%)	240 (99%)	3 (1%)	0	100	100
1	C	232/262 (88%)	228 (98%)	4 (2%)	0	100	100
1	D	235/262 (90%)	231 (98%)	4 (2%)	0	100	100
1	E	237/262 (90%)	230 (97%)	7 (3%)	0	100	100
1	F	235/262 (90%)	231 (98%)	4 (2%)	0	100	100
1	G	230/262 (88%)	225 (98%)	5 (2%)	0	100	100
1	H	203/262 (78%)	199 (98%)	4 (2%)	0	100	100
2	P	1/5 (20%)	1 (100%)	0	0	100	100
2	Q	2/5 (40%)	2 (100%)	0	0	100	100
2	R	1/5 (20%)	1 (100%)	0	0	100	100
2	S	2/5 (40%)	1 (50%)	1 (50%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	1/5 (20%)	1 (100%)	0	0	100	100
2	U	1/5 (20%)	1 (100%)	0	0	100	100
2	V	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1862/2131 (87%)	1825 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/222 (92%)	203 (99%)	2 (1%)	76	86
1	B	208/222 (94%)	206 (99%)	2 (1%)	76	86
1	C	200/222 (90%)	198 (99%)	2 (1%)	76	86
1	D	203/222 (91%)	200 (98%)	3 (2%)	65	81
1	E	204/222 (92%)	197 (97%)	7 (3%)	37	65
1	F	203/222 (91%)	202 (100%)	1 (0%)	88	93
1	G	201/222 (90%)	194 (96%)	7 (4%)	36	64
1	H	27/222 (12%)	27 (100%)	0	100	100
2	P	3/4 (75%)	3 (100%)	0	100	100
2	Q	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	R	3/4 (75%)	3 (100%)	0	100	100
2	S	4/4 (100%)	4 (100%)	0	100	100
2	T	3/4 (75%)	2 (67%)	1 (33%)	0	1
2	U	3/4 (75%)	3 (100%)	0	100	100
2	V	4/4 (100%)	2 (50%)	2 (50%)	0	0
All	All	1475/1804 (82%)	1447 (98%)	28 (2%)	57	77

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	183	PHE
2	V	677	ASN
2	T	674	PHE
1	G	183	PHE
1	E	231	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	74	GLN
1	E	135	HIS
1	H	11	ASN
1	G	57	ASN
1	G	135	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
2	SEP	S	676	2	8,9,10	0.82	0	8,12,14	1.22	0
2	SEP	U	676	2	8,9,10	0.75	0	8,12,14	1.07	0
2	SEP	Q	676	2	8,9,10	0.77	0	8,12,14	1.50	1 (12%)
2	SEP	V	676	2	8,9,10	0.74	0	8,12,14	1.12	0
4	SEP	W	701	2	8,9,10	0.77	0	8,12,14	1.14	0
2	SEP	T	676	2	8,9,10	0.83	0	8,12,14	1.18	0
2	SEP	P	676	2	8,9,10	0.74	0	8,12,14	1.09	0
2	SEP	R	676	2	8,9,10	0.75	0	8,12,14	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	S	676	2	-	0/5/8/10	-
2	SEP	U	676	2	-	0/5/8/10	-
2	SEP	Q	676	2	-	0/5/8/10	-
2	SEP	V	676	2	-	0/5/8/10	-
4	SEP	W	701	2	-	4/5/8/10	-
2	SEP	T	676	2	-	0/5/8/10	-
2	SEP	P	676	2	-	1/5/8/10	-
2	SEP	R	676	2	-	0/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	676	SEP	OG-CB-CA	3.18	111.24	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	W	701	SEP	N-CA-CB-OG
4	W	701	SEP	CB-OG-P-O2P
4	W	701	SEP	CB-OG-P-O3P
4	W	701	SEP	CB-OG-P-O1P
2	P	676	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	FSC	F	301	-	46,51,51	1.27	3 (6%)	47,77,77	1.70	8 (17%)
3	FSC	E	301	-	46,51,51	1.28	3 (6%)	47,77,77	1.71	8 (17%)
3	FSC	G	301	-	46,51,51	1.28	3 (6%)	47,77,77	1.73	8 (17%)
3	FSC	D	301	-	46,51,51	1.25	3 (6%)	47,77,77	1.66	7 (14%)
4	SEP	W	701	2	8,9,10	0.77	0	8,12,14	1.14	0
3	FSC	C	301	-	46,51,51	1.28	3 (6%)	47,77,77	1.72	8 (17%)
3	FSC	A	301	-	46,51,51	1.28	3 (6%)	47,77,77	1.76	9 (19%)
3	FSC	B	301	-	46,51,51	1.29	3 (6%)	47,77,77	1.72	8 (17%)

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	FSC	F	301	-	-	0/29/103/103	0/4/4/4
3	FSC	E	301	-	-	2/29/103/103	0/4/4/4
3	FSC	G	301	-	-	2/29/103/103	0/4/4/4
3	FSC	D	301	-	-	1/29/103/103	0/4/4/4
4	SEP	W	701	2	-	4/5/8/10	-
3	FSC	C	301	-	-	3/29/103/103	0/4/4/4
3	FSC	A	301	-	-	4/29/103/103	0/4/4/4
3	FSC	B	301	-	-	2/29/103/103	0/4/4/4

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	FSC	C19-C15	-5.25	1.52	1.56
3	A	301	FSC	C19-C15	-5.21	1.52	1.56
3	C	301	FSC	C19-C15	-5.16	1.52	1.56
3	E	301	FSC	C19-C15	-5.12	1.52	1.56
3	F	301	FSC	C19-C15	-5.01	1.52	1.56

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	301	FSC	C15-C19-C12	-5.80	110.68	118.11
3	D	301	FSC	C15-C19-C12	-5.75	110.75	118.11
3	C	301	FSC	C15-C19-C12	-5.68	110.83	118.11
3	B	301	FSC	C15-C19-C12	-5.68	110.84	118.11
3	A	301	FSC	C15-C19-C12	-5.65	110.87	118.11

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	301	FSC	C1-C3-O8-C14
4	W	701	SEP	N-CA-CB-OG
4	W	701	SEP	CB-OG-P-O2P
4	W	701	SEP	CB-OG-P-O3P
3	A	301	FSC	C42-C40-O34-C28

There are no ring outliers.

7 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	301	FSC	15	0
3	E	301	FSC	15	0
3	G	301	FSC	20	0
3	D	301	FSC	13	0
3	C	301	FSC	11	0
3	A	301	FSC	14	0
3	B	301	FSC	14	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 FSC F 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FSC E 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FSC G 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FSC D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FSC C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FSC A 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FSC B 301

Bond lengths

Bond angles

Torsions

Rings
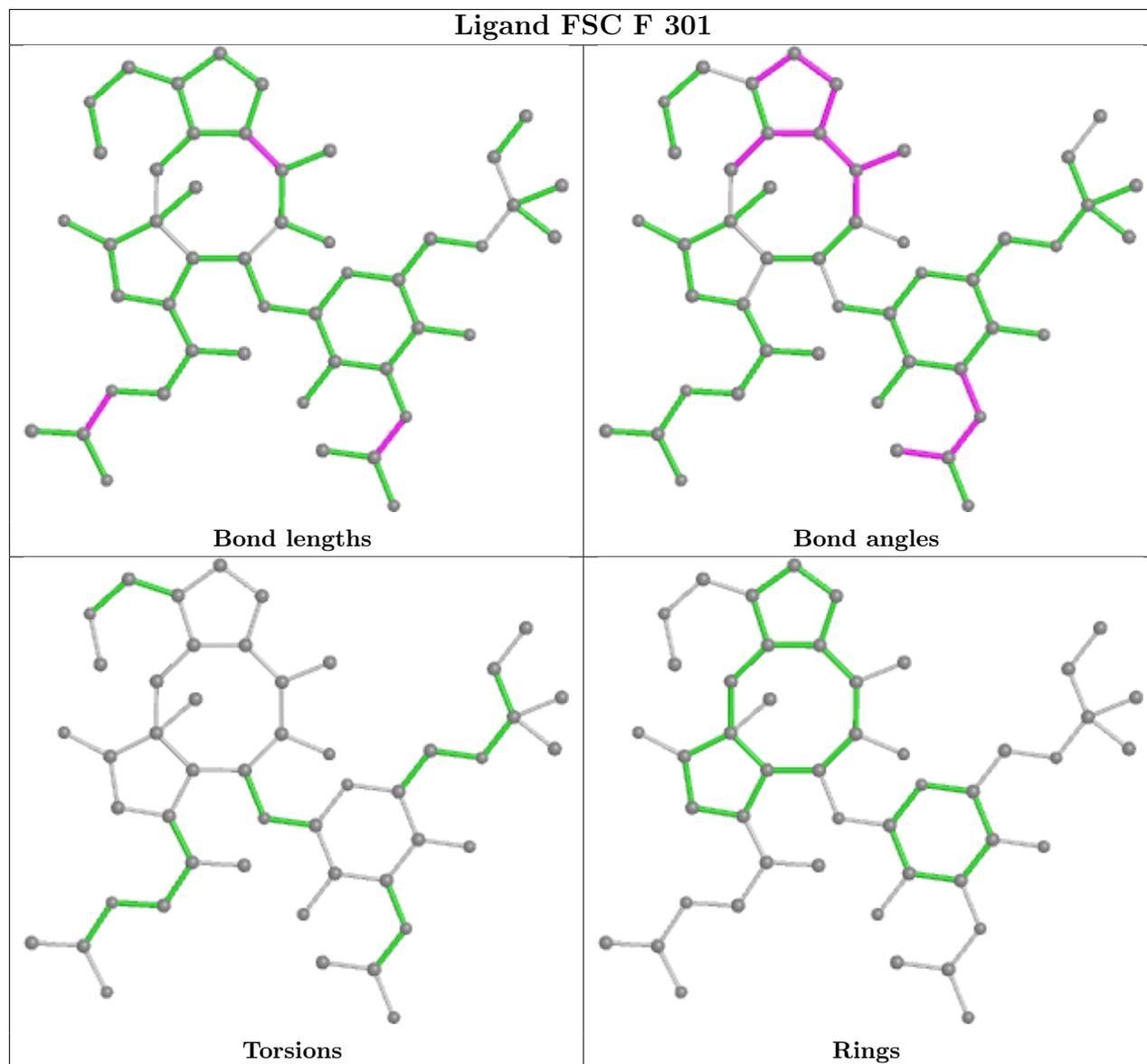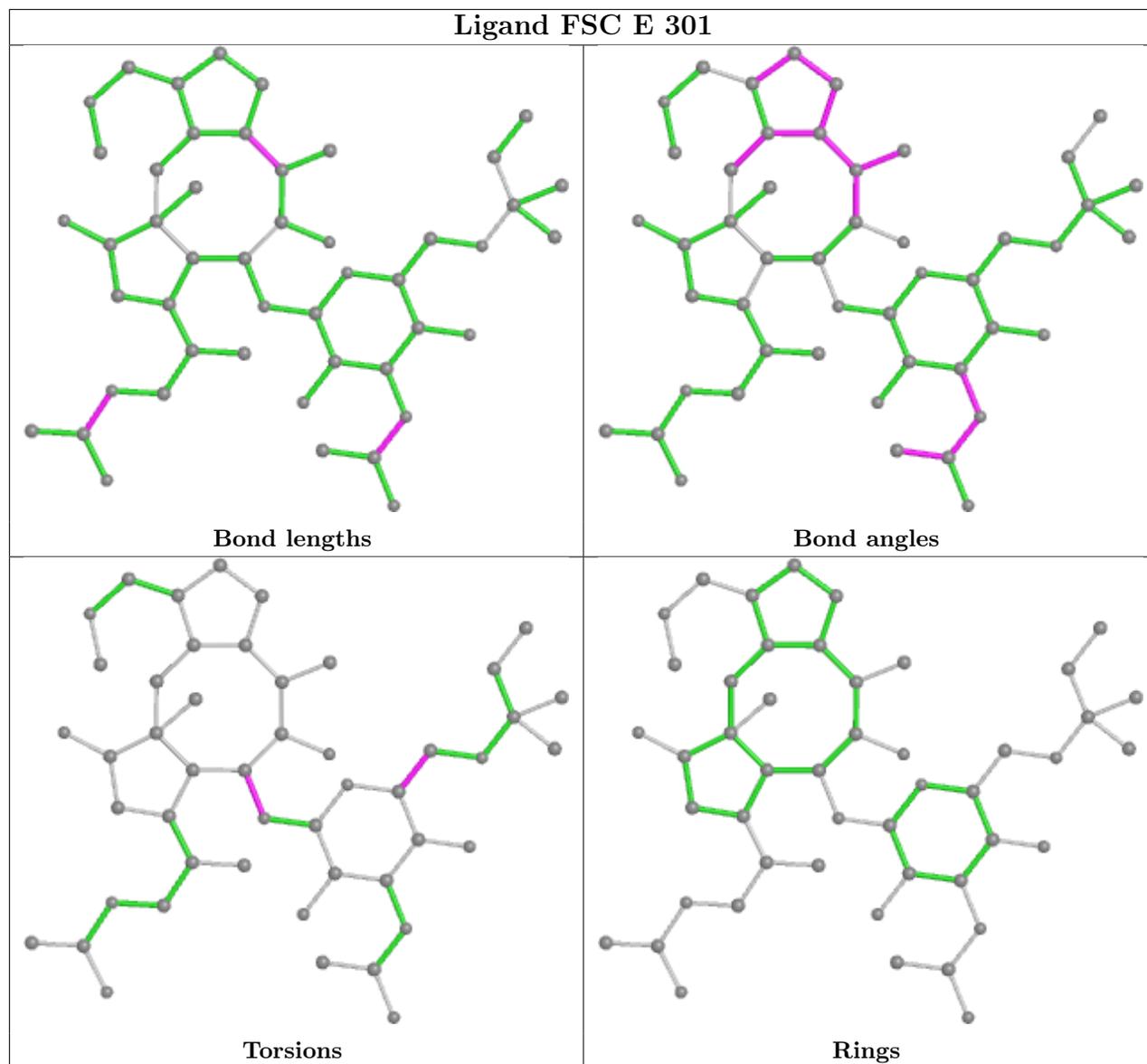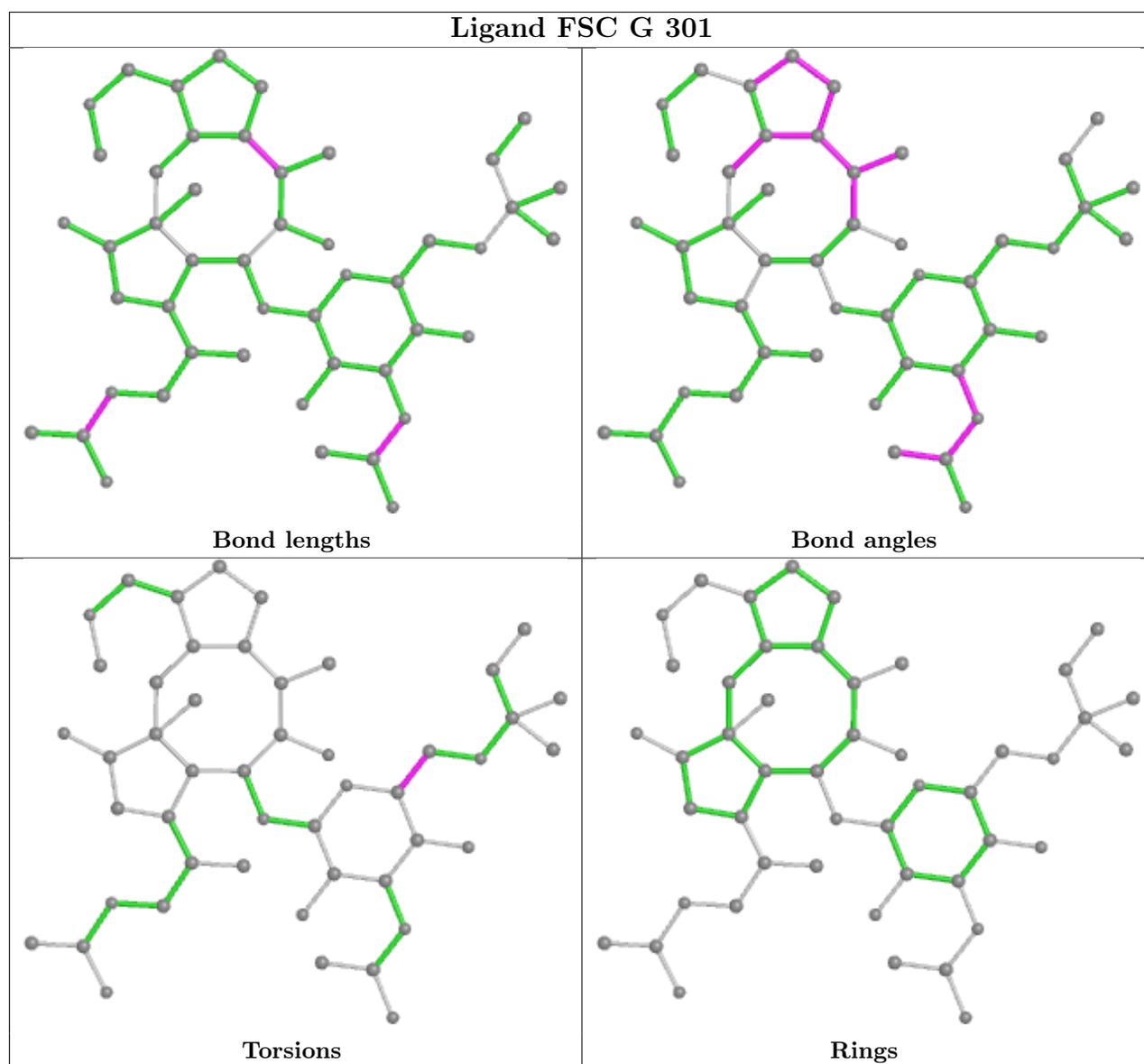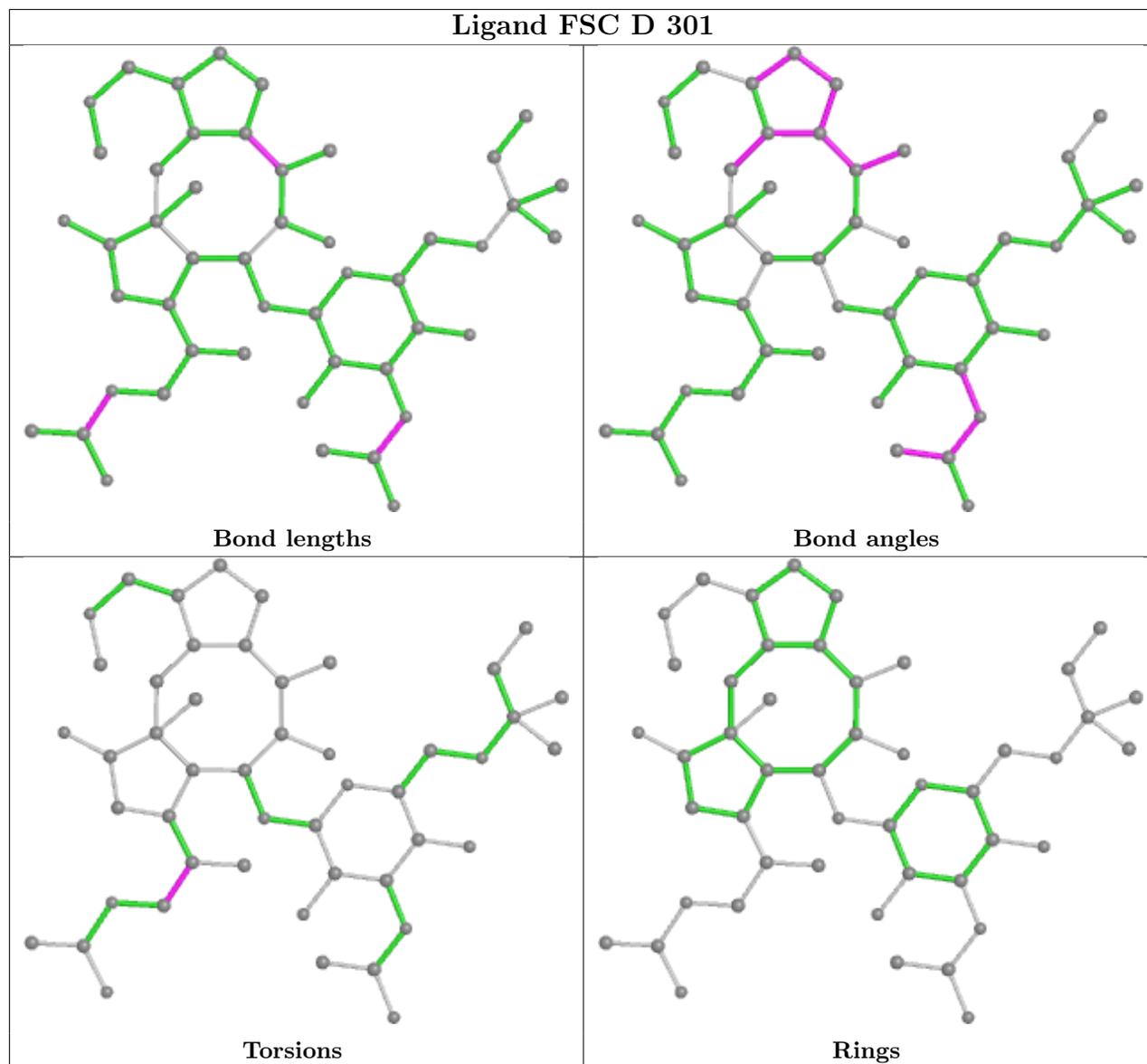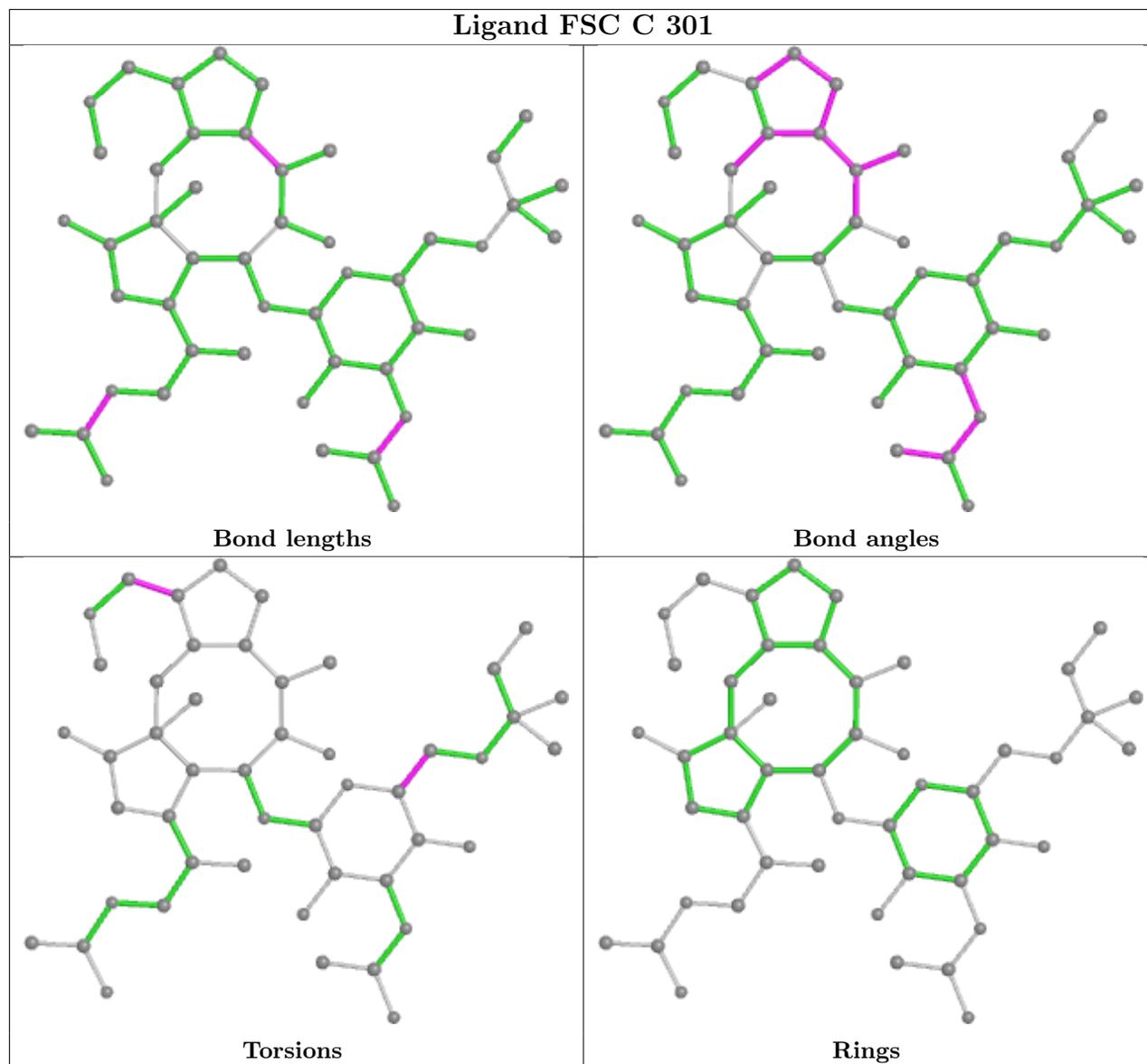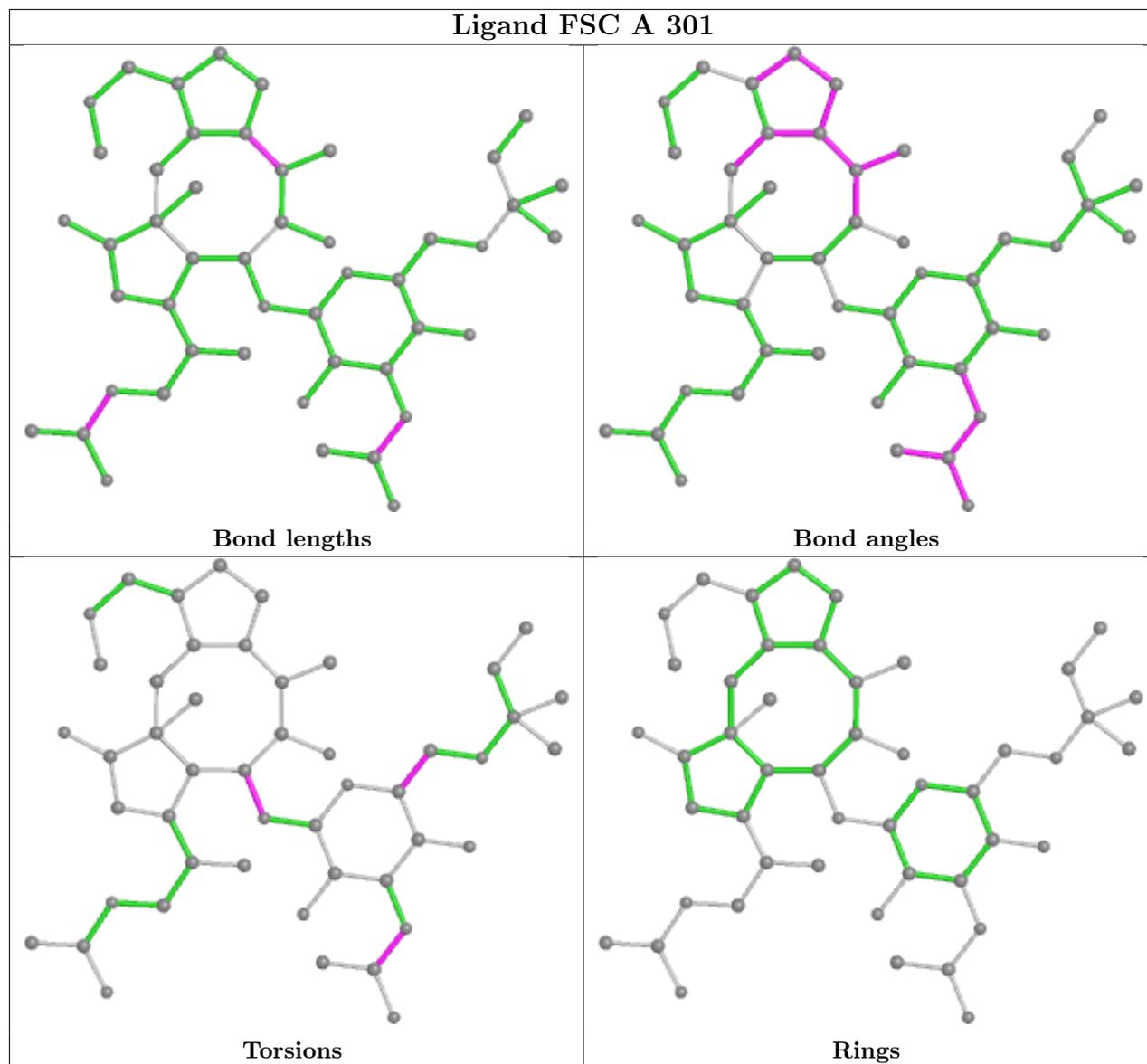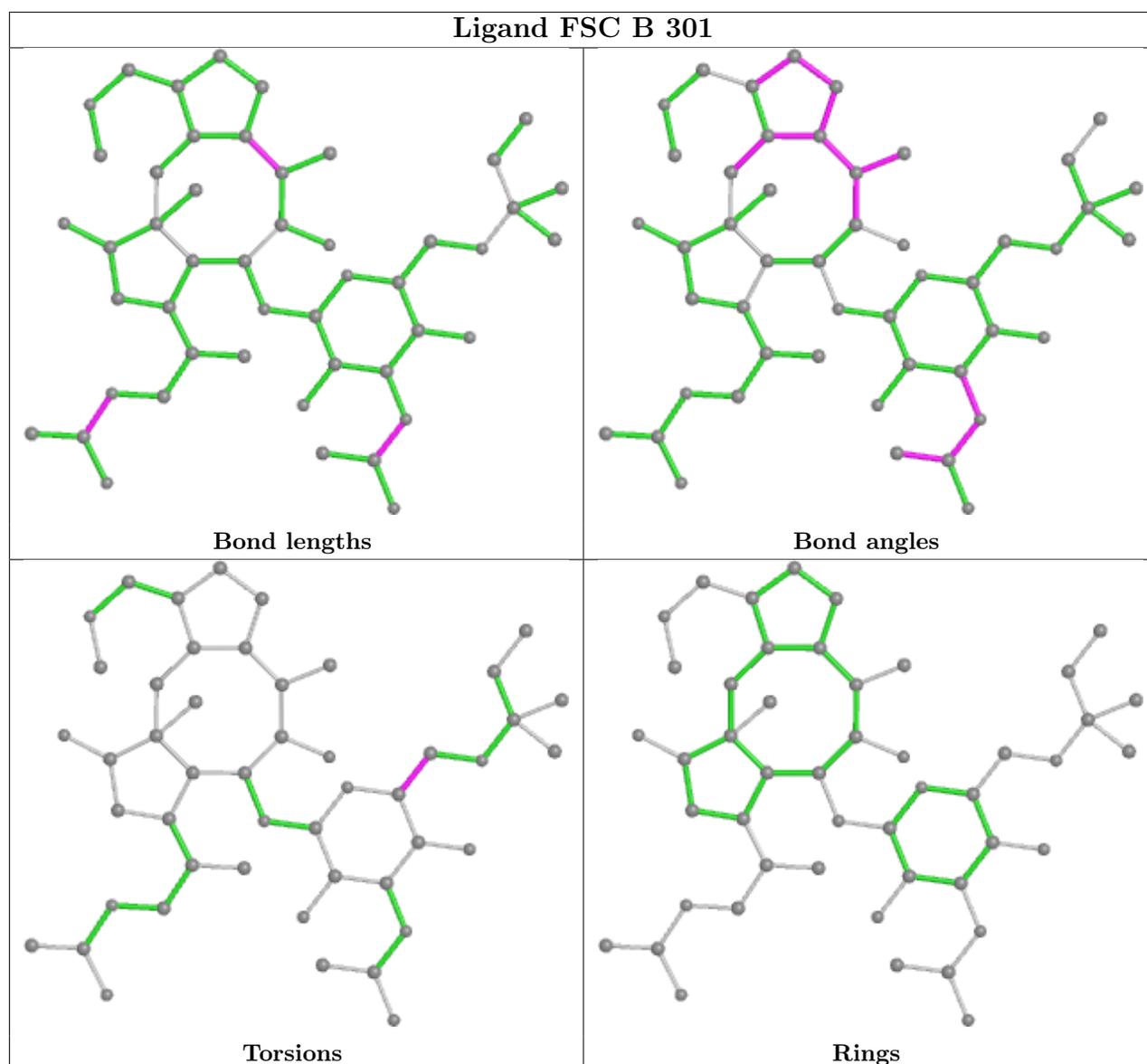
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	239/262 (91%)	-0.47	1 (0%)	92	93	24, 45, 81, 105	0
1	B	245/262 (93%)	-0.46	2 (0%)	86	86	31, 54, 92, 115	0
1	C	234/262 (89%)	-0.53	0	100	100	22, 45, 73, 95	0
1	D	236/262 (90%)	-0.50	0	100	100	22, 48, 84, 109	0
1	E	238/262 (90%)	-0.46	0	100	100	24, 48, 83, 107	0
1	F	237/262 (90%)	-0.38	1 (0%)	92	93	28, 57, 90, 107	0
1	G	234/262 (89%)	-0.22	3 (1%)	77	77	49, 75, 112, 129	0
1	H	213/262 (81%)	0.87	48 (22%)	0	1	87, 137, 196, 203	0
2	P	3/5 (60%)	0.28	0	100	100	86, 86, 97, 104	0
2	Q	4/5 (80%)	-0.09	0	100	100	65, 69, 79, 112	0
2	R	3/5 (60%)	-0.17	0	100	100	63, 63, 75, 82	0
2	S	4/5 (80%)	0.06	0	100	100	69, 75, 97, 107	0
2	T	3/5 (60%)	-0.56	0	100	100	42, 42, 54, 67	0
2	U	3/5 (60%)	0.02	0	100	100	71, 71, 87, 102	0
2	V	4/5 (80%)	0.36	0	100	100	86, 92, 95, 115	0
2	W	1/5 (20%)	1.62	0	100	100	149, 149, 149, 149	0
All	All	1901/2136 (88%)	-0.28	55 (2%)	51	50	22, 56, 142, 203	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	209	ILE	5.9
1	H	235	THR	5.5
1	H	185	VAL	5.3
1	G	218	GLU	5.0
1	G	243	ASP	5.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SEP	W	701	10/11	0.83	0.26	115,123,142,145	0
2	SEP	Q	676	10/11	0.90	0.19	69,81,88,90	0
2	SEP	V	676	10/11	0.92	0.14	82,88,92,93	0
2	SEP	R	676	10/11	0.93	0.17	42,52,64,65	0
2	SEP	S	676	10/11	0.93	0.22	65,67,73,84	0
2	SEP	P	676	10/11	0.95	0.21	61,73,85,86	0
2	SEP	T	676	10/11	0.95	0.13	39,44,52,53	0
2	SEP	U	676	10/11	0.96	0.17	57,69,86,89	0

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SEP	W	701	10/11	0.83	0.26	115,123,142,145	0
3	FSC	G	301	48/48	0.84	0.33	64,81,95,99	0
3	FSC	E	301	48/48	0.94	0.20	31,44,60,64	0
3	FSC	F	301	48/48	0.94	0.21	16,39,46,52	0
3	FSC	A	301	48/48	0.94	0.21	40,55,83,88	0
3	FSC	B	301	48/48	0.94	0.18	39,54,58,66	0
3	FSC	C	301	48/48	0.95	0.18	15,44,69,70	0
3	FSC	D	301	48/48	0.95	0.17	32,46,56,61	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.
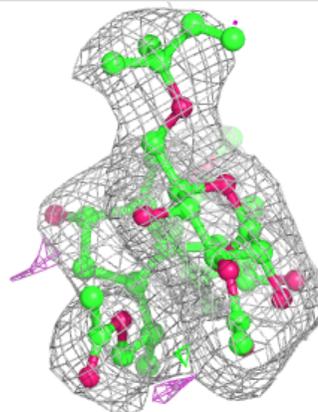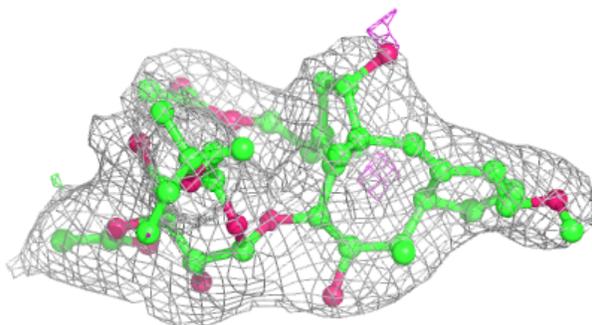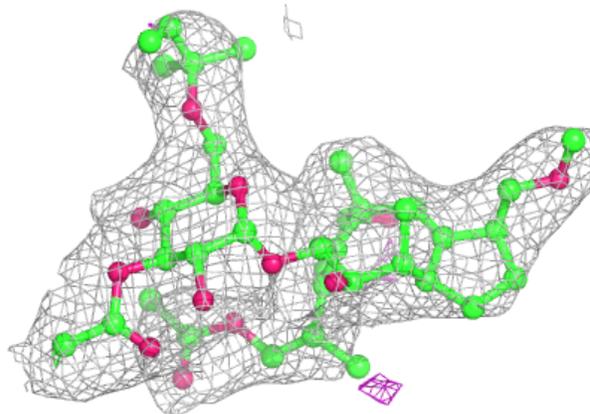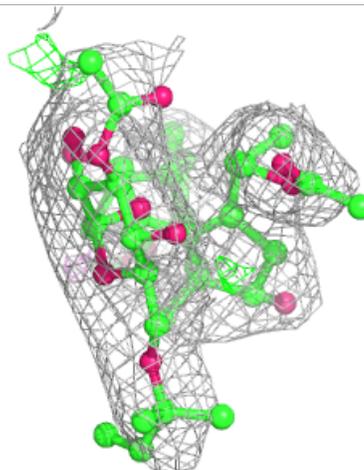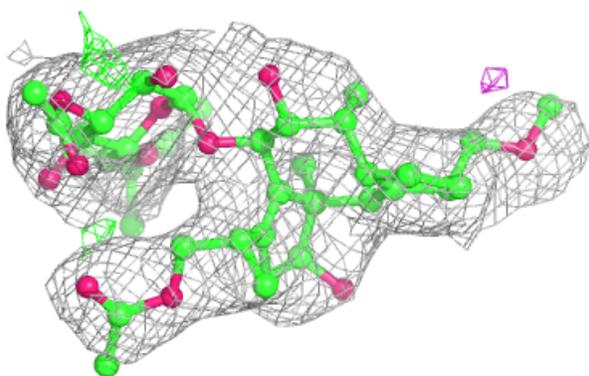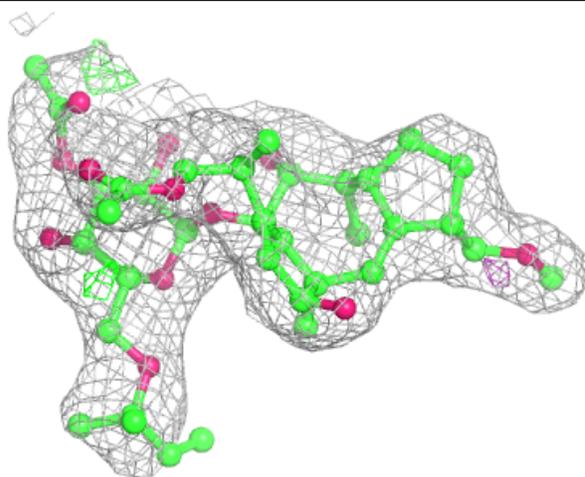
Electron density around FSC G 301:

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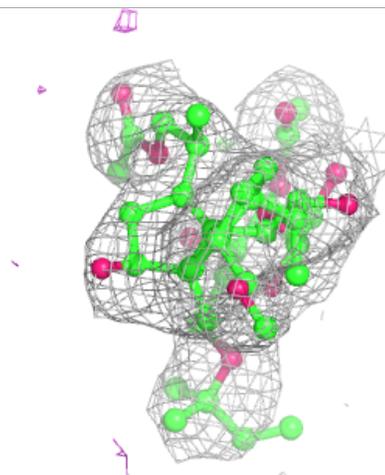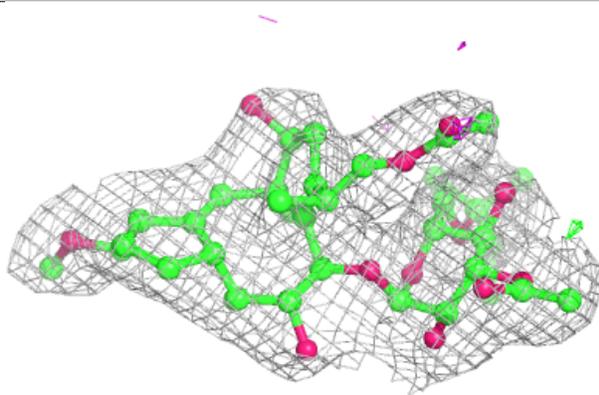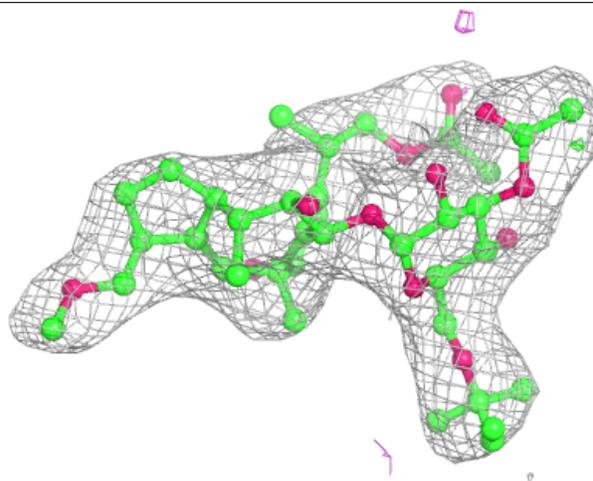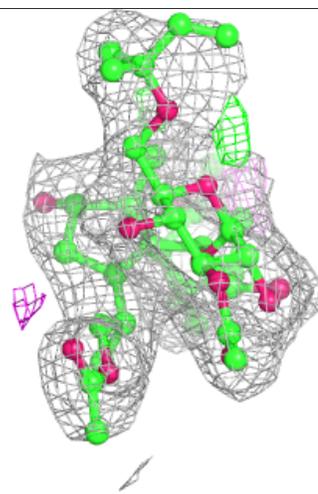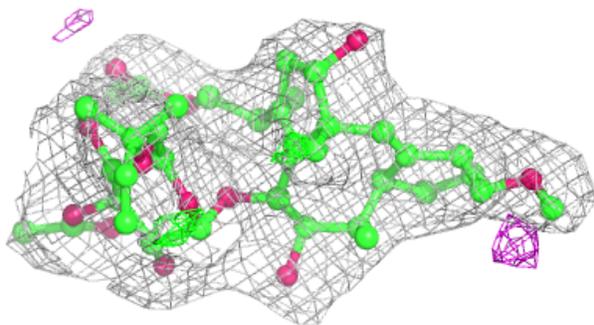mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
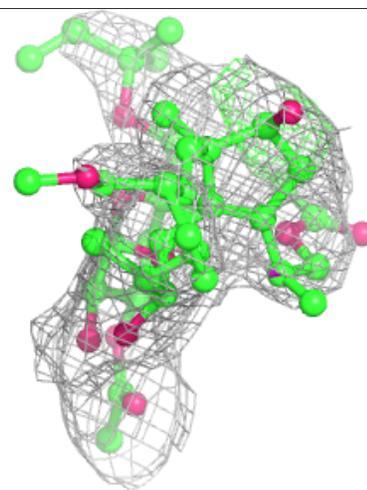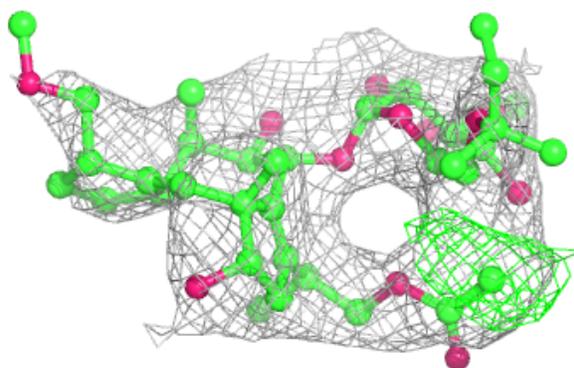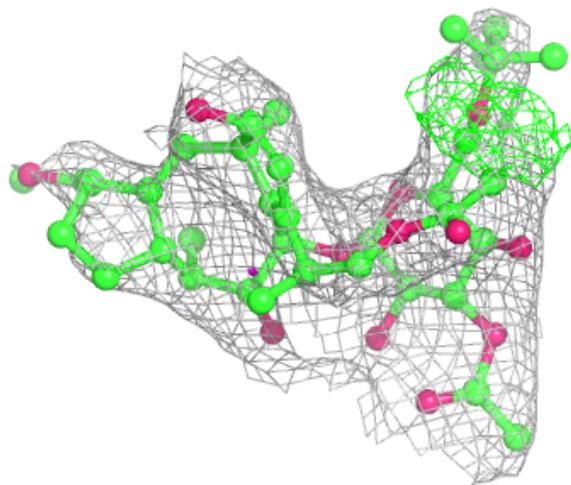
Electron density around FSC E 301:

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$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
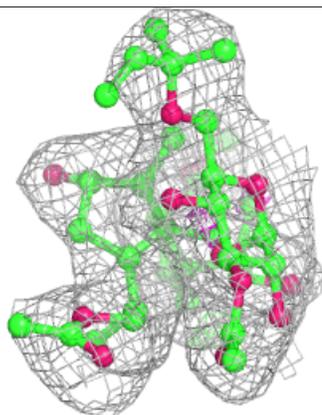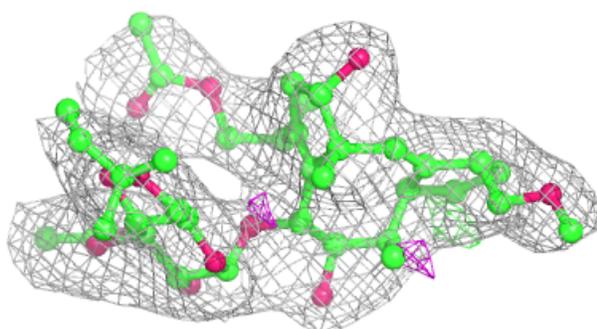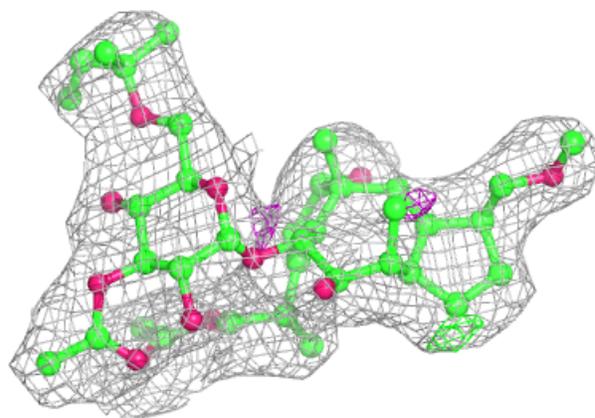
Electron density around FSC F 301:

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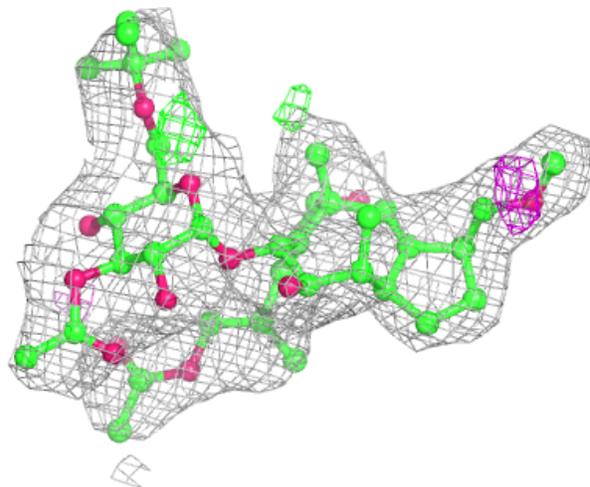$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around FSC A 301:

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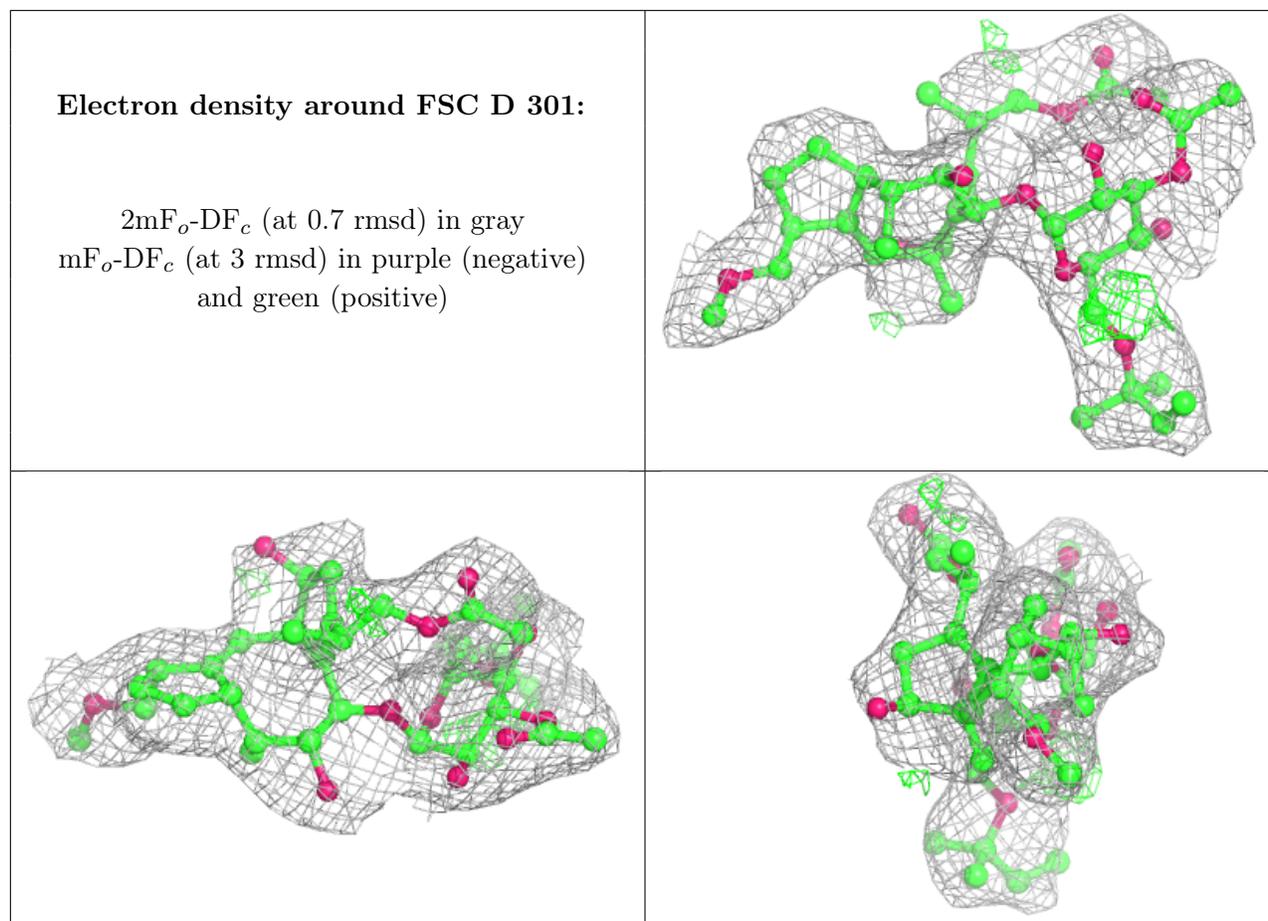and green (positive)

Electron density around FSC B 301:

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

Electron density around FSC C 301:

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

Electron density around FSC D 301:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.