



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:45 pm BST

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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

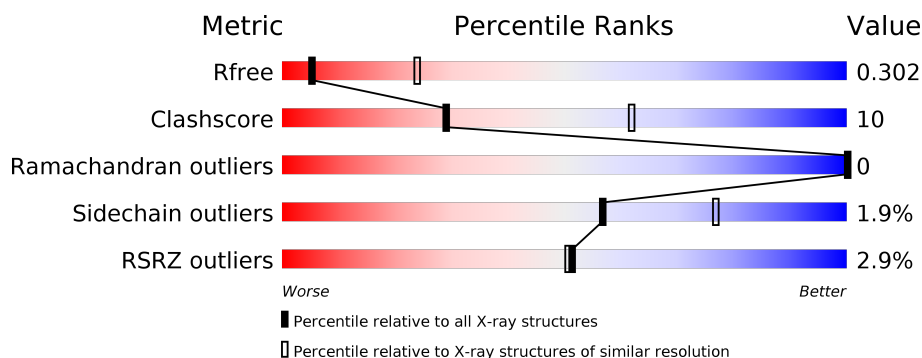
1 Overall quality at a glance

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	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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	262	<div> <div></div> <div>79%12%9%</div> </div>
1	B	262	<div> <div></div> <div>%80%13%6%</div> </div>
1	C	262	<div> <div></div> <div>78%11%11%</div> </div>
1	D	262	<div> <div></div> <div>77%13%10%</div> </div>
1	E	262	<div> <div></div> <div>76%15%9%</div> </div>
1	F	262	<div> <div></div> <div>74%16%10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	262	<div><div>%</div><div><div></div><div>75%</div><div>14%</div><div>11%</div></div></div>
1	H	262	<div><div>18%</div><div><div></div><div>78%</div><div>19%</div></div></div>
2	P	5	<div><div></div><div><div>80%</div><div>20%</div></div></div>
2	Q	5	<div><div></div><div><div>60%</div><div>40%</div></div></div>
2	R	5	<div><div></div><div><div>60%</div><div>20%</div><div>20%</div></div></div>
2	S	5	<div><div></div><div><div>100%</div></div></div>
2	T	5	<div><div></div><div><div>60%</div><div>20%</div><div>20%</div></div></div>
2	U	5	<div><div></div><div><div>60%</div><div>20%</div><div>20%</div></div></div>
2	V	5	<div><div></div><div><div>40%</div><div>40%</div><div>20%</div></div></div>
2	W	5	<div><div></div><div><div>20%</div><div>80%</div></div></div>

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

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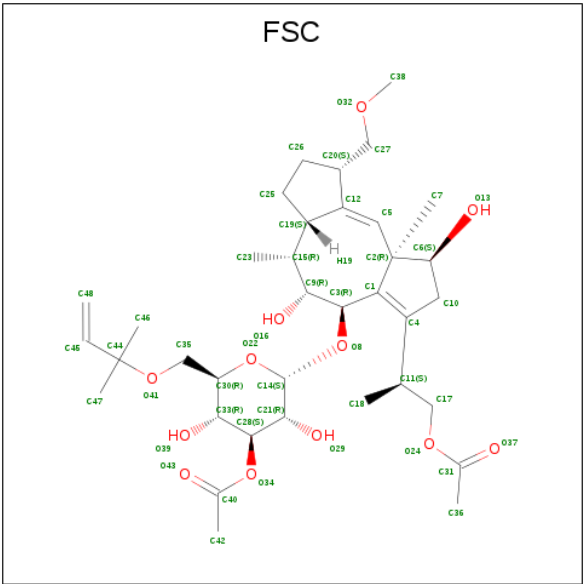
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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLY	-	expression tag	UNP Q5KTN5
H	-1	PRO	-	expression tag	UNP Q5KTN5
H	0	GLY	-	expression tag	UNP Q5KTN5

- Molecule 2 is a protein called Potassium channel KAT1.

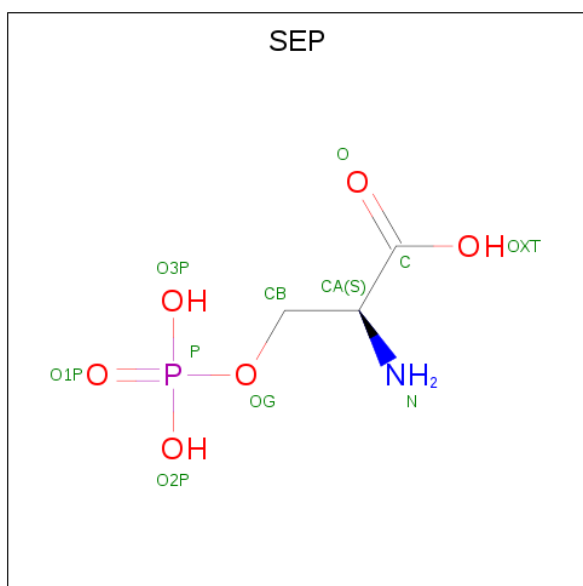
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	4	Total	C	N	O	P	0	0	0
			36	19	5	11	1			
2	Q	5	Total	C	N	O	P	0	0	0
			48	28	6	13	1			
2	R	4	Total	C	N	O	P	0	0	0
			36	19	5	11	1			
2	S	5	Total	C	N	O	P	0	0	0
			48	28	6	13	1			
2	T	4	Total	C	N	O	P	0	0	0
			36	19	5	11	1			
2	U	4	Total	C	N	O	P	0	0	0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

- Molecule 3 is FUSICOCCIN (three-letter code: FSC) (formula: C₃₆H₅₆O₁₂).



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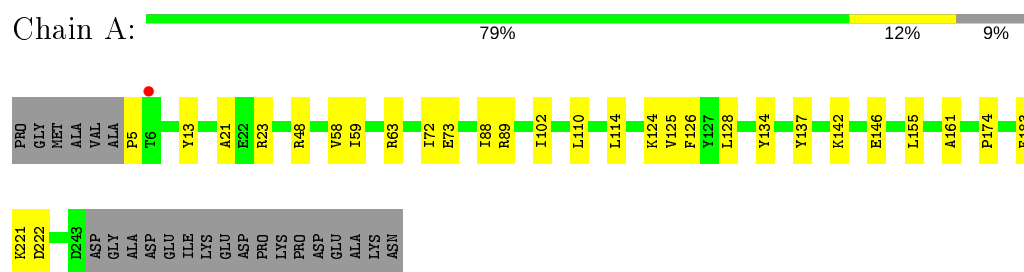
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Q	1	Total 1	O 1	0	0
5	C	15	Total 15	O 15	0	0
5	R	1	Total 1	O 1	0	0
5	D	13	Total 13	O 13	0	0
5	E	21	Total 21	O 21	0	0
5	T	2	Total 2	O 2	0	0
5	F	14	Total 14	O 14	0	0
5	G	7	Total 7	O 7	0	0
5	V	1	Total 1	O 1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

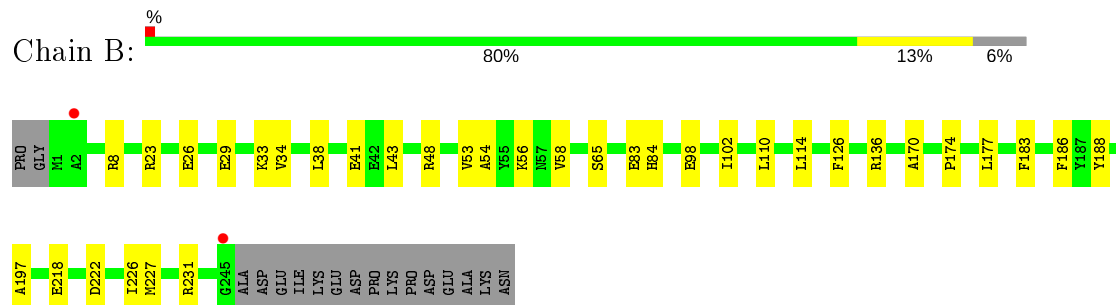
3 Residue-property plots

These plots are drawn for all protein, RNA 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.

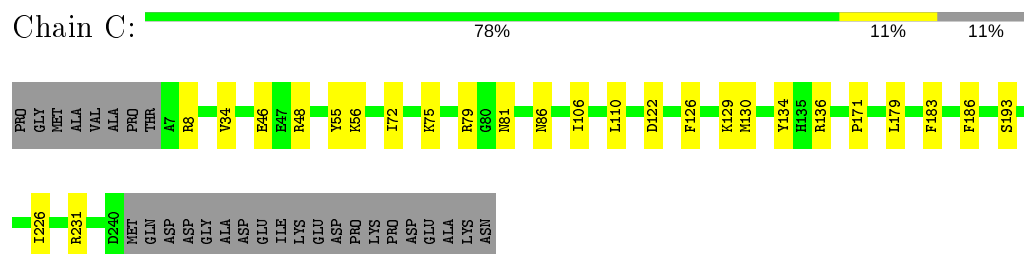
• Molecule 1: 14-3-3 c-1 protein



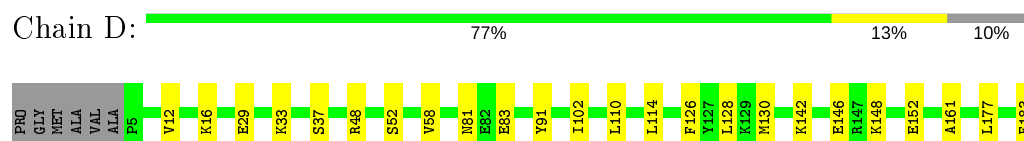
• Molecule 1: 14-3-3 c-1 protein

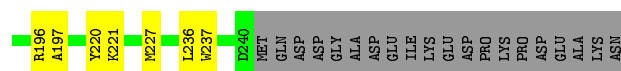


• Molecule 1: 14-3-3 c-1 protein



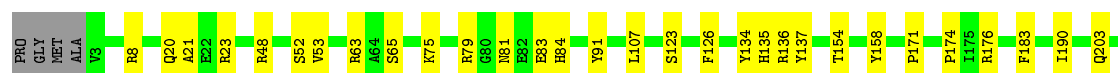
• Molecule 1: 14-3-3 c-1 protein





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

Chain E: 76% 15% 9%



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

Chain F: 74% 16% 10%



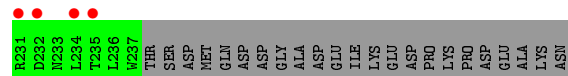
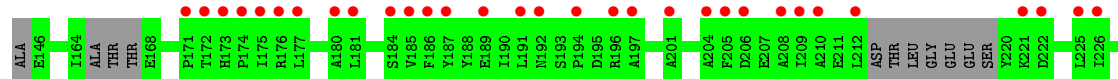
- Molecule 1: 14-3-3 c-1 protein

Chain G: 75% 14% 11%




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

Chain H: 18% 78% 19%



- Molecule 2: Potassium channel KAT1

Chain P:  80% 20%



- Molecule 2: Potassium channel KAT1

Chain Q:  60% 40%



- Molecule 2: Potassium channel KAT1

Chain R:  60% 20% 20%



- 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%



- Molecule 2: Potassium channel KAT1

Chain U:  60% 20% 20%



- Molecule 2: Potassium channel KAT1

Chain V:  40% 40% 20%



- Molecule 2: Potassium channel KAT1

Chain W:  20% 80%



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	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.*

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: FSC, SEP

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(°)	Ideal(°)
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.

All (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:G:110:LEU:HD21	1:G:130:MET:HE3	1.15	1.08
1:B:38:LEU:HD22	1:B:41:GLU:HG3	1.25	1.08
1:C:79:ARG:NH1	1:E:207:GLU:CG	2.16	1.06
1:C:79:ARG:HH11	1:E:207:GLU:CG	1.70	1.05
3:G:301:FSC:H271	3:G:301:FSC:H233	1.32	1.05
1:A:5:PRO:HD3	1:B:83:GLU:OE1	1.55	1.04
1:B:38:LEU:HD22	1:B:41:GLU:CG	1.91	1.00
1:F:81:ASN:OD1	1:F:84:HIS:ND1	1.94	1.00
1:G:110:LEU:CD2	1:G:130:MET:HE2	1.81	0.97
1:G:110:LEU:CD2	1:G:130:MET:HE3	1.79	0.97
1:C:79:ARG:HH12	1:E:207:GLU:HG2	1.30	0.96
3:B:301:FSC:H19	3:B:301:FSC:H182	1.49	0.94
1:G:110:LEU:HD21	1:G:130:MET:HE2	0.93	0.94
1:C:46:GLU:HG3	3:C:301:FSC:H482	1.48	0.93
3:B:301:FSC:H7C2	3:B:301:FSC:H232	1.51	0.90
3:D:301:FSC:H182	3:D:301:FSC:H19	1.54	0.88
1:G:110:LEU:CG	1:G:130:MET:HE3	2.04	0.88
3:D:301:FSC:C40	3:D:301:FSC:H363	2.03	0.87
1:C:106:ILE:HG21	1:C:134:TYR:CD2	2.09	0.87
1:B:38:LEU:CD2	1:B:41:GLU:HG3	2.04	0.87
3:G:301:FSC:O39	3:G:301:FSC:H363	1.75	0.87
1:A:174:PRO:CB	1:A:222:ASP:OD2	2.23	0.86
3:G:301:FSC:C27	3:G:301:FSC:H233	2.07	0.85
1:A:174:PRO:HB3	1:A:222:ASP:OD2	1.77	0.85
1:C:72:ILE:HD12	1:E:214:THR:O	1.79	0.82
1:F:46:GLU:HG2	3:F:301:FSC:H482	1.61	0.80
1:A:126:PHE:CD1	3:A:301:FSC:H382	2.16	0.80
3:C:301:FSC:H232	3:C:301:FSC:H7C2	1.62	0.80
3:B:301:FSC:H363	3:B:301:FSC:O39	1.82	0.79
1:C:75:LYS:HB3	1:E:214:THR:HG22	1.64	0.78
3:F:301:FSC:H182	3:F:301:FSC:H19	1.66	0.77
1:C:106:ILE:HG21	1:C:134:TYR:CE2	2.19	0.76
1:C:72:ILE:CD1	1:E:214:THR:O	2.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:VAL:HG21	3:E:301:FSC:H462	1.67	0.75
1:B:174:PRO:HG2	1:B:222:ASP:OD2	1.86	0.75
1:G:110:LEU:HD21	1:G:130:MET:HE1	1.58	0.74
1:C:55:TYR:CB	1:C:134:TYR:OH	2.35	0.74
3:A:301:FSC:H7C2	3:A:301:FSC:H232	1.69	0.73
1:F:83:GLU:N	1:F:83:GLU:OE1	2.21	0.73
1:C:79:ARG:HH11	1:E:207:GLU:HG2	0.90	0.72
3:B:301:FSC:C7	3:B:301:FSC:H232	2.20	0.72
1:C:75:LYS:CB	1:E:214:THR:HG22	2.20	0.71
1:B:38:LEU:CD2	1:B:41:GLU:CG	2.67	0.70
3:E:301:FSC:H7C2	3:E:301:FSC:H232	1.74	0.70
1:F:221:LYS:HD2	3:F:301:FSC:H421	1.72	0.69
1:D:37:SER:HA	1:G:113:LYS:HG2	1.75	0.69
1:A:13:TYR:CE1	1:B:84:HIS:CE1	2.82	0.67
3:D:301:FSC:H363	3:D:301:FSC:O43	1.94	0.67
3:D:301:FSC:H271	3:D:301:FSC:H233	1.79	0.65
1:E:203:GLN:O	1:E:207:GLU:HG3	1.95	0.65
1:A:126:PHE:CE1	3:A:301:FSC:C38	2.81	0.65
1:C:221:LYS:HB2	3:C:301:FSC:H421	1.79	0.64
3:F:301:FSC:O39	3:F:301:FSC:H363	1.97	0.63
1:E:221:LYS:HD3	1:E:221:LYS:H	1.63	0.63
3:F:301:FSC:H7C3	3:F:301:FSC:H352	1.81	0.63
1:G:110:LEU:HD11	1:G:130:MET:HG2	1.80	0.62
3:G:301:FSC:H351	3:G:301:FSC:C36	2.29	0.62
1:B:8:ARG:HG3	1:B:34:VAL:HG13	1.81	0.62
3:E:301:FSC:H11	3:E:301:FSC:H9	1.80	0.62
1:G:131:LYS:HG3	1:G:135:HIS:HD2	1.64	0.62
1:E:107:LEU:HD21	1:E:135:HIS:CD2	2.34	0.61
1:G:126:PHE:CZ	3:G:301:FSC:H383	2.35	0.61
1:B:53:VAL:HG21	3:B:301:FSC:C47	2.30	0.61
1:F:81:ASN:CG	1:F:84:HIS:HD1	1.97	0.61
1:F:83:GLU:CD	1:F:83:GLU:H	2.03	0.61
1:B:53:VAL:HG21	3:B:301:FSC:H472	1.83	0.61
3:C:301:FSC:H232	3:C:301:FSC:C7	2.30	0.61
3:F:301:FSC:H233	3:F:301:FSC:H271	1.84	0.60
1:A:5:PRO:HD3	1:B:83:GLU:CD	2.22	0.60
3:A:301:FSC:H9	3:A:301:FSC:H11	1.82	0.59
1:G:124:LYS:O	1:G:128:LEU:HG	2.03	0.59
1:A:221:LYS:HZ2	1:A:221:LYS:HB2	1.68	0.59
1:D:29:GLU:O	1:D:33:LYS:HG3	2.02	0.59
1:A:174:PRO:CG	1:A:222:ASP:OD2	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:301:FSC:C5	3:B:301:FSC:H232	2.32	0.59
1:A:126:PHE:CE1	3:A:301:FSC:H383	2.39	0.58
1:D:193:SER:HB3	1:D:196:ARG:HG3	1.86	0.57
1:G:48:ARG:HG2	1:G:126:PHE:CZ	2.39	0.57
1:A:13:TYR:CD1	1:B:84:HIS:CE1	2.92	0.57
3:C:301:FSC:H232	3:C:301:FSC:C5	2.34	0.57
1:E:136:ARG:HB2	1:E:154:THR:HG21	1.87	0.57
3:B:301:FSC:C2	3:B:301:FSC:H232	2.35	0.57
1:C:86:ASN:ND2	5:C:402:HOH:O	2.38	0.57
1:C:129:LYS:HB2	1:C:179:LEU:HD13	1.86	0.56
1:F:96:GLU:HA	1:F:99:LEU:HD12	1.87	0.56
1:C:136:ARG:HD3	1:C:186:PHE:HB2	1.87	0.56
1:E:83:GLU:OE1	1:E:83:GLU:HA	2.06	0.56
3:F:301:FSC:H7C2	3:F:301:FSC:H232	1.87	0.56
1:E:20:GLN:HG2	1:F:72:ILE:HD11	1.87	0.56
1:A:125:VAL:HG13	1:A:161:ALA:HB1	1.88	0.55
1:G:201:ALA:HB3	1:G:234:LEU:HD21	1.88	0.55
3:G:301:FSC:H351	3:G:301:FSC:H363	1.88	0.55
1:C:79:ARG:NH2	1:C:81:ASN:OD1	2.38	0.55
3:D:301:FSC:C27	3:D:301:FSC:H233	2.37	0.55
3:B:301:FSC:H19	3:B:301:FSC:C18	2.31	0.55
1:E:65:SER:HB3	1:F:21:ALA:HB1	1.88	0.55
1:G:240:ASP:OD1	1:G:241:MET:SD	2.65	0.55
3:D:301:FSC:C19	3:D:301:FSC:C1	2.85	0.55
3:G:301:FSC:C35	3:G:301:FSC:H362	2.37	0.55
3:A:301:FSC:C5	3:A:301:FSC:H232	2.37	0.54
3:B:301:FSC:C1	3:B:301:FSC:C19	2.85	0.54
3:G:301:FSC:C35	3:G:301:FSC:C36	2.86	0.54
3:A:301:FSC:C1	3:A:301:FSC:C19	2.85	0.54
3:E:301:FSC:H271	3:E:301:FSC:H233	1.89	0.54
1:F:174:PRO:HB3	1:F:222:ASP:HB3	1.88	0.54
3:F:301:FSC:C19	3:F:301:FSC:C1	2.85	0.54
1:A:174:PRO:HB3	1:A:222:ASP:CG	2.28	0.54
1:A:126:PHE:CE1	3:A:301:FSC:H382	2.43	0.54
3:G:301:FSC:O43	3:G:301:FSC:O29	2.24	0.53
3:E:301:FSC:C1	3:E:301:FSC:C19	2.85	0.53
3:E:301:FSC:C5	3:E:301:FSC:H232	2.38	0.53
1:D:142:LYS:HD3	1:D:146:GLU:HB3	1.91	0.53
1:A:221:LYS:NZ	1:A:221:LYS:HB2	2.24	0.53
3:D:301:FSC:H19	3:D:301:FSC:C1	2.39	0.53
3:E:301:FSC:C1	3:E:301:FSC:H19	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:HG2	1:A:126:PHE:CE2	2.45	0.52
3:A:301:FSC:C7	3:A:301:FSC:H232	2.38	0.52
3:F:301:FSC:C1	3:F:301:FSC:H19	2.39	0.52
1:A:221:LYS:HB2	3:A:301:FSC:H421	1.92	0.52
3:C:301:FSC:C1	3:C:301:FSC:C19	2.87	0.52
3:D:301:FSC:H232	3:D:301:FSC:H7C2	1.92	0.52
3:A:301:FSC:C1	3:A:301:FSC:H19	2.40	0.52
1:D:81:ASN:HB2	1:D:83:GLU:OE2	2.09	0.52
1:F:136:ARG:HD3	1:F:186:PHE:HB2	1.92	0.51
3:B:301:FSC:C1	3:B:301:FSC:H19	2.40	0.51
1:A:221:LYS:CB	1:A:221:LYS:NZ	2.73	0.51
3:C:301:FSC:H232	3:C:301:FSC:C2	2.41	0.51
1:G:71:SER:O	1:G:75:LYS:HG2	2.11	0.51
3:F:301:FSC:H233	3:F:301:FSC:C27	2.40	0.51
3:F:301:FSC:C5	3:F:301:FSC:H232	2.41	0.51
3:G:301:FSC:C1	3:G:301:FSC:C19	2.89	0.50
1:B:136:ARG:HD3	1:B:186:PHE:HB2	1.92	0.50
1:G:142:LYS:HD3	1:G:146:GLU:HB3	1.92	0.50
1:A:5:PRO:CD	1:B:83:GLU:OE1	2.45	0.50
1:E:174:PRO:HG3	1:E:223:SER:HB2	1.94	0.50
3:D:301:FSC:C5	3:D:301:FSC:H232	2.42	0.50
3:D:301:FSC:H9	3:D:301:FSC:H11	1.93	0.50
1:D:177:LEU:HD13	1:D:227:MET:HG3	1.94	0.50
3:G:301:FSC:C1	3:G:301:FSC:H19	2.42	0.50
1:E:21:ALA:HB2	1:F:69:ILE:HD13	1.93	0.49
1:G:84:HIS:O	1:G:88:ILE:HG13	2.12	0.49
1:H:75:LYS:O	1:H:79:ARG:HG2	2.12	0.49
3:C:301:FSC:H19	3:C:301:FSC:C1	2.43	0.49
1:B:174:PRO:CG	1:B:222:ASP:OD2	2.60	0.49
1:B:48:ARG:HG2	1:B:126:PHE:CE2	2.48	0.49
1:A:73:GLU:OE2	1:A:89:ARG:HG2	2.13	0.48
1:C:171:PRO:HD2	1:C:211:GLU:HG3	1.96	0.48
1:E:48:ARG:NH1	1:E:123:SER:HB3	2.28	0.48
3:D:301:FSC:C18	3:D:301:FSC:H19	2.35	0.48
1:G:181:LEU:HD13	1:G:230:LEU:HD23	1.95	0.48
1:G:71:SER:O	1:G:74:GLN:HG2	2.14	0.48
1:F:62:ARG:HD2	1:F:98:GLU:OE2	2.14	0.48
1:E:136:ARG:HG3	1:E:190:ILE:HG13	1.95	0.48
1:B:177:LEU:HD13	1:B:227:MET:HG3	1.96	0.48
1:F:73:GLU:HB2	1:F:88:ILE:HG21	1.95	0.48
1:C:48:ARG:HG2	1:C:126:PHE:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:GLU:HG3	1:D:190:ILE:HG12	1.94	0.47
1:F:110:LEU:HD11	1:F:130:MET:HG2	1.96	0.47
1:C:226:ILE:HD11	3:C:301:FSC:H252	1.97	0.47
1:D:221:LYS:HD3	1:D:221:LYS:O	2.14	0.47
3:E:301:FSC:C27	3:E:301:FSC:H233	2.43	0.47
1:C:75:LYS:HB3	1:E:214:THR:CG2	2.40	0.47
3:F:301:FSC:H11	3:F:301:FSC:H9	1.97	0.47
1:G:110:LEU:CD1	1:G:130:MET:HE3	2.44	0.47
1:B:218:GLU:OE2	1:B:218:GLU:HA	2.14	0.47
3:D:301:FSC:O43	3:D:301:FSC:O29	2.23	0.47
1:E:134:TYR:HA	1:E:137:TYR:CD2	2.49	0.47
1:B:58:VAL:HG12	1:B:102:ILE:HD13	1.97	0.47
3:E:301:FSC:C7	3:E:301:FSC:H232	2.42	0.47
1:G:173:HIS:HE1	1:G:175:ILE:HD12	1.80	0.46
1:G:21:ALA:HB1	1:H:65:SER:HB3	1.97	0.46
1:A:124:LYS:O	1:A:128:LEU:HG	2.15	0.46
1:F:56:LYS:HD2	2:U:677:ASN:HD22	1.80	0.46
3:G:301:FSC:H11	3:G:301:FSC:H9	1.97	0.46
1:C:8:ARG:HG3	1:C:34:VAL:HG13	1.96	0.46
3:D:301:FSC:C40	3:D:301:FSC:C36	2.86	0.46
1:A:142:LYS:HD3	1:A:146:GLU:HB3	1.97	0.46
1:G:110:LEU:HG	1:G:130:MET:HE3	1.91	0.46
3:G:301:FSC:H351	3:G:301:FSC:H362	1.95	0.46
1:A:23:ARG:NH1	1:B:98:GLU:OE2	2.36	0.46
1:D:58:VAL:HG12	1:D:102:ILE:HD13	1.96	0.46
1:C:55:TYR:HB3	1:C:134:TYR:HH	1.75	0.46
1:B:126:PHE:CD1	3:B:301:FSC:H382	2.51	0.46
1:E:21:ALA:HB2	1:F:69:ILE:CD1	2.46	0.46
1:G:56:LYS:NZ	3:G:301:FSC:O13	2.49	0.46
1:B:188:TYR:HB2	1:B:197:ALA:CB	2.45	0.45
1:G:230:LEU:O	1:G:234:LEU:HG	2.16	0.45
1:B:29:GLU:O	1:B:33:LYS:HG3	2.16	0.45
1:E:52:SER:OG	3:E:301:FSC:H7C1	2.16	0.45
3:B:301:FSC:C23	3:B:301:FSC:C5	2.91	0.45
1:B:170:ALA:HB2	1:C:46:GLU:OE2	2.16	0.45
1:B:54:ALA:O	1:B:58:VAL:HG23	2.16	0.45
1:F:32:GLU:HG2	1:F:109:LEU:HD22	1.98	0.45
1:B:56:LYS:HZ1	2:Q:677:ASN:HB2	1.82	0.45
1:A:13:TYR:CE1	1:B:84:HIS:ND1	2.85	0.45
1:E:107:LEU:CD2	1:E:135:HIS:CD2	2.99	0.45
1:A:58:VAL:HG12	1:A:102:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:HD11	1:B:43:LEU:HD23	1.99	0.45
1:B:56:LYS:NZ	2:Q:677:ASN:HB2	2.32	0.45
1:C:75:LYS:CD	1:E:214:THR:HA	2.47	0.45
1:G:201:ALA:HB1	1:G:230:LEU:HD22	1.98	0.45
1:A:59:ILE:HG13	1:A:63:ARG:HD2	1.98	0.44
1:A:72:ILE:HG22	1:A:88:ILE:HD13	1.98	0.44
1:G:91:TYR:OH	1:H:23:ARG:HD2	2.17	0.44
1:C:231:ARG:HA	1:C:231:ARG:HE	1.82	0.44
1:D:197:ALA:HB1	1:D:237:TRP:CZ3	2.53	0.44
1:G:126:PHE:CD2	3:G:301:FSC:H382	2.52	0.44
1:G:48:ARG:HD2	1:G:126:PHE:CG	2.52	0.44
1:H:70:SER:HA	1:H:92:ARG:HH21	1.82	0.44
1:A:185:VAL:O	1:A:189:GLU:HG2	2.17	0.44
1:D:48:ARG:HG2	1:D:126:PHE:CE1	2.52	0.44
1:E:226:ILE:HD12	1:E:226:ILE:H	1.83	0.44
1:E:107:LEU:HD21	1:E:135:HIS:HD2	1.82	0.44
3:E:301:FSC:H28	3:E:301:FSC:H171	1.99	0.44
1:F:202:LYS:HE3	1:F:206:ASP:OD2	2.17	0.44
3:F:301:FSC:O29	3:F:301:FSC:O43	2.25	0.44
1:E:221:LYS:HD3	1:E:221:LYS:N	2.32	0.44
1:F:226:ILE:HD11	3:F:301:FSC:H182	1.98	0.44
1:C:75:LYS:CD	1:E:214:THR:HG22	2.47	0.43
1:C:72:ILE:HD11	1:E:214:THR:O	2.13	0.43
1:F:126:PHE:CD1	3:F:301:FSC:H382	2.54	0.43
1:A:126:PHE:CD1	3:A:301:FSC:C38	2.92	0.43
1:F:136:ARG:HB2	1:F:154:THR:HG21	2.00	0.43
3:A:301:FSC:C2	3:A:301:FSC:H232	2.48	0.43
1:F:58:VAL:HG12	1:F:102:ILE:HD13	2.00	0.43
1:A:21:ALA:HB1	1:B:65:SER:HB3	2.00	0.43
1:E:220:TYR:HB2	1:E:223:SER:H	1.83	0.43
1:G:88:ILE:HD11	1:H:13:TYR:OH	2.19	0.43
1:H:81:ASN:HB3	1:H:84:HIS:HB2	2.00	0.43
1:C:56:LYS:HE2	2:R:677:ASN:HD22	1.84	0.43
1:B:23:ARG:NH2	1:B:26:GLU:OE1	2.51	0.43
1:B:226:ILE:HD11	3:B:301:FSC:C18	2.48	0.42
3:C:301:FSC:H11	3:C:301:FSC:H9	2.00	0.42
1:G:201:ALA:CB	1:G:234:LEU:HD21	2.49	0.42
1:F:69:ILE:HG23	1:F:88:ILE:HG23	2.01	0.42
3:G:301:FSC:C27	3:G:301:FSC:C23	2.90	0.42
1:A:110:LEU:HD23	1:A:114:LEU:HD12	2.01	0.42
1:E:53:VAL:HG21	3:E:301:FSC:C46	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:ALA:HB1	1:F:65:SER:HB3	2.01	0.42
1:D:128:LEU:HB3	1:D:161:ALA:HB2	2.01	0.42
1:E:220:TYR:HB2	1:E:223:SER:CB	2.50	0.42
1:E:75:LYS:O	1:E:79:ARG:HG2	2.20	0.42
1:F:44:THR:O	1:F:48:ARG:HB2	2.19	0.41
1:D:148:LYS:O	1:D:152:GLU:HB2	2.20	0.41
1:D:220:TYR:HA	1:E:221:LYS:HE3	2.02	0.41
1:G:173:HIS:HA	1:G:174:PRO:HD2	1.89	0.41
1:E:220:TYR:HB2	1:E:223:SER:HB3	2.02	0.41
1:E:171:PRO:HA	1:E:176:ARG:HD3	2.02	0.41
1:B:110:LEU:HA	1:B:114:LEU:HB2	2.01	0.41
1:C:75:LYS:HD3	1:E:214:THR:HG22	2.03	0.41
1:E:81:ASN:HB3	1:E:84:HIS:HB2	2.02	0.41
1:G:110:LEU:HD11	1:G:130:MET:HE3	2.02	0.41
3:G:301:FSC:C11	3:G:301:FSC:H9	2.50	0.41
1:D:110:LEU:HD23	1:D:114:LEU:HD12	2.02	0.41
1:E:126:PHE:HE2	3:E:301:FSC:H233	1.86	0.41
3:E:301:FSC:H352	3:E:301:FSC:H472	1.76	0.41
1:F:181:LEU:HD13	1:F:230:LEU:HD23	2.02	0.41
3:E:301:FSC:C2	3:E:301:FSC:H232	2.51	0.41
1:F:177:LEU:HD13	1:F:227:MET:HG3	2.03	0.41
1:G:62:ARG:HB3	1:G:99:LEU:HD21	2.03	0.41
1:D:12:VAL:O	1:D:16:LYS:HG3	2.20	0.41
1:F:71:SER:O	1:F:75:LYS:HG2	2.21	0.41
1:G:126:PHE:CE2	3:G:301:FSC:H383	2.55	0.41
1:C:110:LEU:HD11	1:C:130:MET:HG2	2.03	0.41
1:F:38:LEU:HD22	1:F:41:GLU:HG3	2.02	0.40
3:G:301:FSC:H472	3:G:301:FSC:H352	1.71	0.40
1:C:193:SER:HB3	1:C:196:ARG:HH21	1.86	0.40
3:C:301:FSC:C23	3:C:301:FSC:C5	2.93	0.40
1:C:79:ARG:O	1:C:79:ARG:HG2	2.21	0.40
1:A:134:TYR:HA	1:A:137:TYR:CD2	2.56	0.40
1:D:110:LEU:HD11	1:D:130:MET:HG2	2.03	0.40
1:E:63:ARG:CZ	1:E:137:TYR:CE1	3.04	0.40
3:A:301:FSC:C27	3:A:301:FSC:H233	2.51	0.40
1:D:52:SER:HB2	1:D:126:PHE:HZ	1.86	0.40
1:G:48:ARG:NH1	1:G:123:SER:HA	2.37	0.40
1:G:185:VAL:HG21	2:V:675:SER:O	2.22	0.40
1:E:233:ASN:HB3	1:E:237:TRP:CE2	2.56	0.40
1:F:47:GLU:HA	1:F:50:LEU:HB2	2.03	0.40
3:G:301:FSC:O13	2:V:677:ASN:OD1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LEU
1	A	183	PHE
1	B	183	PHE
1	B	231	ARG
2	Q	673	TYR
1	C	122	ASP
1	C	183	PHE
1	D	91	TYR
1	D	183	PHE
1	D	236	LEU
1	E	8	ARG
1	E	23	ARG
1	E	91	TYR
1	E	158	TYR
1	E	183	PHE

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Mol	Chain	Res	Type
1	E	221	LYS
1	E	231	ARG
2	T	674	PHE
1	F	183	PHE
1	G	62	ARG
1	G	63	ARG
1	G	83	GLU
1	G	159	LYS
1	G	163	ASP
1	G	183	PHE
1	G	222	ASP
2	V	673	TYR
2	V	677	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	97	ASN
1	B	162	GLN
1	C	74	GLN
1	C	86	ASN
1	C	173	HIS
2	R	677	ASN
2	S	677	ASN
1	E	74	GLN
1	E	135	HIS
1	E	203	GLN
1	G	49	ASN
1	G	57	ASN
1	G	135	HIS
1	H	11	ASN

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	Q	676	2	8,9,10	0.77	0	8,12,14	1.50	1 (12%)
2	SEP	U	676	2	8,9,10	0.75	0	8,12,14	1.07	0
2	SEP	P	676	2	8,9,10	0.74	0	8,12,14	1.09	0
2	SEP	V	676	2	8,9,10	0.74	0	8,12,14	1.12	0
2	SEP	T	676	2	8,9,10	0.83	0	8,12,14	1.18	0
4	SEP	W	701	2	8,9,10	0.77	0	8,12,14	1.14	0
2	SEP	R	676	2	8,9,10	0.75	0	8,12,14	1.07	0
2	SEP	S	676	2	8,9,10	0.82	0	8,12,14	1.22	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	Q	676	2	-	0/5/8/10	-
2	SEP	U	676	2	-	0/5/8/10	-
2	SEP	P	676	2	-	1/5/8/10	-
2	SEP	V	676	2	-	0/5/8/10	-
2	SEP	T	676	2	-	0/5/8/10	-
4	SEP	W	701	2	-	4/5/8/10	-
2	SEP	R	676	2	-	0/5/8/10	-
2	SEP	S	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	D	301	-	46,51,51	1.25	3 (6%)	47,77,77	1.66	7 (14%)
3	FSC	G	301	-	46,51,51	1.28	3 (6%)	47,77,77	1.73	8 (17%)
3	FSC	F	301	-	46,51,51	1.27	3 (6%)	47,77,77	1.70	8 (17%)
3	FSC	C	301	-	46,51,51	1.28	3 (6%)	47,77,77	1.72	8 (17%)
3	FSC	B	301	-	46,51,51	1.29	3 (6%)	47,77,77	1.72	8 (17%)
3	FSC	E	301	-	46,51,51	1.28	3 (6%)	47,77,77	1.71	8 (17%)
3	FSC	A	301	-	46,51,51	1.28	3 (6%)	47,77,77	1.76	9 (19%)
4	SEP	W	701	2	8,9,10	0.77	0	8,12,14	1.14	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
3	FSC	D	301	-	-	1/29/103/103	0/4/4/4
3	FSC	G	301	-	-	2/29/103/103	0/4/4/4
3	FSC	F	301	-	-	0/29/103/103	0/4/4/4
3	FSC	C	301	-	-	3/29/103/103	0/4/4/4
3	FSC	B	301	-	-	2/29/103/103	0/4/4/4
3	FSC	E	301	-	-	2/29/103/103	0/4/4/4
3	FSC	A	301	-	-	4/29/103/103	0/4/4/4
4	SEP	W	701	2	-	4/5/8/10	-

All (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
3	G	301	FSC	C19-C15	-5.00	1.52	1.56
3	G	301	FSC	O34-C40	4.88	1.46	1.35
3	E	301	FSC	O34-C40	4.83	1.46	1.35
3	D	301	FSC	C19-C15	-4.82	1.52	1.56
3	B	301	FSC	O34-C40	4.81	1.46	1.35
3	C	301	FSC	O34-C40	4.80	1.46	1.35
3	F	301	FSC	O34-C40	4.80	1.46	1.35
3	D	301	FSC	O34-C40	4.79	1.46	1.35
3	A	301	FSC	O34-C40	4.72	1.45	1.35
3	G	301	FSC	O24-C31	2.53	1.45	1.33
3	A	301	FSC	O24-C31	2.52	1.45	1.33
3	F	301	FSC	O24-C31	2.52	1.45	1.33
3	D	301	FSC	O24-C31	2.52	1.45	1.33
3	E	301	FSC	O24-C31	2.51	1.45	1.33
3	B	301	FSC	O24-C31	2.51	1.45	1.33
3	C	301	FSC	O24-C31	2.51	1.45	1.33

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	FSC	C15-C19-C12	-5.64	110.89	118.11
3	F	301	FSC	C15-C19-C12	-5.58	110.96	118.11
3	B	301	FSC	C19-C12-C5	-5.04	125.23	130.72
3	C	301	FSC	C19-C12-C5	-4.93	125.35	130.72
3	E	301	FSC	C19-C12-C5	-4.90	125.39	130.72
3	A	301	FSC	C19-C12-C5	-4.89	125.39	130.72
3	F	301	FSC	C19-C12-C5	-4.67	125.64	130.72
3	D	301	FSC	C19-C12-C5	-4.56	125.76	130.72
3	G	301	FSC	C19-C12-C5	-4.44	125.89	130.72
3	A	301	FSC	O34-C40-C42	4.38	119.14	111.09
3	F	301	FSC	O34-C40-C42	4.27	118.95	111.09
3	C	301	FSC	O34-C40-C42	4.27	118.95	111.09
3	E	301	FSC	O34-C40-C42	4.26	118.94	111.09
3	D	301	FSC	O34-C40-C42	4.26	118.92	111.09
3	G	301	FSC	O34-C40-C42	4.24	118.89	111.09
3	B	301	FSC	O34-C40-C42	4.23	118.88	111.09
3	A	301	FSC	C28-O34-C40	-3.57	112.20	117.72
3	G	301	FSC	C19-C15-C9	-3.42	108.79	112.39
3	B	301	FSC	C19-C15-C9	-3.25	108.97	112.39
3	G	301	FSC	C23-C15-C19	-3.13	112.29	114.85
3	C	301	FSC	C19-C15-C9	-2.99	109.24	112.39
3	F	301	FSC	C23-C15-C19	-2.99	112.41	114.85
3	A	301	FSC	C19-C15-C9	-2.96	109.28	112.39
3	D	301	FSC	C23-C15-C19	-2.96	112.43	114.85
3	F	301	FSC	C28-O34-C40	-2.93	113.18	117.72
3	B	301	FSC	C25-C26-C20	2.89	108.44	103.66
3	C	301	FSC	C28-O34-C40	-2.89	113.25	117.72
3	E	301	FSC	C28-O34-C40	-2.84	113.33	117.72
3	E	301	FSC	C19-C15-C9	-2.83	109.41	112.39
3	D	301	FSC	C28-O34-C40	-2.83	113.34	117.72
3	G	301	FSC	C28-O34-C40	-2.82	113.35	117.72
3	C	301	FSC	C25-C26-C20	2.79	108.27	103.66
3	A	301	FSC	C25-C26-C20	2.77	108.25	103.66
3	E	301	FSC	C25-C26-C20	2.76	108.22	103.66
3	C	301	FSC	C23-C15-C19	-2.74	112.61	114.85
3	F	301	FSC	C25-C26-C20	2.73	108.18	103.66
3	A	301	FSC	C23-C15-C19	-2.73	112.62	114.85
3	D	301	FSC	C25-C26-C20	2.72	108.16	103.66
3	B	301	FSC	C28-O34-C40	-2.70	113.54	117.72
3	B	301	FSC	C23-C15-C19	-2.68	112.66	114.85
3	G	301	FSC	C25-C26-C20	2.64	108.03	103.66
3	E	301	FSC	C23-C15-C19	-2.55	112.77	114.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	FSC	C19-C15-C9	-2.49	109.77	112.39
3	C	301	FSC	C26-C25-C19	2.37	108.72	104.55
3	A	301	FSC	C26-C25-C19	2.33	108.66	104.55
3	F	301	FSC	C26-C25-C19	2.31	108.62	104.55
3	E	301	FSC	C26-C25-C19	2.29	108.59	104.55
3	D	301	FSC	C26-C25-C19	2.29	108.58	104.55
3	B	301	FSC	C26-C25-C19	2.24	108.50	104.55
3	A	301	FSC	O34-C40-O43	-2.23	118.53	122.96
3	G	301	FSC	C26-C25-C19	2.19	108.42	104.55

There are no chirality outliers.

All (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
3	A	301	FSC	O22-C30-C35-O41
3	G	301	FSC	O22-C30-C35-O41
4	W	701	SEP	CB-OG-P-O1P
3	A	301	FSC	O43-C40-O34-C28
3	G	301	FSC	C33-C30-C35-O41
3	B	301	FSC	O22-C30-C35-O41
3	C	301	FSC	O22-C30-C35-O41
3	B	301	FSC	C33-C30-C35-O41
3	C	301	FSC	C33-C30-C35-O41
3	E	301	FSC	O22-C30-C35-O41
3	D	301	FSC	C4-C11-C17-O24
3	A	301	FSC	C1-C3-O8-C14
3	C	301	FSC	C12-C20-C27-O32

There are no ring outliers.

7 monomers are involved in 102 short contacts:

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

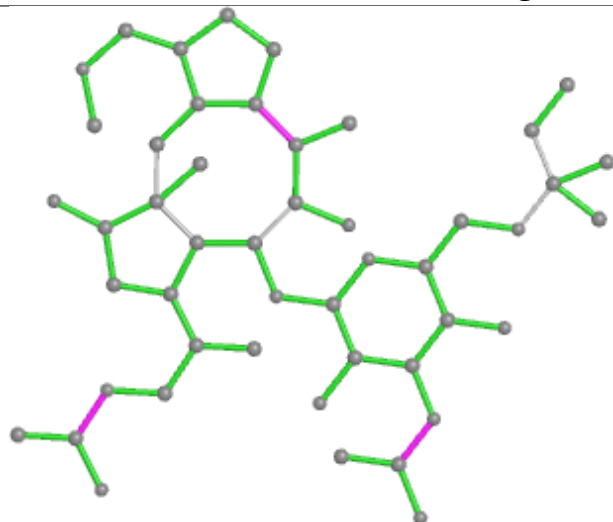
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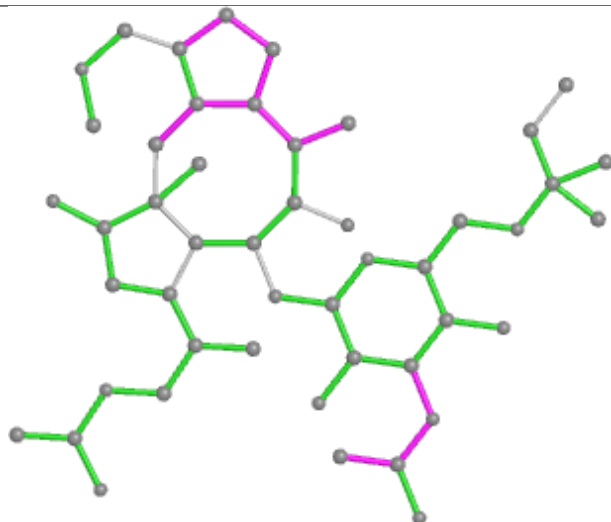
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	FSC	14	0
3	E	301	FSC	15	0
3	A	301	FSC	14	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

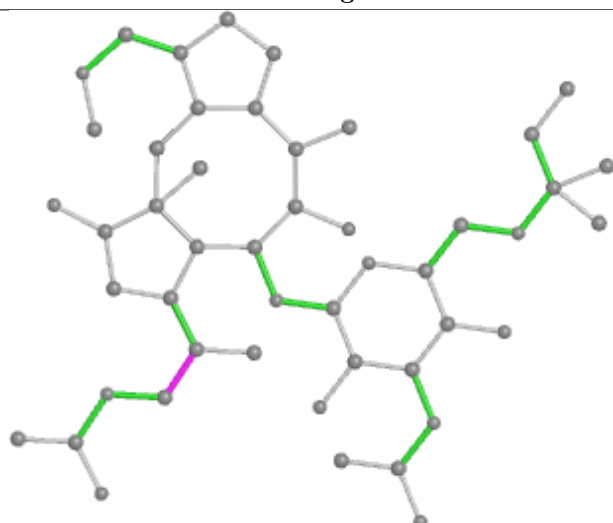
Ligand FSC D 301



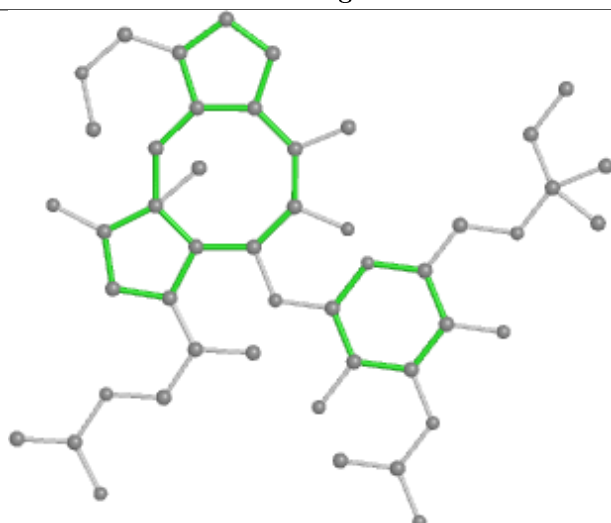
Bond lengths



Bond angles

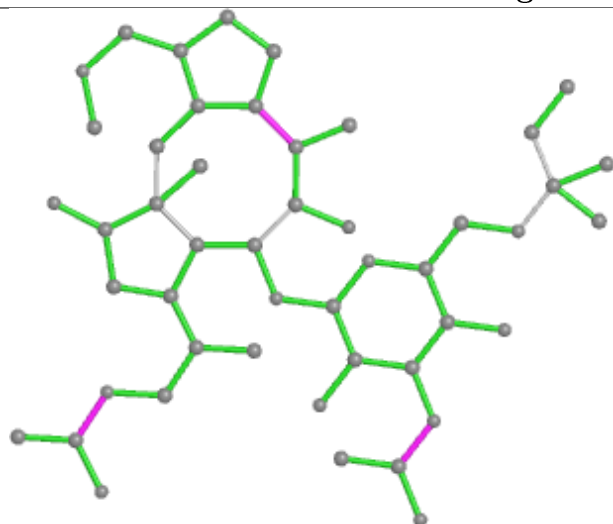


Torsions

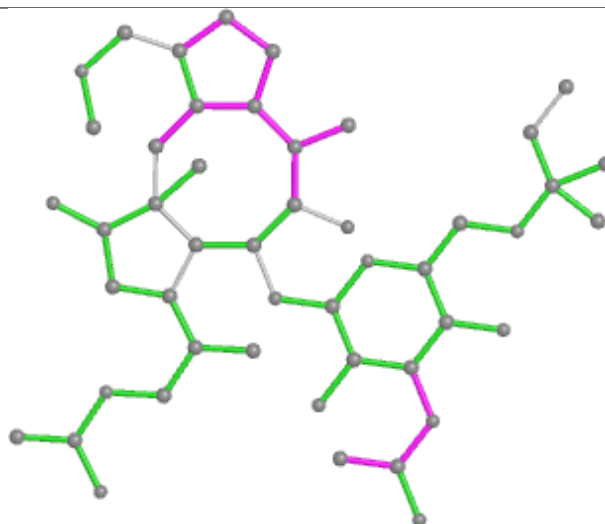


Rings

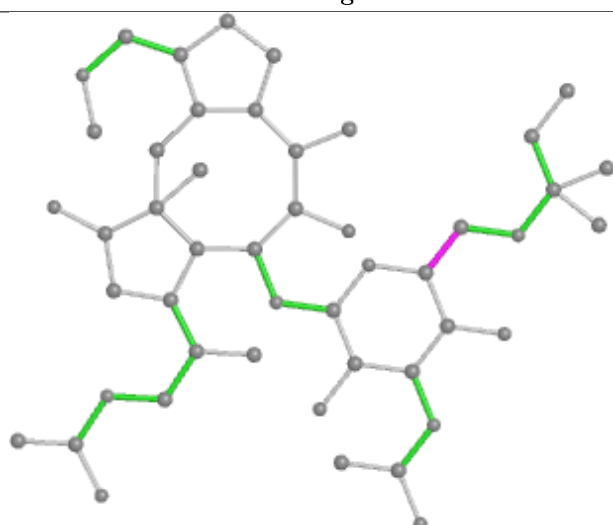
Ligand FSC G 301



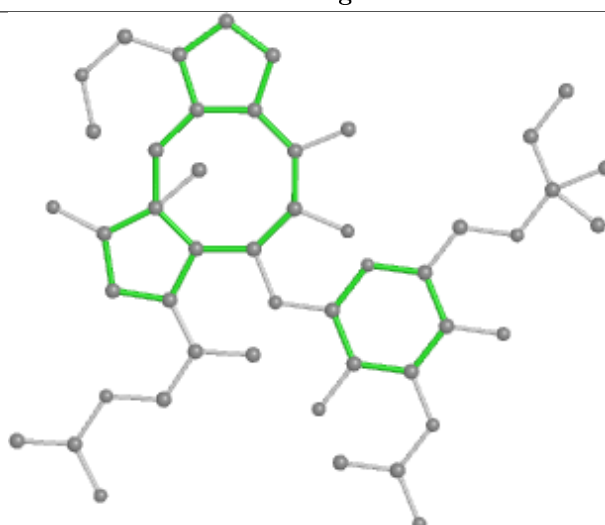
Bond lengths



Bond angles

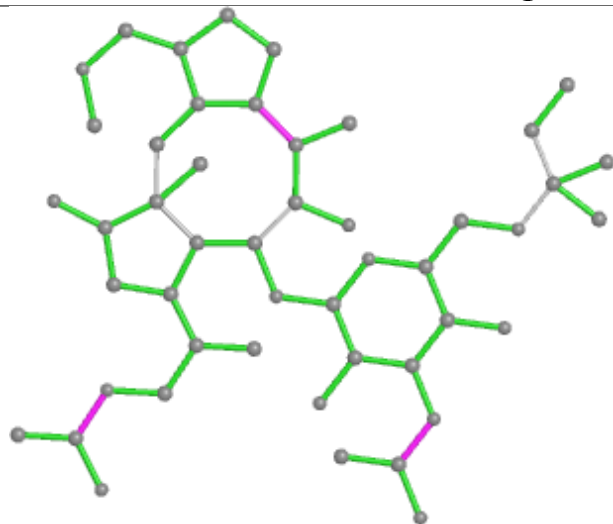


Torsions

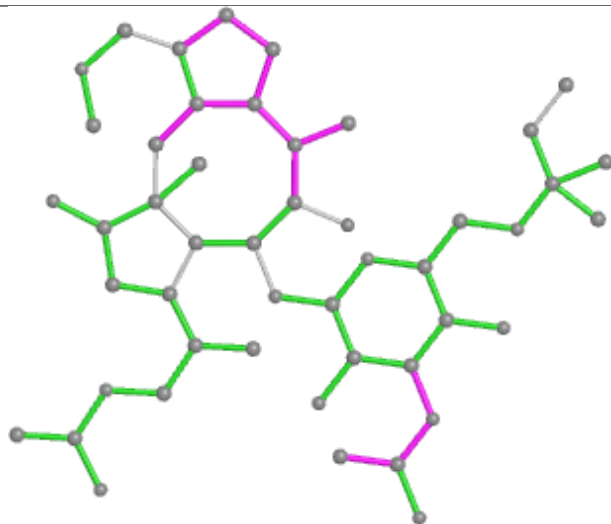


Rings

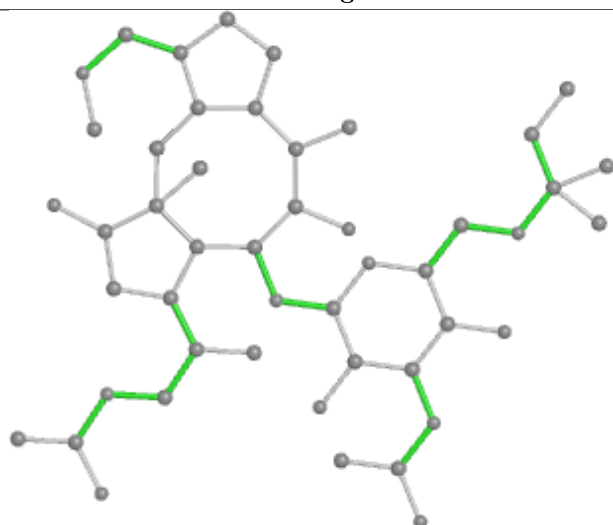
Ligand FSC F 301



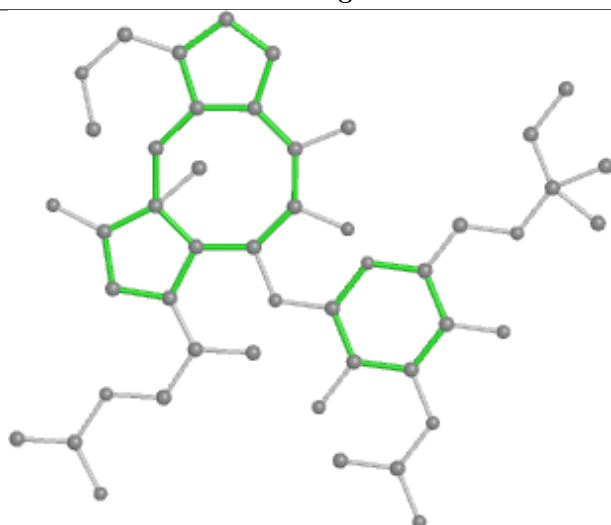
Bond lengths



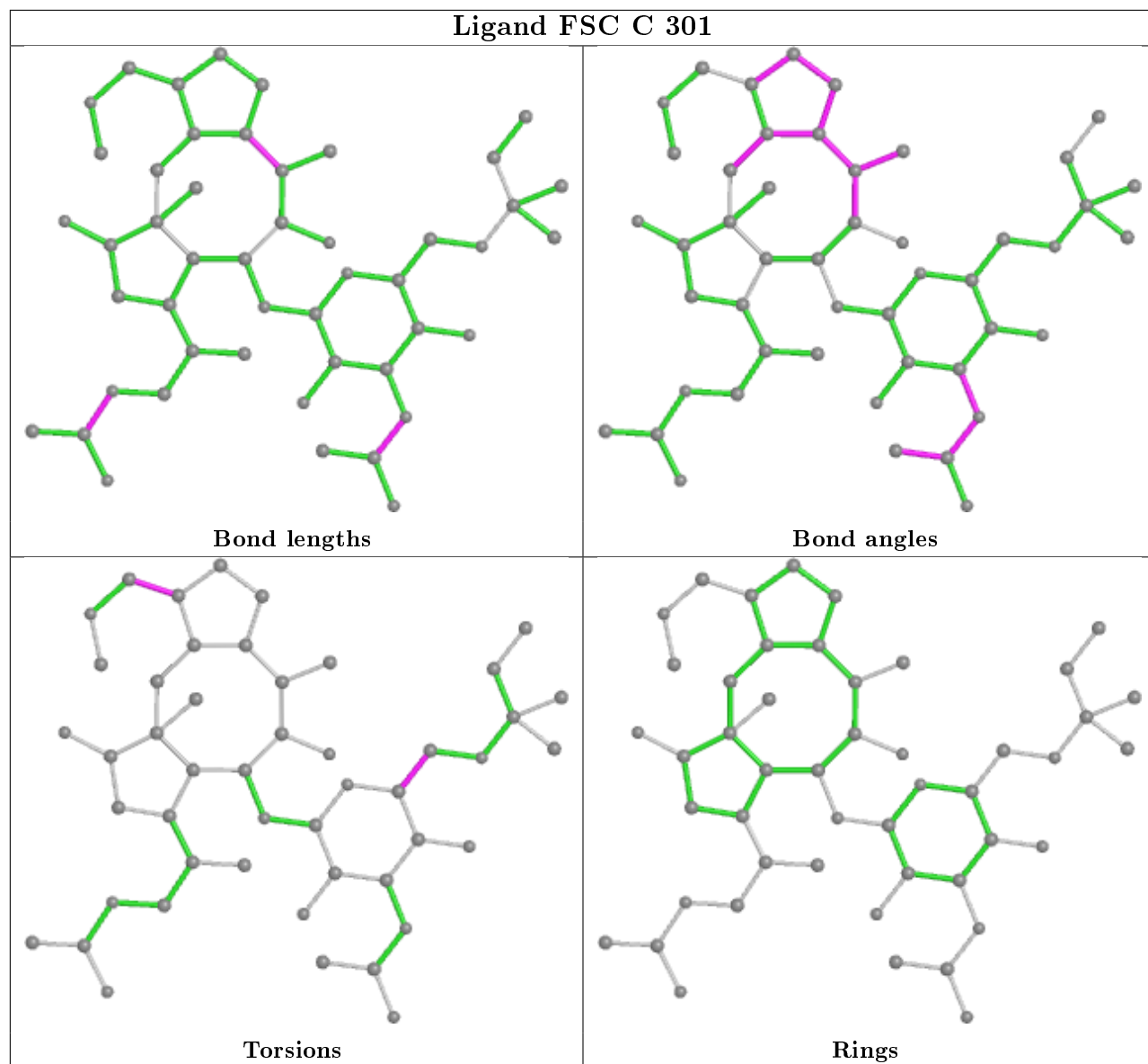
Bond angles

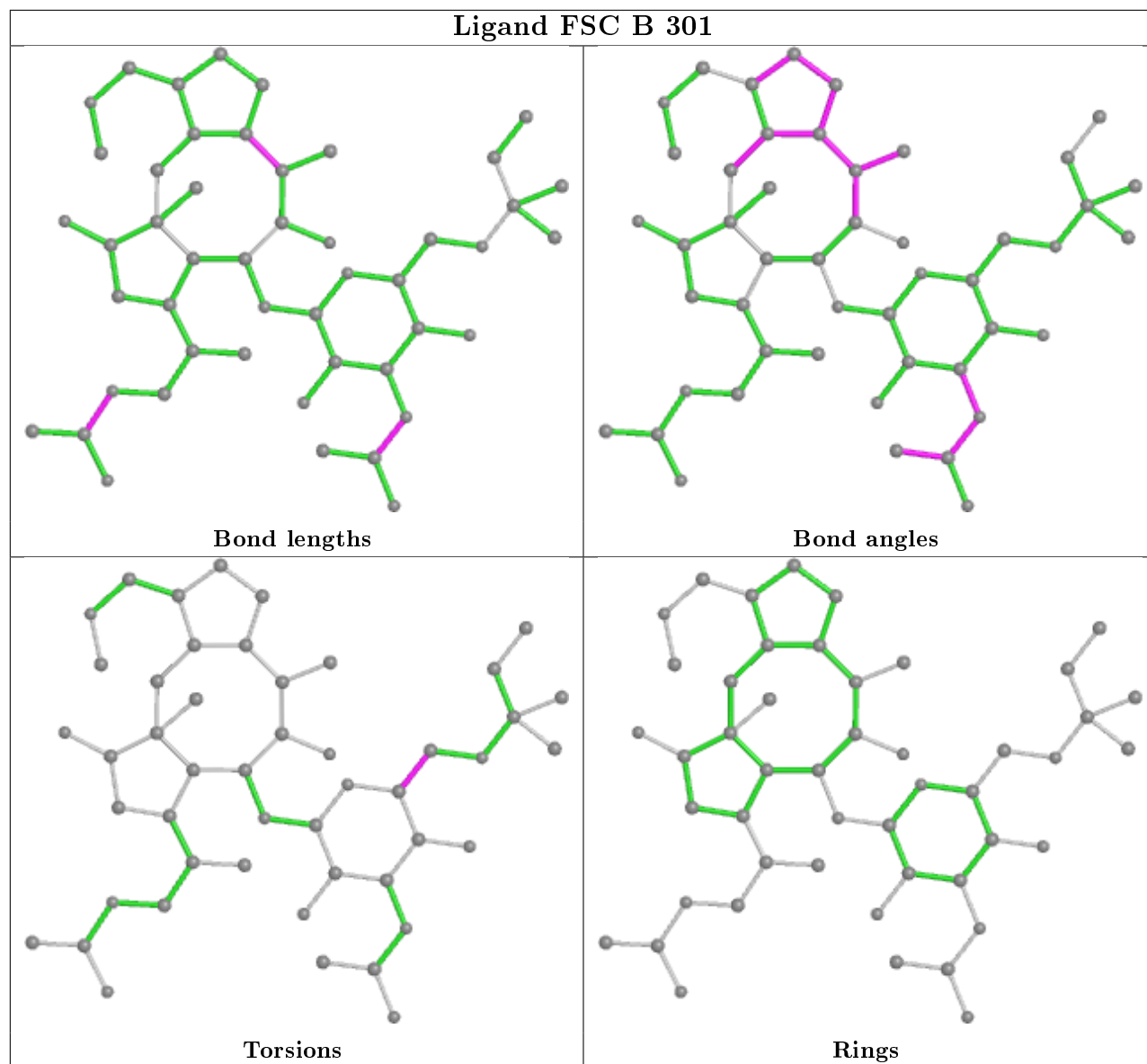


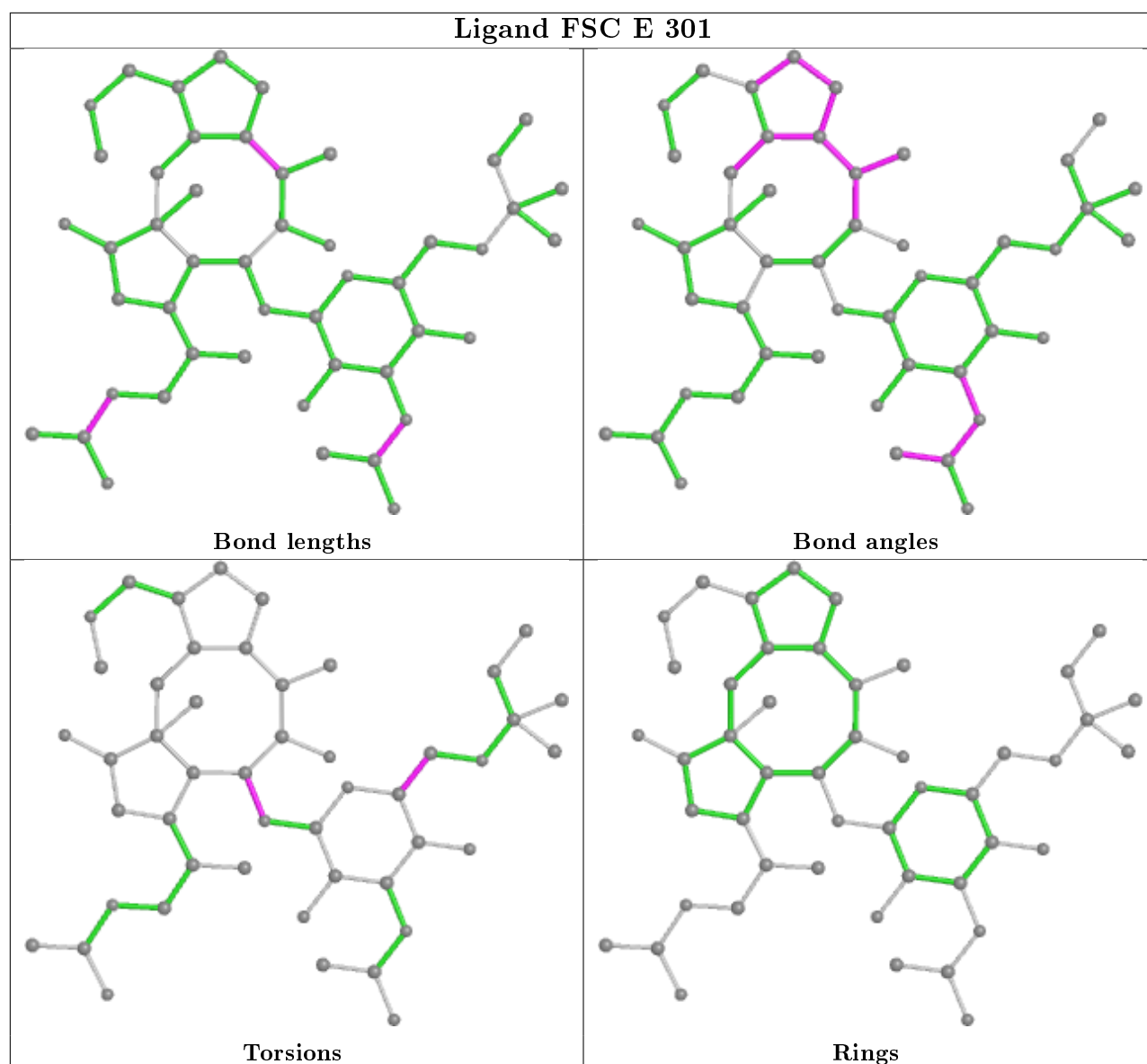
Torsions

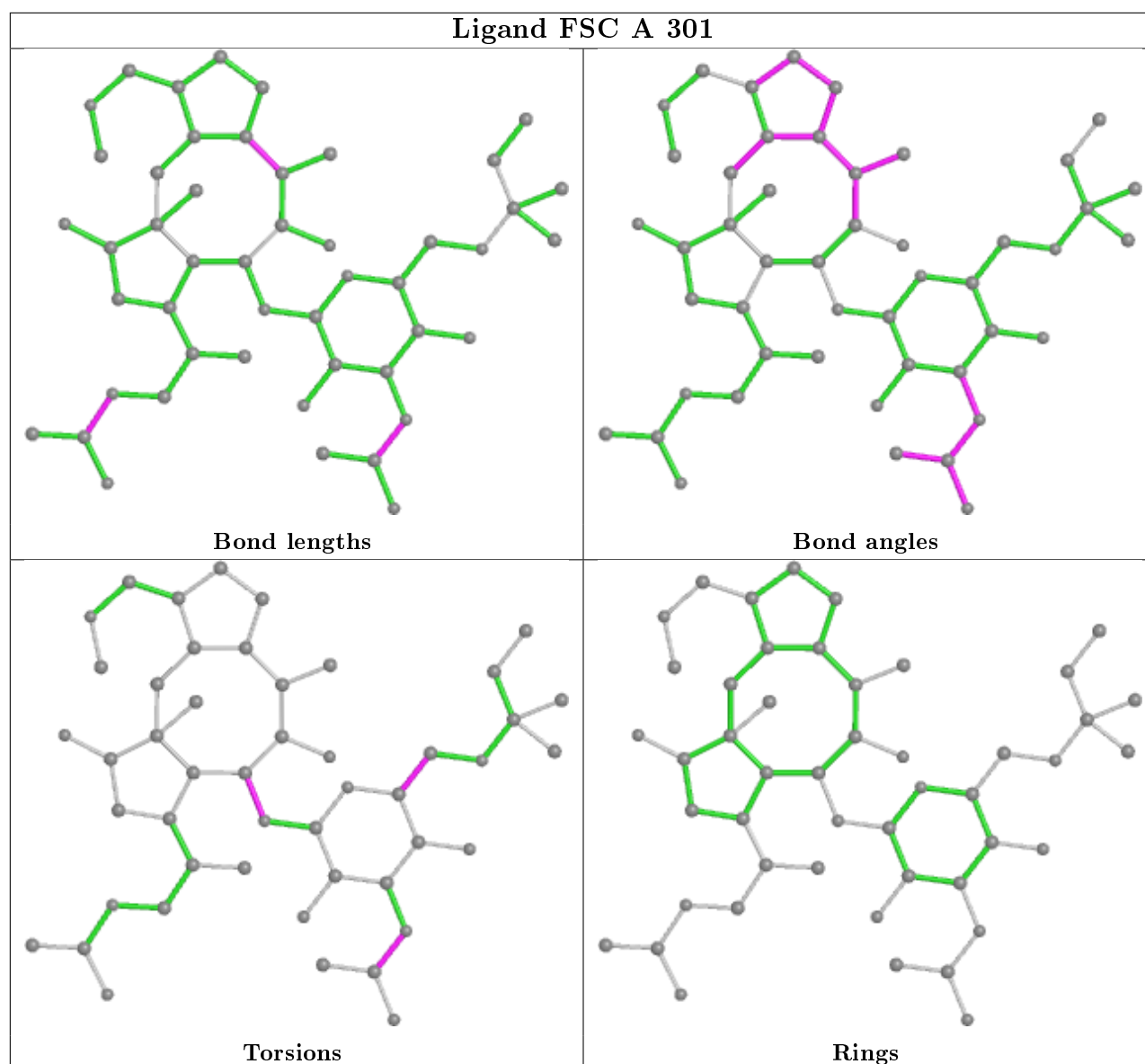


Rings









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

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	23, 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

All (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

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Mol	Chain	Res	Type	RSRZ
1	H	205	PHE	4.5
1	H	225	LEU	4.4
1	H	139	ALA	4.3
1	H	204	ALA	4.3
1	H	210	ALA	4.2
1	H	197	ALA	4.1
1	H	174	PRO	3.8
1	H	191	LEU	3.8
1	H	208	ALA	3.7
1	H	171	PRO	3.6
1	H	192	ASN	3.5
1	H	206	ASP	3.5
1	H	186	PHE	3.5
1	H	232	ASP	3.5
1	H	137	TYR	3.4
1	H	231	ARG	3.3
1	H	173	HIS	3.3
1	H	221	LYS	3.3
1	G	19	GLU	3.2
1	H	175	ILE	3.1
1	H	184	SER	3.1
1	H	37	SER	3.0
1	H	46	GLU	2.8
1	H	176	ARG	2.8
1	H	180	ALA	2.7
1	H	34	VAL	2.7
1	H	116	PRO	2.7
1	H	172	THR	2.6
1	A	6	THR	2.6
1	H	111	ASP	2.5
1	H	181	LEU	2.5
1	H	189	GLU	2.4
1	H	119	ALA	2.4
1	H	196	ARG	2.4
1	H	187	TYR	2.4
1	H	194	PRO	2.4
1	H	222	ASP	2.3
1	H	212	LEU	2.3
1	H	55	TYR	2.3
1	H	201	ALA	2.3
1	B	245	GLY	2.3
1	H	52	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	177	LEU	2.3
1	H	45	VAL	2.3
1	H	234	LEU	2.2
1	B	2	ALA	2.1
1	H	115	ILE	2.1
1	H	126	PHE	2.1
1	F	192	ASN	2.1
1	H	226	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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	T	676	10/11	0.95	0.13	39,44,52,53	0
2	SEP	P	676	10/11	0.95	0.21	61,73,85,86	0
2	SEP	U	676	10/11	0.96	0.17	57,69,86,89	0

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(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

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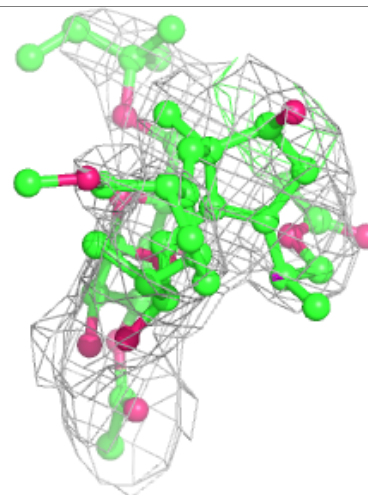
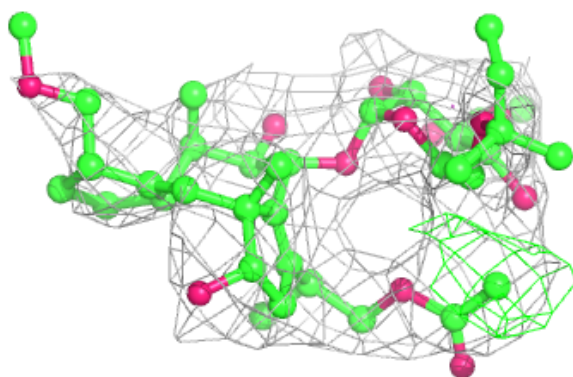
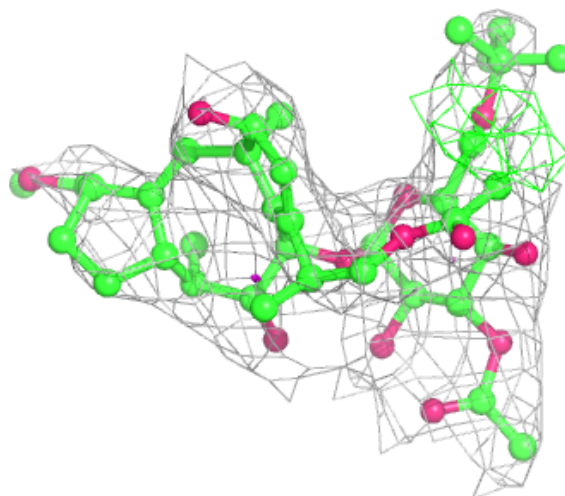
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FSC	B	301	48/48	0.94	0.18	39,54,58,66	0
3	FSC	E	301	48/48	0.94	0.20	31,44,60,64	0
3	FSC	A	301	48/48	0.94	0.21	40,55,83,88	0
3	FSC	F	301	48/48	0.94	0.21	16,39,46,52	0
3	FSC	D	301	48/48	0.95	0.17	32,46,56,61	0
3	FSC	C	301	48/48	0.95	0.18	15,44,69,70	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.

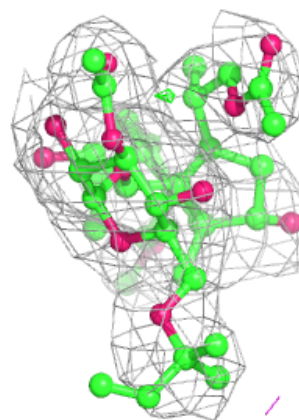
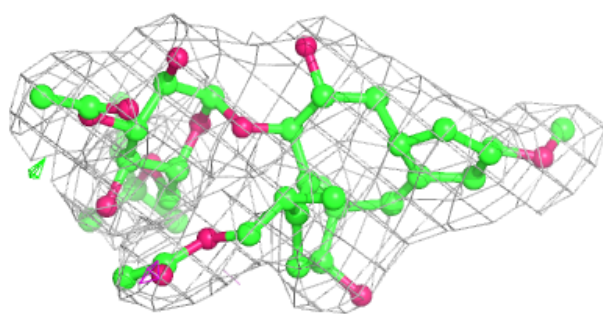
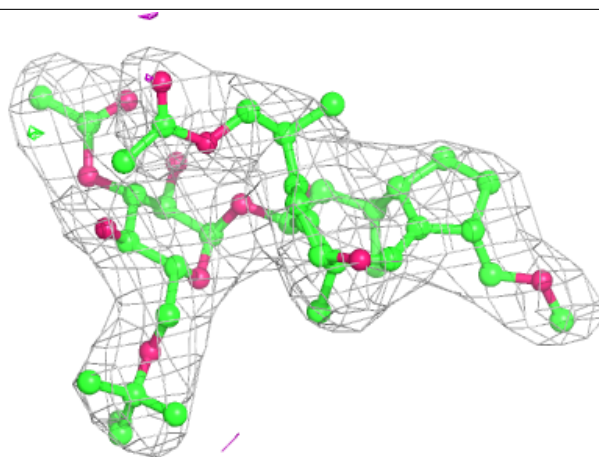
Electron density around FSC G 301:

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



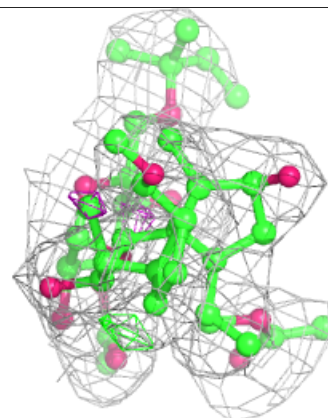
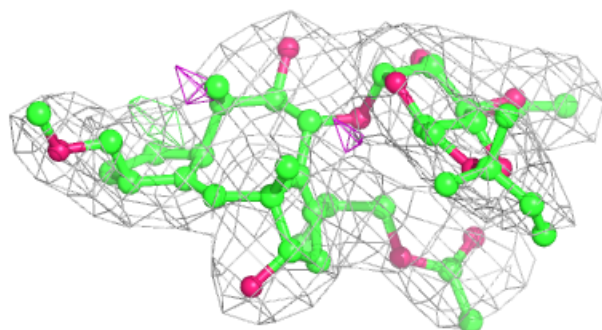
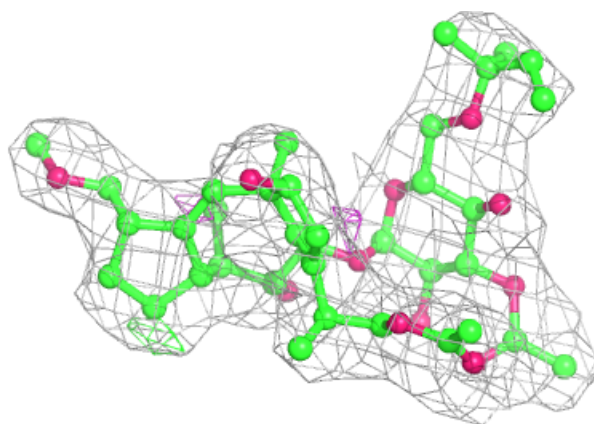
Electron density around FSC B 301:

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and green (positive)



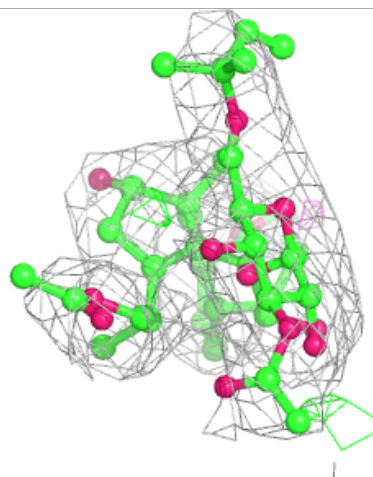
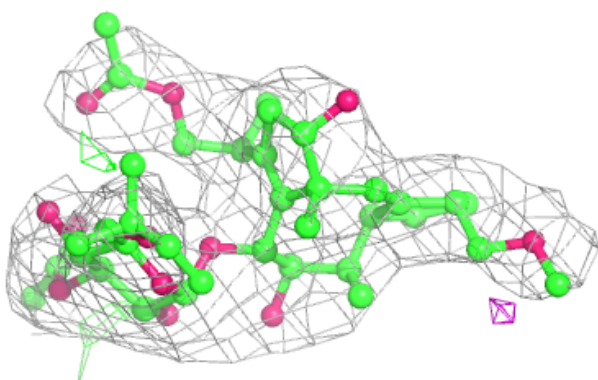
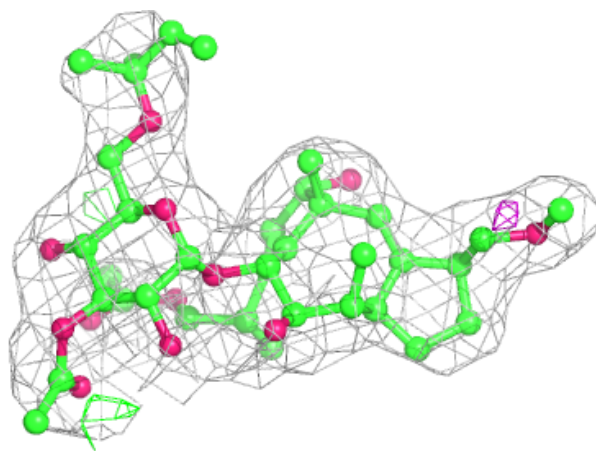
Electron density around FSC E 301:

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and green (positive)



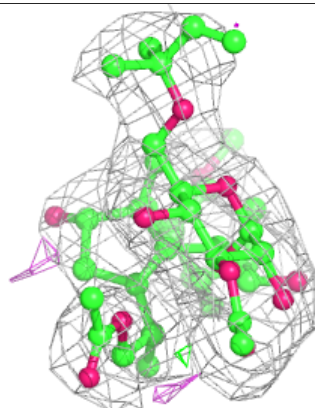
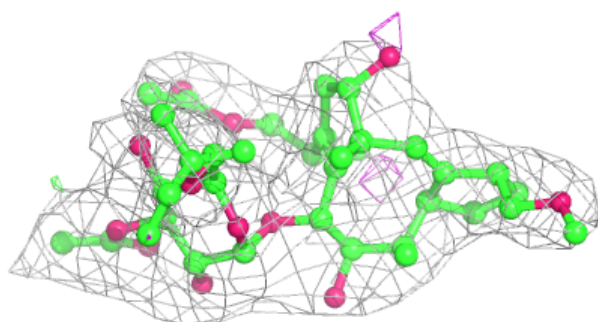
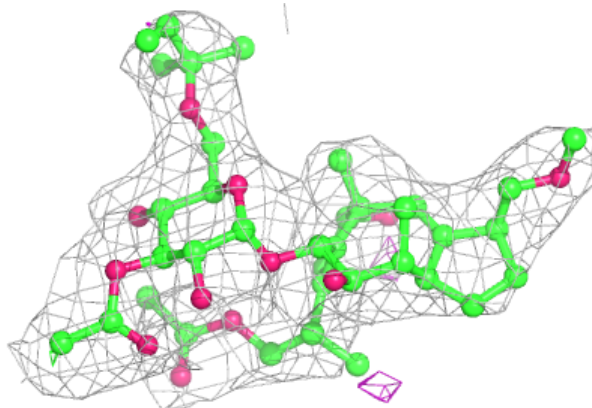
Electron density around FSC A 301:

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



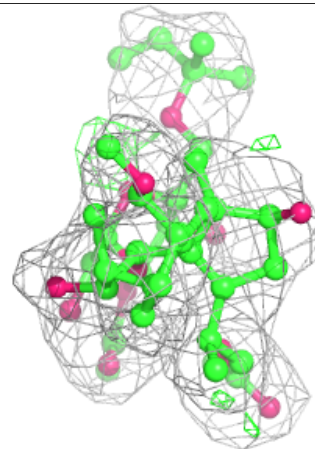
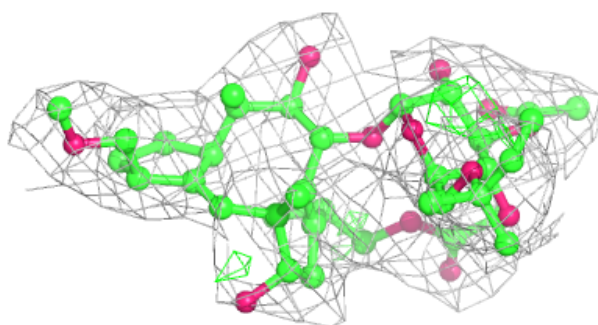
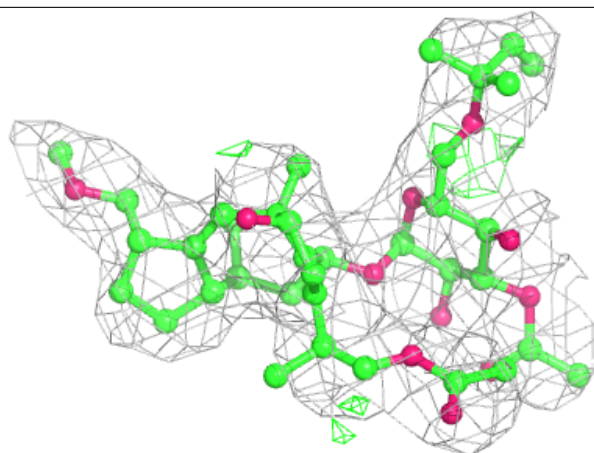
Electron density around FSC F 301:

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and green (positive)



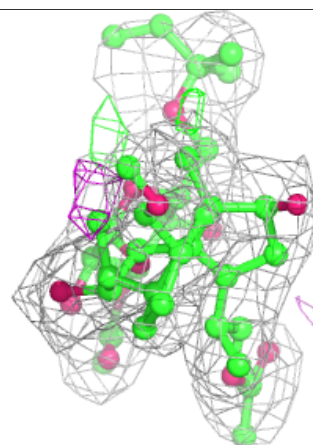
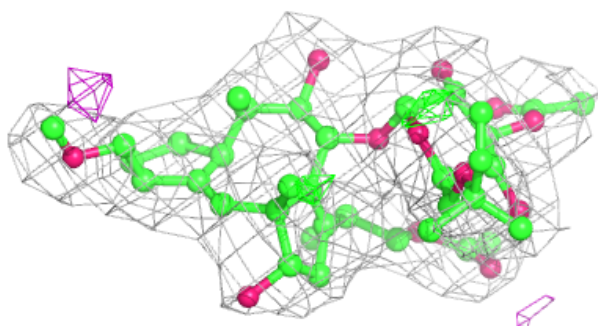
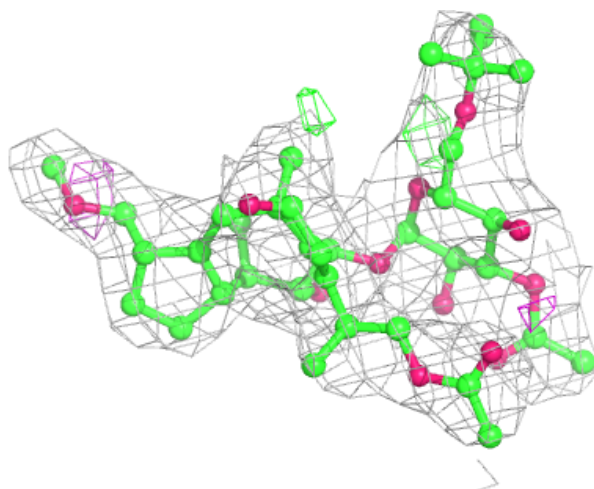
Electron density around FSC D 301:

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



Electron density around FSC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.