



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 03:43 pm BST

PDB ID : 4ACA
Title : CRYSTAL STRUCTURE OF TRANSLATION ELONGATION FACTOR
SELB FROM METHANOCOCCUS MARIPALUDIS, APO FORM
Authors : Leibundgut, M.; Frick, C.; Thanbichler, M.; Boeck, A.; Ban, N.
Deposited on : 2011-12-14
Resolution : 3.15 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 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

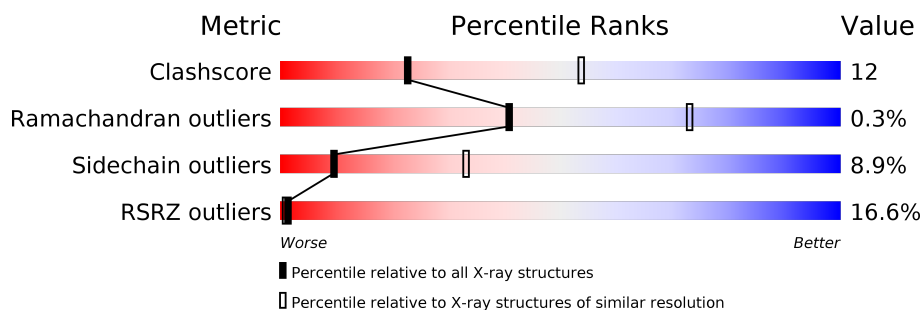
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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))
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	482	<div> <div>16%</div> <div>63%</div> <div>27%</div> <div>7%</div> </div>
1	B	482	<div> <div>15%</div> <div>65%</div> <div>27%</div> <div>5%</div> </div>
1	C	482	<div> <div>4%</div> <div>73%</div> <div>22%</div> <div>• •</div> </div>
1	D	482	<div> <div>29%</div> <div>65%</div> <div>28%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CMH	A	340	-	-	X	-
1	CMH	B	371	-	-	X	-
2	SO4	B	1471	-	-	-	X
2	SO4	C	1474	-	-	-	X
2	SO4	C	1481	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14529 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 TRANSLATION ELONGATION FACTOR SELB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	448	Total	C	Hg	N	O	S	0	0	0
			3475	2220	4	593	644	14			
1	B	456	Total	C	Hg	N	O	S	0	0	0
			3533	2257	4	603	655	14			
1	C	471	Total	C	Hg	N	O	S	0	0	0
			3651	2327	4	627	679	14			
1	D	467	Total	C	Hg	N	O	S	0	0	0
			3615	2305	4	618	675	13			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q8J307
A	-12	HIS	-	expression tag	UNP Q8J307
A	-11	HIS	-	expression tag	UNP Q8J307
A	-10	HIS	-	expression tag	UNP Q8J307
A	-9	HIS	-	expression tag	UNP Q8J307
A	-8	HIS	-	expression tag	UNP Q8J307
A	-7	HIS	-	expression tag	UNP Q8J307
A	-6	SER	-	expression tag	UNP Q8J307
A	-5	ILE	-	expression tag	UNP Q8J307
A	-4	GLU	-	expression tag	UNP Q8J307
A	-3	GLY	-	expression tag	UNP Q8J307
A	-2	ARG	-	expression tag	UNP Q8J307
A	-1	PRO	-	expression tag	UNP Q8J307
A	0	HIS	-	expression tag	UNP Q8J307
B	-13	MET	-	expression tag	UNP Q8J307
B	-12	HIS	-	expression tag	UNP Q8J307
B	-11	HIS	-	expression tag	UNP Q8J307
B	-10	HIS	-	expression tag	UNP Q8J307
B	-9	HIS	-	expression tag	UNP Q8J307
B	-8	HIS	-	expression tag	UNP Q8J307
B	-7	HIS	-	expression tag	UNP Q8J307

Continued on next page...

Continued from previous page...

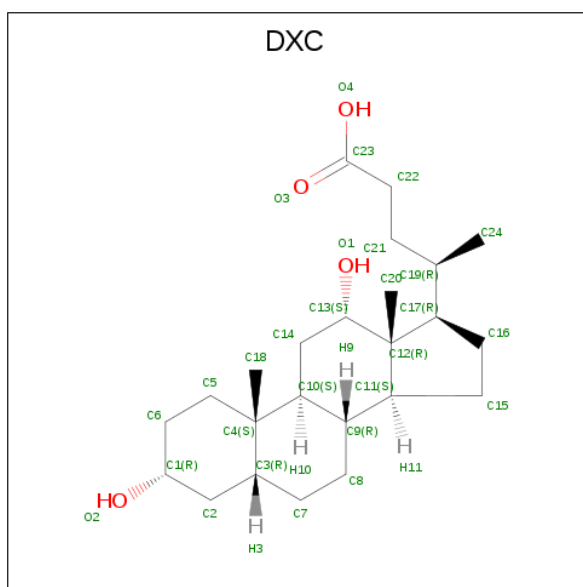
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	SER	-	expression tag	UNP Q8J307
B	-5	ILE	-	expression tag	UNP Q8J307
B	-4	GLU	-	expression tag	UNP Q8J307
B	-3	GLY	-	expression tag	UNP Q8J307
B	-2	ARG	-	expression tag	UNP Q8J307
B	-1	PRO	-	expression tag	UNP Q8J307
B	0	HIS	-	expression tag	UNP Q8J307
C	-13	MET	-	expression tag	UNP Q8J307
C	-12	HIS	-	expression tag	UNP Q8J307
C	-11	HIS	-	expression tag	UNP Q8J307
C	-10	HIS	-	expression tag	UNP Q8J307
C	-9	HIS	-	expression tag	UNP Q8J307
C	-8	HIS	-	expression tag	UNP Q8J307
C	-7	HIS	-	expression tag	UNP Q8J307
C	-6	SER	-	expression tag	UNP Q8J307
C	-5	ILE	-	expression tag	UNP Q8J307
C	-4	GLU	-	expression tag	UNP Q8J307
C	-3	GLY	-	expression tag	UNP Q8J307
C	-2	ARG	-	expression tag	UNP Q8J307
C	-1	PRO	-	expression tag	UNP Q8J307
C	0	HIS	-	expression tag	UNP Q8J307
D	-13	MET	-	expression tag	UNP Q8J307
D	-12	HIS	-	expression tag	UNP Q8J307
D	-11	HIS	-	expression tag	UNP Q8J307
D	-10	HIS	-	expression tag	UNP Q8J307
D	-9	HIS	-	expression tag	UNP Q8J307
D	-8	HIS	-	expression tag	UNP Q8J307
D	-7	HIS	-	expression tag	UNP Q8J307
D	-6	SER	-	expression tag	UNP Q8J307
D	-5	ILE	-	expression tag	UNP Q8J307
D	-4	GLU	-	expression tag	UNP Q8J307
D	-3	GLY	-	expression tag	UNP Q8J307
D	-2	ARG	-	expression tag	UNP Q8J307
D	-1	PRO	-	expression tag	UNP Q8J307
D	0	HIS	-	expression tag	UNP Q8J307

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



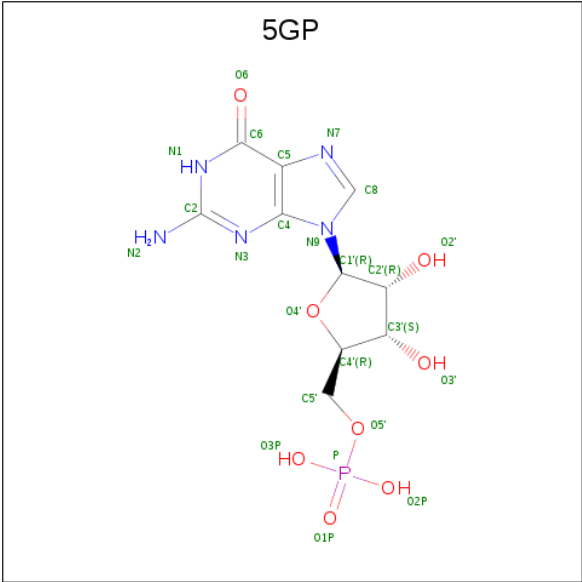
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula: C₂₄H₄₀O₄).

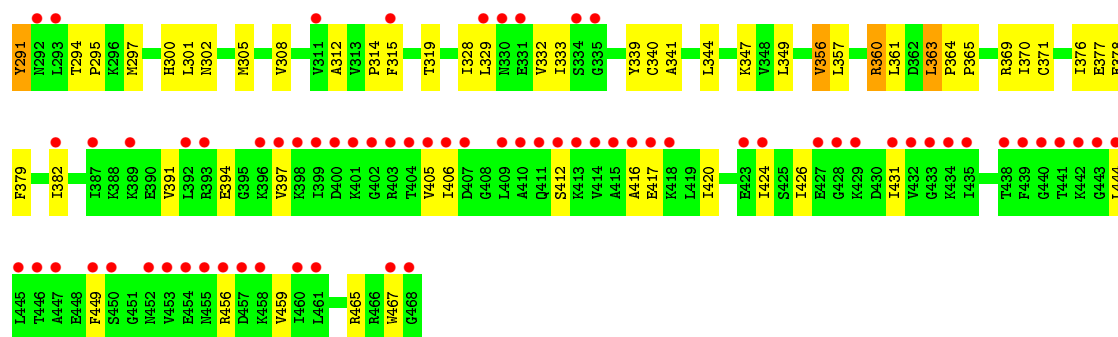


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			28	24	4		
3	C	1	Total	C	O	0	0
			28	24	4		
3	C	1	Total	C	O	0	0
			28	24	4		
3	C	1	Total	C	O	0	0
			28	24	4		
3	C	1	Total	C	O	0	0
			28	24	4		
3	C	1	Total	C	O	0	0
			28	24	4		

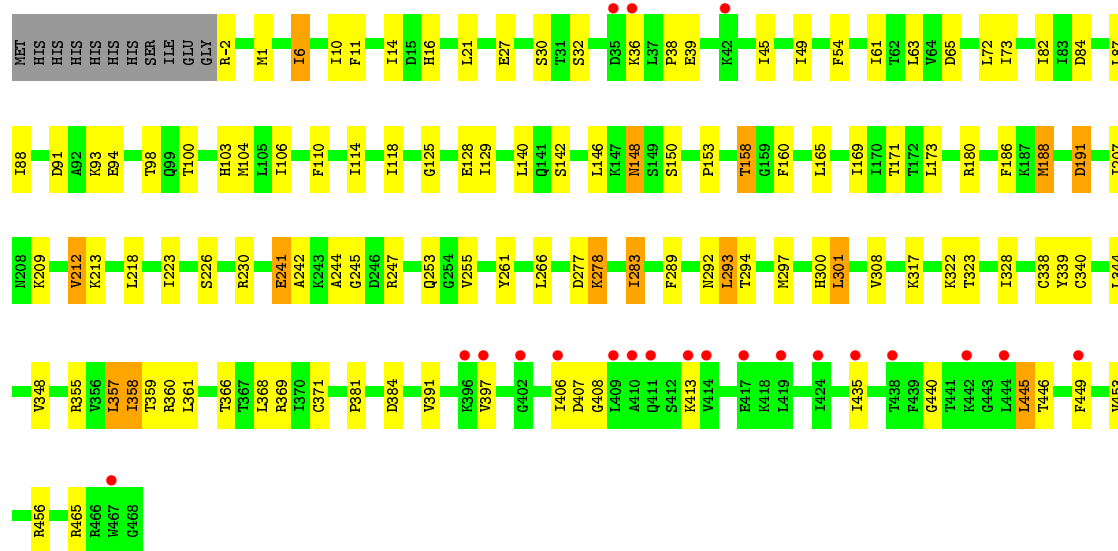
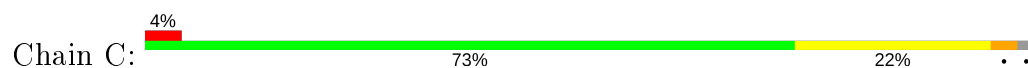
- Molecule 4 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



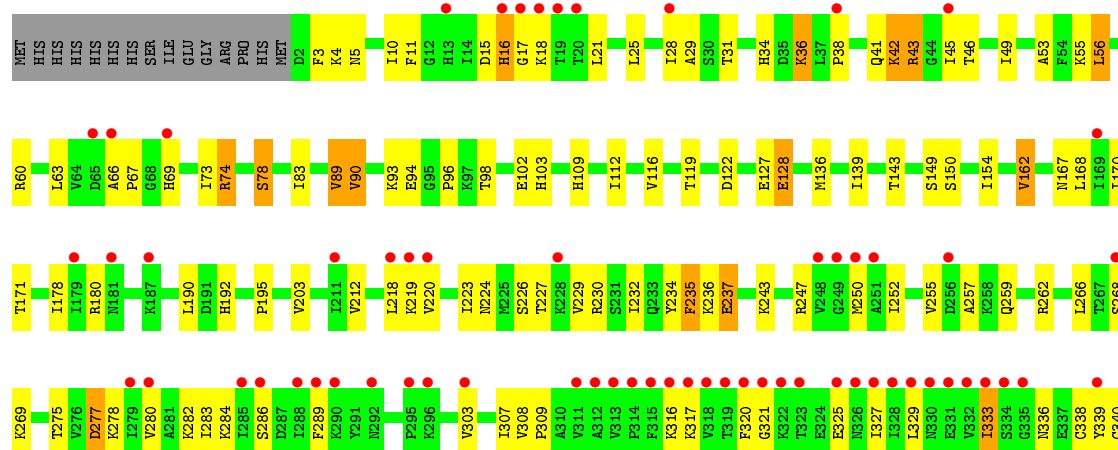
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

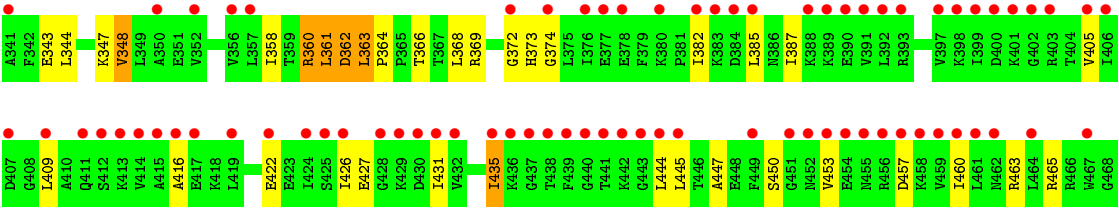


• Molecule 1: TRANSLATION ELONGATION FACTOR SELB



• Molecule 1: TRANSLATION ELONGATION FACTOR SELB





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	146.86Å 146.86Å 297.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 3.15 48.07 – 3.15	Depositor EDS
% Data completeness (in resolution range)	86.9 (19.97-3.15) 90.3 (48.07-3.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8 _1069)	Depositor
R, R_{free}	0.172 , 0.215 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	100.6	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 126.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14529	wwPDB-VP
Average B, all atoms (Å ²)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 5GP, DXC, SO4, CMH

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	0.31	0/3484	0.54	0/4684
1	B	0.34	0/3541	0.57	0/4760
1	C	0.39	0/3664	0.62	0/4929
1	D	0.29	0/3626	0.52	0/4878
All	All	0.33	0/14315	0.56	0/19251

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3475	0	3656	83	0
1	B	3533	0	3728	91	0
1	C	3651	0	3838	70	0
1	D	3615	0	3799	101	0
2	B	10	0	0	1	0
2	C	25	0	0	1	0
3	B	28	0	39	2	0
3	C	168	0	234	11	0
4	B	24	0	12	2	0
All	All	14529	0	15306	343	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 12.

The worst 5 of 343 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:D:283:ILE:HG13	1:D:340:CMH:HB3	1.21	1.15
1:C:338:CMH:HB3	1:C:340:CMH:CM	2.03	0.86
1:D:223:ILE:HG21	1:D:259:GLN:HB3	1.58	0.85
1:D:284:LYS:HG3	1:D:336:ASN:HB2	1.63	0.81
1:D:416:ALA:HB1	1:D:445:LEU:HD21	1.61	0.79

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	440/482 (91%)	420 (96%)	19 (4%)	1 (0%)	47	78
1	B	448/482 (93%)	430 (96%)	18 (4%)	0	100	100
1	C	465/482 (96%)	439 (94%)	26 (6%)	0	100	100
1	D	461/482 (96%)	433 (94%)	24 (5%)	4 (1%)	17	53
All	All	1814/1928 (94%)	1722 (95%)	87 (5%)	5 (0%)	41	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	LYS
1	A	69	HIS
1	D	333	ILE
1	D	321	GLY
1	D	382	ILE

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	382/412 (93%)	346 (91%)	36 (9%)	8	30
1	B	388/412 (94%)	359 (92%)	29 (8%)	13	42
1	C	402/412 (98%)	364 (90%)	38 (10%)	8	30
1	D	398/412 (97%)	361 (91%)	37 (9%)	9	31
All	All	1570/1648 (95%)	1430 (91%)	140 (9%)	9	33

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	394	GLU
1	C	191	ASP
1	D	333	ILE
1	C	6	ILE
1	C	98	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	HIS
1	B	148	ASN
1	D	69	HIS
1	D	373	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

16 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	$\# Z > 2$
1	CMH	D	338	1	5,7,8	0.70	0	1,7,9	0.53	0
1	CMH	B	338	1	5,7,8	0.65	0	1,7,9	0.47	0
1	CMH	D	371	1	5,7,8	0.58	0	1,7,9	0.36	0
1	CMH	B	264	1	5,7,8	0.88	0	1,7,9	1.55	0
1	CMH	A	264	1	5,7,8	0.58	0	1,7,9	0.47	0
1	CMH	B	371	1	5,7,8	0.54	0	1,7,9	1.76	0
1	CMH	C	371	1	5,7,8	0.69	0	1,7,9	1.01	0
1	CMH	A	371	1	5,7,8	0.63	0	1,7,9	1.54	0
1	CMH	C	338	1	5,7,8	0.73	0	1,7,9	0.35	0
1	CMH	C	264	1	5,7,8	0.73	0	1,7,9	1.91	0
1	CMH	D	340	1	5,7,8	0.71	0	1,7,9	0.56	0
1	CMH	B	340	1	5,7,8	0.57	0	1,7,9	0.35	0
1	CMH	C	340	1	5,7,8	0.88	0	1,7,9	1.05	0
1	CMH	A	338	1	5,7,8	0.65	0	1,7,9	0.18	0
1	CMH	A	340	1	5,7,8	0.72	0	1,7,9	0.80	0
1	CMH	D	264	1	5,7,8	0.62	0	1,7,9	0.58	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
1	CMH	D	338	1	-	0/0/6/8	-
1	CMH	B	338	1	-	0/0/6/8	-
1	CMH	D	371	1	-	0/0/6/8	-
1	CMH	B	264	1	-	0/0/6/8	-
1	CMH	A	264	1	-	0/0/6/8	-
1	CMH	B	371	1	-	0/0/6/8	-
1	CMH	C	371	1	-	0/0/6/8	-
1	CMH	A	371	1	-	0/0/6/8	-
1	CMH	C	338	1	-	0/0/6/8	-
1	CMH	C	264	1	-	0/0/6/8	-
1	CMH	D	340	1	-	0/0/6/8	-
1	CMH	B	340	1	-	0/0/6/8	-
1	CMH	C	340	1	-	0/0/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CMH	A	338	1	-	0/0/6/8	-
1	CMH	A	340	1	-	0/0/6/8	-
1	CMH	D	264	1	-	0/0/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	338	CMH	2	0
1	B	371	CMH	4	0
1	C	371	CMH	3	0
1	C	338	CMH	1	0
1	D	340	CMH	1	0
1	B	340	CMH	1	0
1	C	340	CMH	2	0
1	A	338	CMH	2	0
1	A	340	CMH	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 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	DXC	C	1480	-	28,31,31	1.89	8 (28%)	46,49,49	1.84	11 (23%)
3	DXC	B	1473	-	28,31,31	1.49	5 (17%)	46,49,49	1.67	11 (23%)
2	SO4	B	1472	-	4,4,4	0.14	0	6,6,6	0.20	0
3	DXC	C	1475	-	28,31,31	1.82	6 (21%)	46,49,49	1.85	17 (36%)
2	SO4	C	1481	-	4,4,4	0.15	0	6,6,6	0.06	0
3	DXC	C	1479	-	28,31,31	1.57	7 (25%)	46,49,49	1.97	14 (30%)
2	SO4	C	1474	-	4,4,4	0.18	0	6,6,6	0.19	0
2	SO4	C	1473	-	4,4,4	0.14	0	6,6,6	0.09	0
3	DXC	C	1477	-	28,31,31	1.66	6 (21%)	46,49,49	1.59	12 (26%)
3	DXC	C	1478	-	28,31,31	1.56	7 (25%)	46,49,49	1.94	15 (32%)
2	SO4	C	1471	-	4,4,4	0.12	0	6,6,6	0.34	0
2	SO4	C	1472	-	4,4,4	0.15	0	6,6,6	0.09	0
3	DXC	C	1476	-	28,31,31	1.69	5 (17%)	46,49,49	1.67	10 (21%)
2	SO4	B	1471	-	4,4,4	0.14	0	6,6,6	0.07	0
4	5GP	B	1474	-	22,26,26	0.59	0	27,40,40	1.70	5 (18%)

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	DXC	C	1480	-	-	0/7/71/71	0/4/4/4
3	DXC	B	1473	-	-	0/7/71/71	0/4/4/4
3	DXC	C	1475	-	-	0/7/71/71	0/4/4/4
3	DXC	C	1479	-	-	7/7/71/71	0/4/4/4
3	DXC	C	1477	-	-	2/7/71/71	0/4/4/4
3	DXC	C	1478	-	-	1/7/71/71	0/4/4/4
3	DXC	C	1476	-	-	2/7/71/71	0/4/4/4
4	5GP	B	1474	-	-	2/6/26/26	0/3/3/3

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1475	DXC	C12-C13	-4.68	1.47	1.54
3	C	1480	DXC	C12-C13	-4.28	1.47	1.54
3	C	1477	DXC	C12-C13	-4.01	1.48	1.54
3	C	1480	DXC	C18-C4	-3.94	1.47	1.54
3	C	1476	DXC	C12-C13	-3.58	1.49	1.54

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1478	DXC	C7-C8-C9	-4.79	104.25	112.14
3	C	1480	DXC	C18-C4-C5	-4.75	100.60	108.26
3	C	1478	DXC	C10-C14-C13	-4.60	108.23	114.30
3	C	1476	DXC	C18-C4-C3	-4.55	102.64	110.36
3	C	1480	DXC	C22-C21-C19	-4.48	108.68	114.72

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1474	5GP	C3'-C4'-C5'-O5'
3	C	1479	DXC	C16-C17-C19-C24
3	C	1479	DXC	C12-C17-C19-C24
3	C	1479	DXC	C24-C19-C21-C22
3	C	1476	DXC	C24-C19-C21-C22

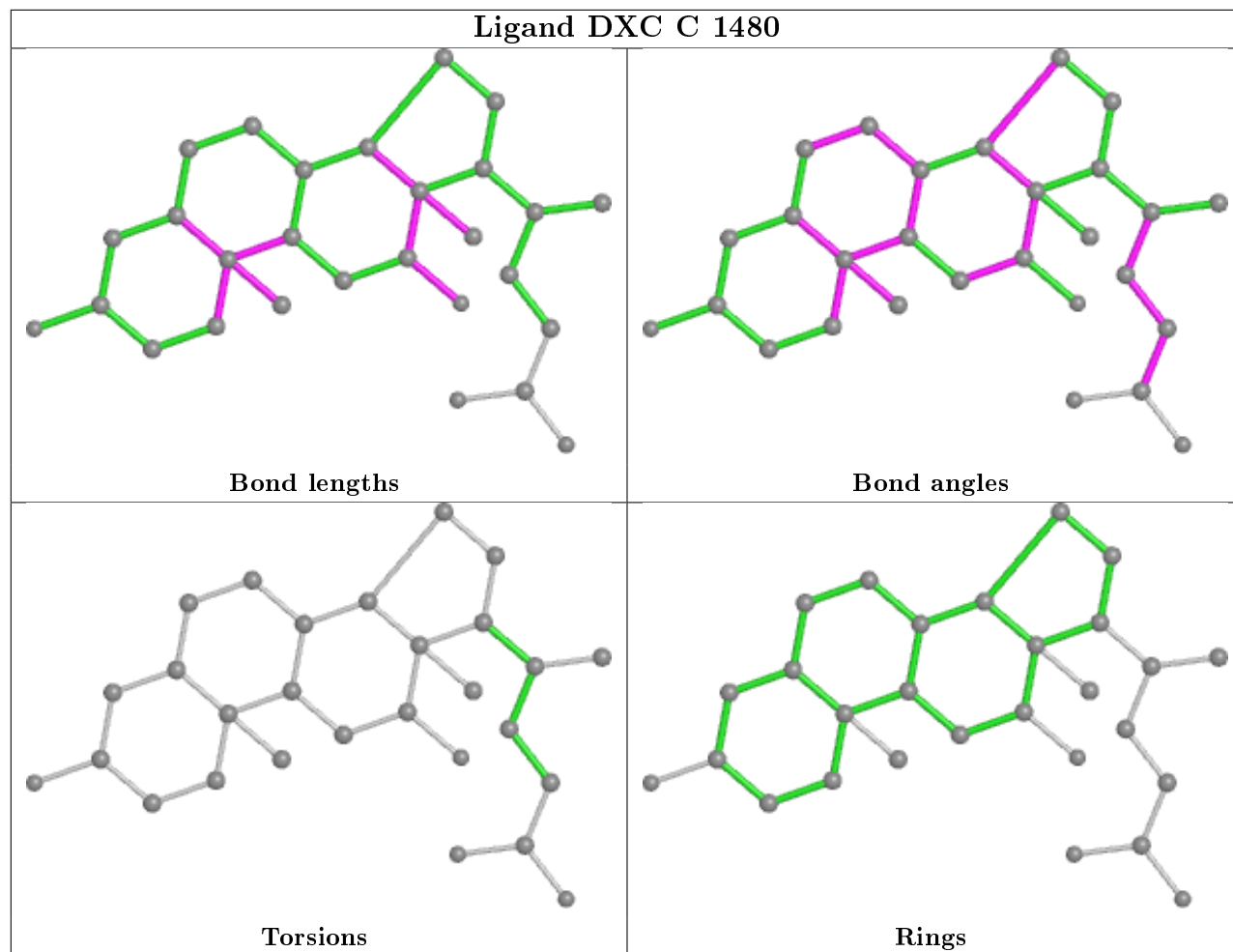
There are no ring outliers.

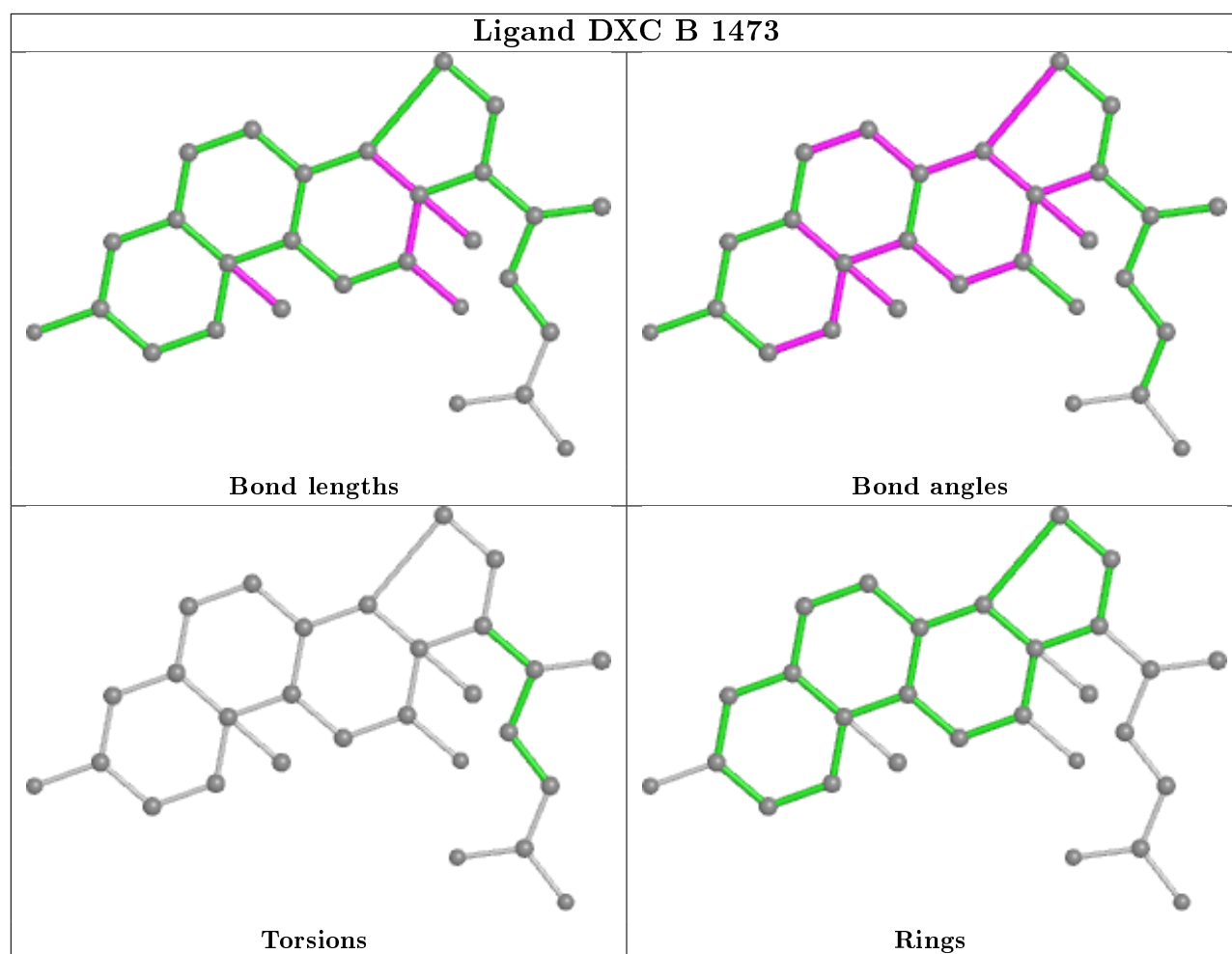
9 monomers are involved in 17 short contacts:

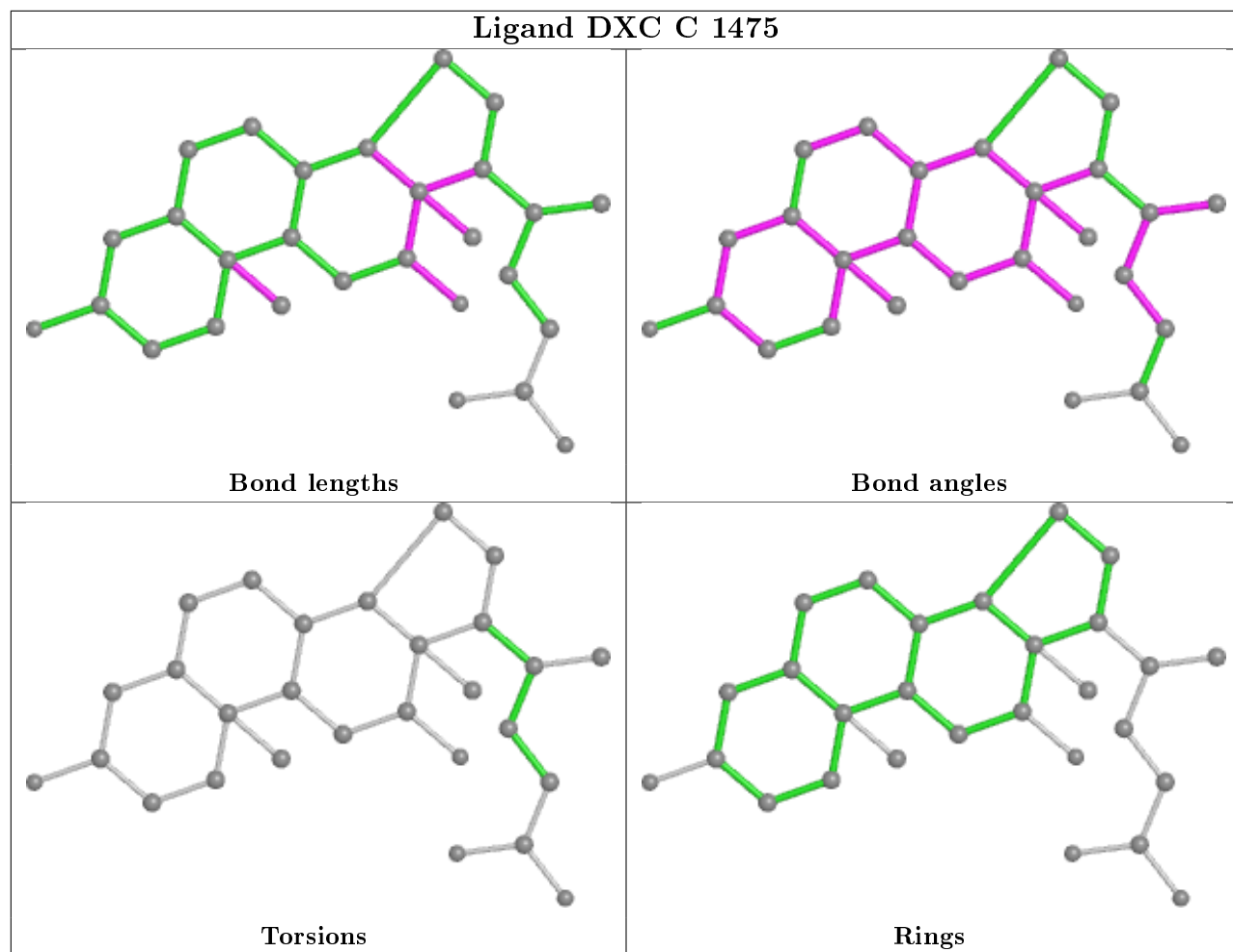
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1480	DXC	1	0
3	B	1473	DXC	2	0
3	C	1475	DXC	2	0
3	C	1479	DXC	3	0
2	C	1473	SO4	1	0
3	C	1478	DXC	2	0
3	C	1476	DXC	3	0
2	B	1471	SO4	1	0
4	B	1474	5GP	2	0

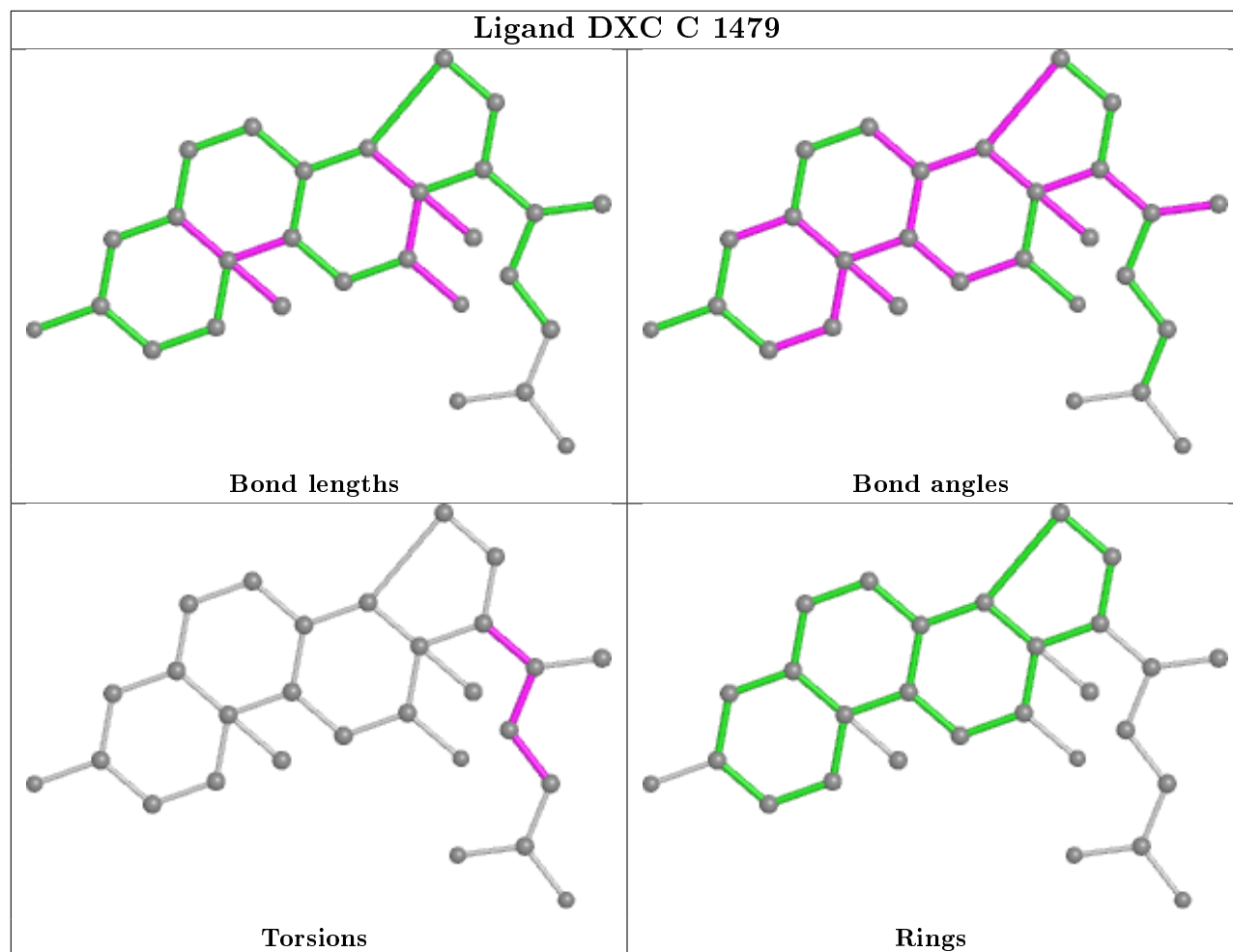
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

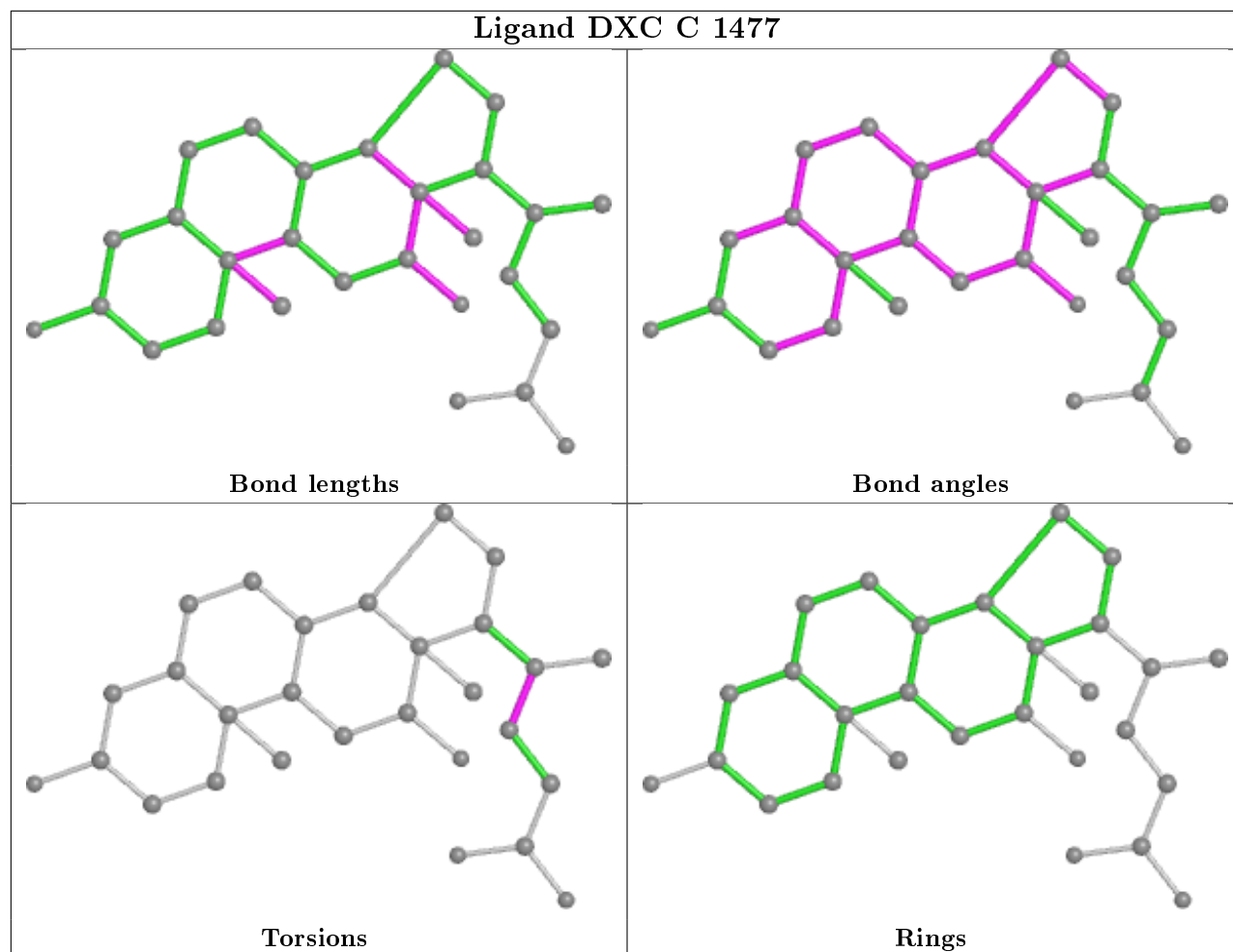
equivalents in the CSD to analyse the geometry.

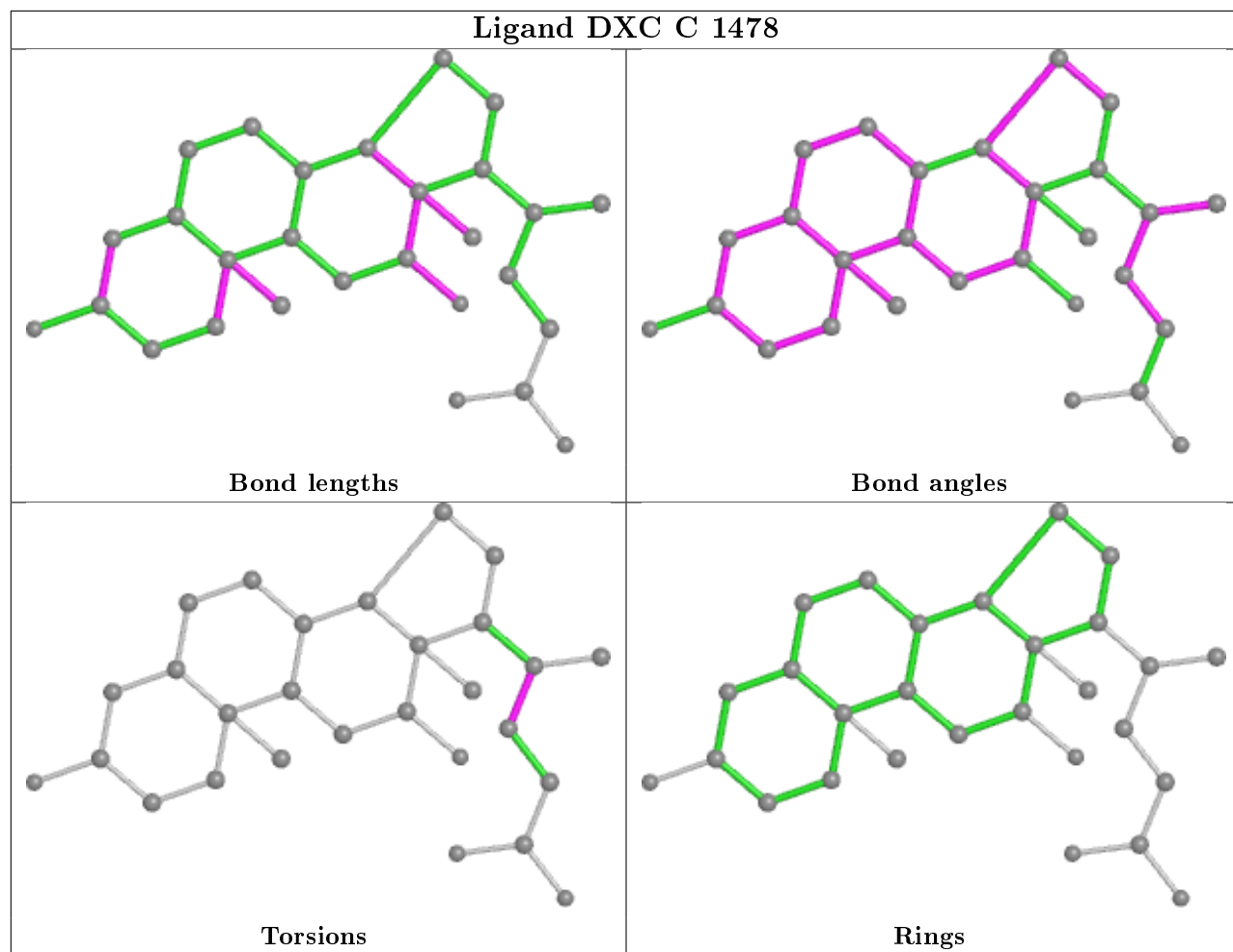


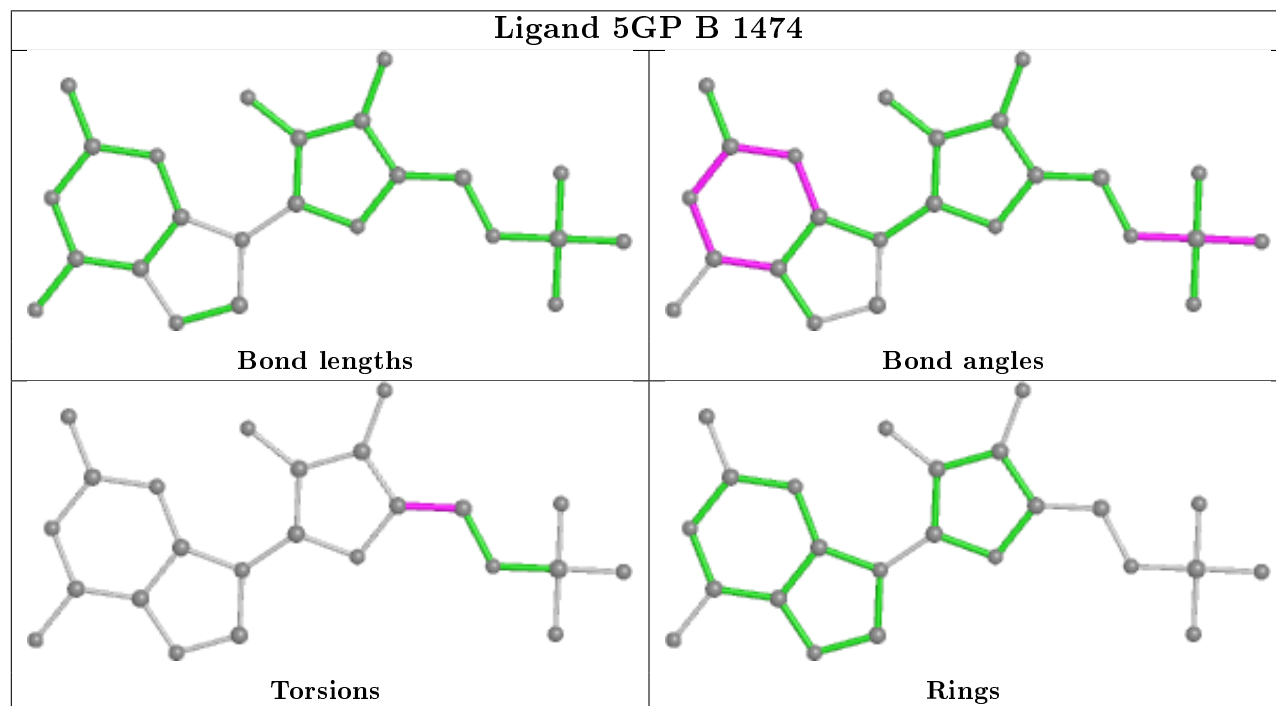
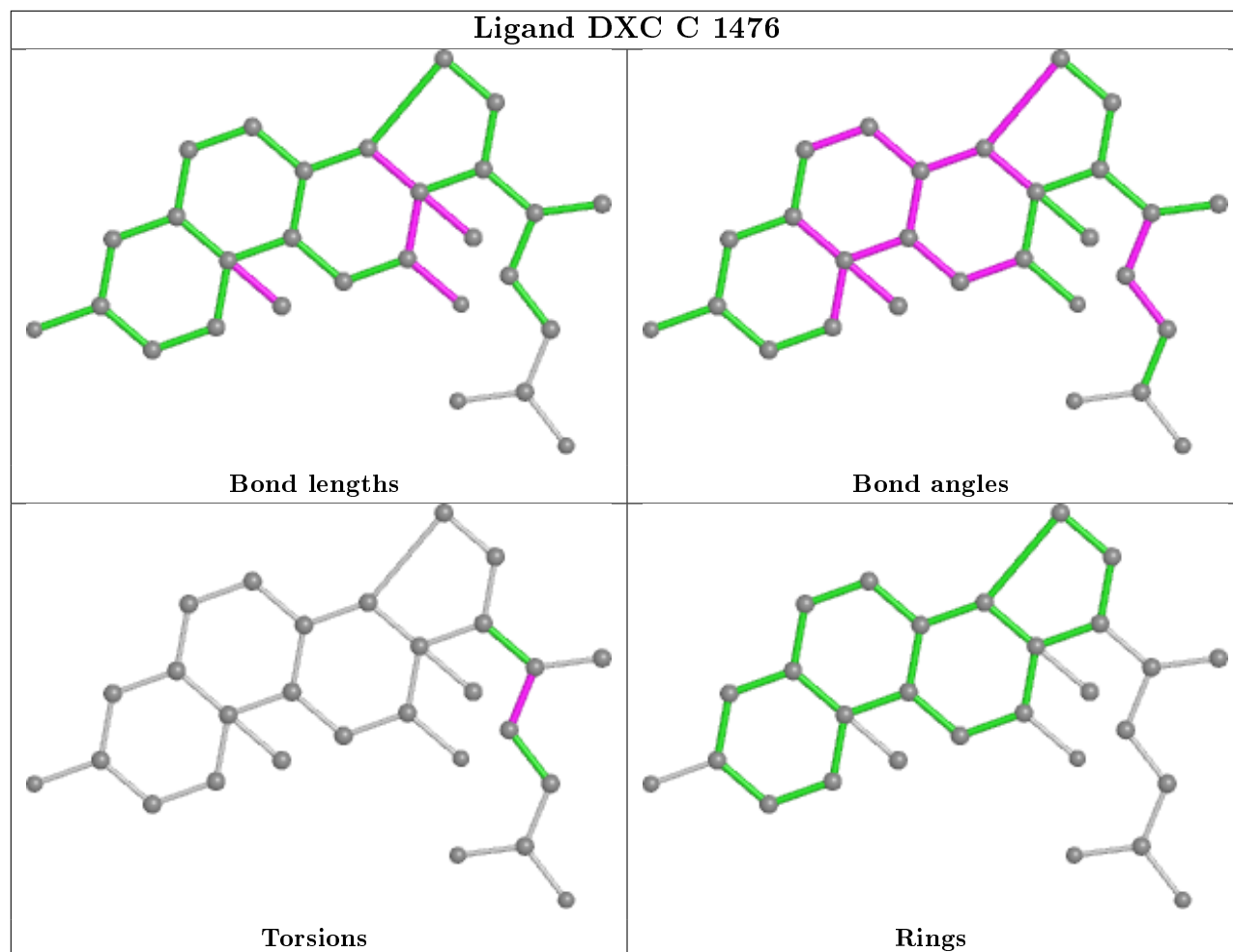












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/482 (92%)	0.76	75 (16%) 1 1	89, 172, 246, 330	0
1	B	452/482 (93%)	0.81	70 (15%) 2 1	67, 130, 321, 373	0
1	C	467/482 (96%)	0.24	21 (4%) 33 19	65, 105, 204, 279	0
1	D	463/482 (96%)	1.62	138 (29%) 0 0	117, 220, 320, 374	0
All	All	1826/1928 (94%)	0.86	304 (16%) 1 1	65, 163, 299, 374	0

The worst 5 of 304 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	THR	16.5
1	D	442	LYS	12.3
1	D	441	THR	12.2
1	D	453	VAL	11.4
1	B	441	THR	10.9

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
1	CMH	D	338	8/9	0.75	0.17	187,264,268,302	2
1	CMH	A	371	8/9	0.91	0.34	154,165,195,202	2
1	CMH	B	371	8/9	0.94	0.13	141,161,218,263	2
1	CMH	A	338	8/9	0.94	0.21	149,179,204,211	2
1	CMH	B	338	8/9	0.95	0.15	157,190,227,235	2
1	CMH	D	340	8/9	0.96	0.24	155,269,276,276	2
1	CMH	D	371	8/9	0.96	0.21	129,151,184,191	2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CMH	C	338	8/9	0.97	0.19	72,94,152,200	2
1	CMH	B	340	8/9	0.98	0.17	141,161,259,276	2
1	CMH	C	340	8/9	0.98	0.16	58,87,108,131	2
1	CMH	A	264	8/9	0.98	0.17	166,181,195,201	2
1	CMH	A	340	8/9	0.98	0.22	150,189,198,212	2
1	CMH	D	264	8/9	0.98	0.24	164,180,206,220	2
1	CMH	B	264	8/9	1.00	0.23	57,72,95,100	2
1	CMH	C	371	8/9	1.00	0.19	55,102,148,154	2
1	CMH	C	264	8/9	1.00	0.17	61,95,114,120	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.

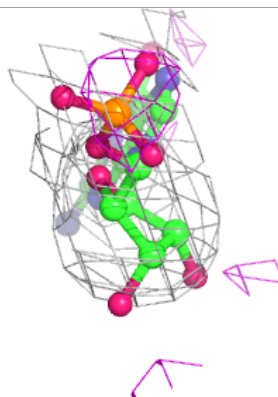
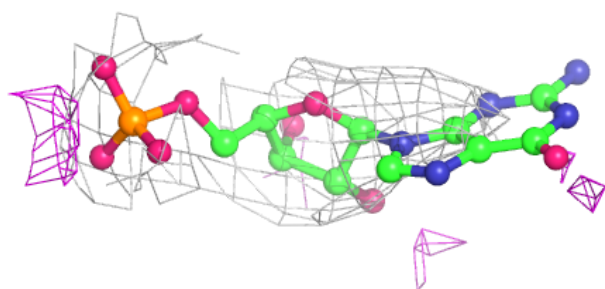
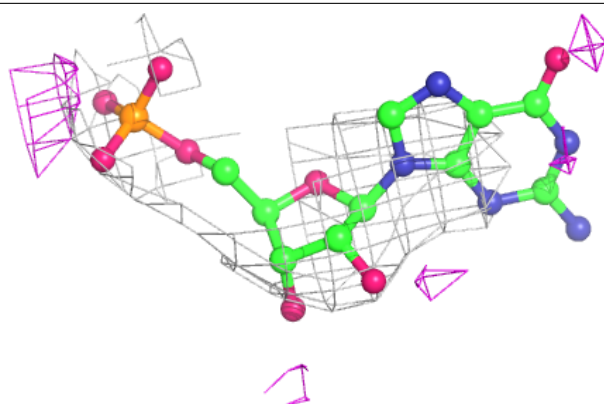
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	C	1474	5/5	0.57	0.62	156,216,245,297	5
2	SO4	C	1481	5/5	0.67	0.85	157,190,196,199	5
2	SO4	B	1471	5/5	0.73	0.41	172,203,237,246	0
4	5GP	B	1474	24/24	0.87	0.41	204,243,284,292	0
2	SO4	C	1473	5/5	0.88	0.11	138,173,210,226	5
3	DXC	C	1476	28/28	0.89	0.34	139,146,204,235	0
2	SO4	B	1472	5/5	0.91	0.42	94,222,224,320	0
3	DXC	C	1479	28/28	0.93	0.34	72,89,173,216	28
3	DXC	C	1477	28/28	0.95	0.30	67,90,157,199	0
3	DXC	C	1478	28/28	0.96	0.31	73,105,138,168	0
2	SO4	C	1471	5/5	0.96	0.24	93,127,147,181	0
2	SO4	C	1472	5/5	0.96	0.17	112,131,153,180	0
3	DXC	C	1475	28/28	0.97	0.26	64,79,119,144	0
3	DXC	B	1473	28/28	0.98	0.26	62,82,119,128	0
3	DXC	C	1480	28/28	0.98	0.23	64,76,98,107	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.

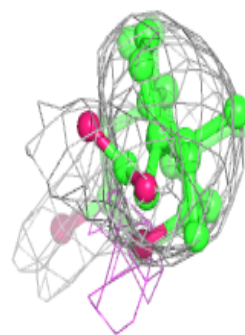
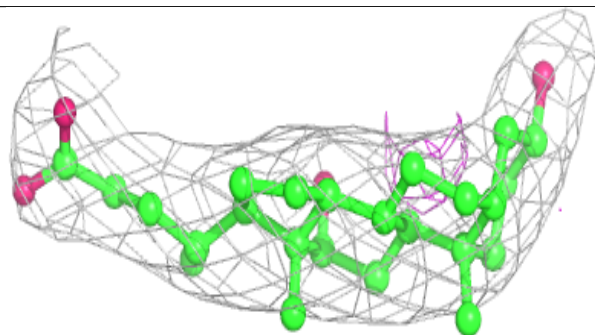
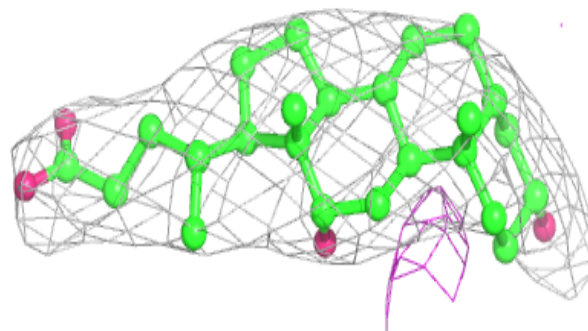
Electron density around 5GP B 1474:

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



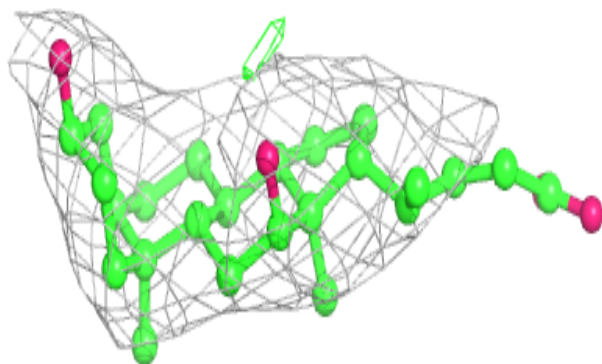
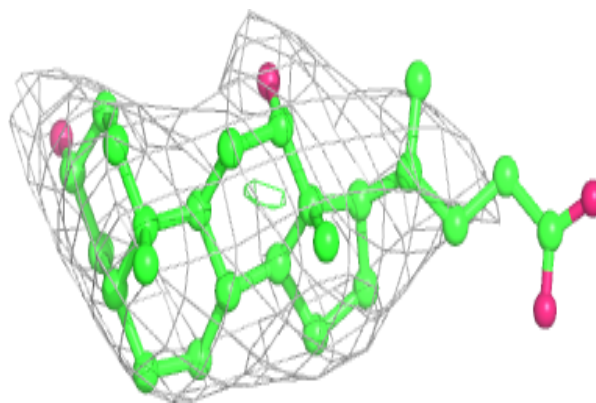
Electron density around DXC C 1476:

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

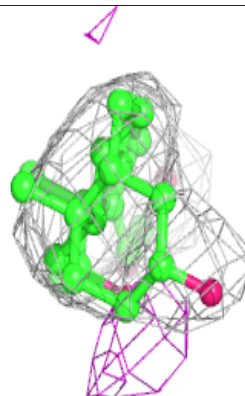
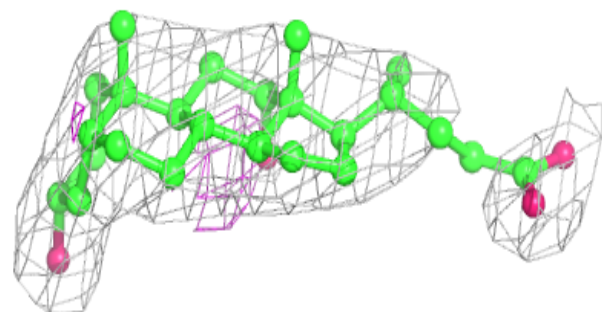
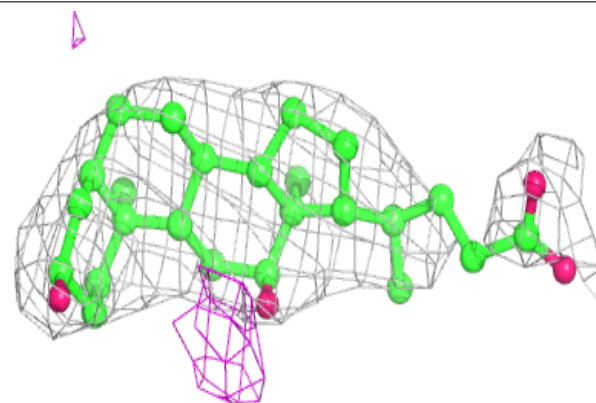


Electron density around DXC C 1479:

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

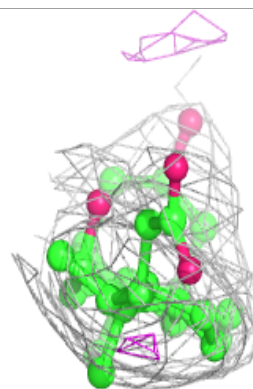
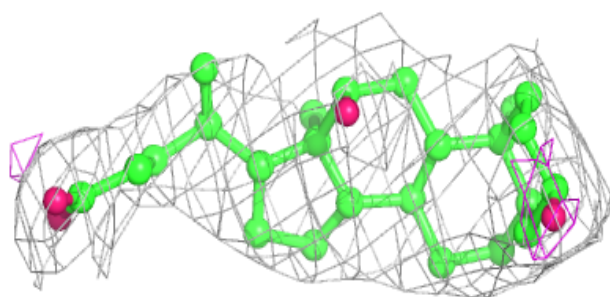
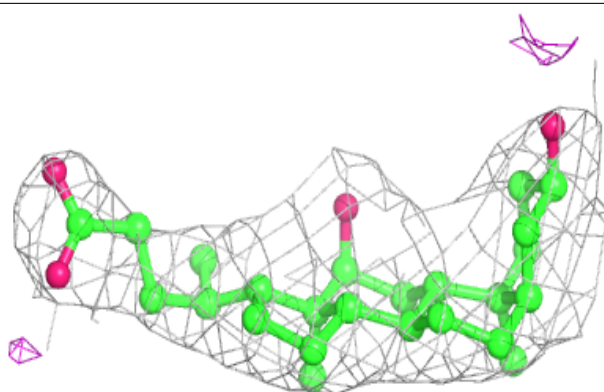
**Electron density around DXC C 1477:**

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

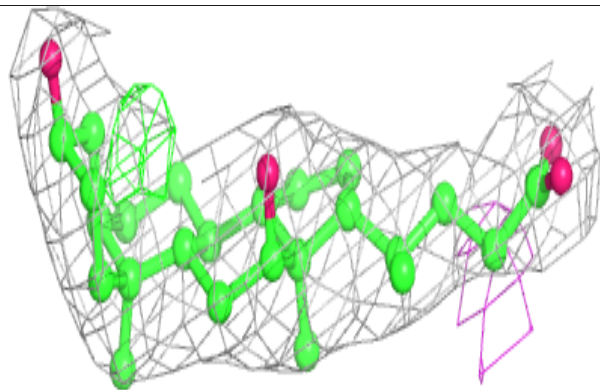
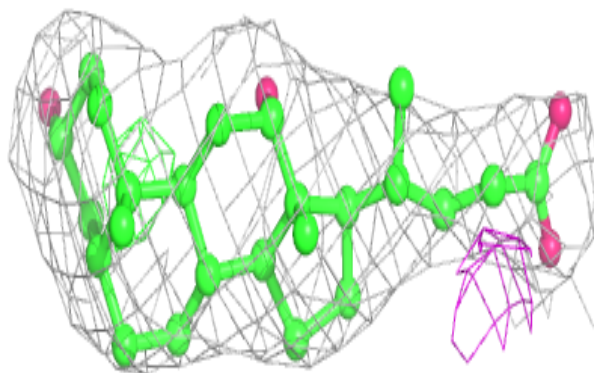


Electron density around DXC C 1478:

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

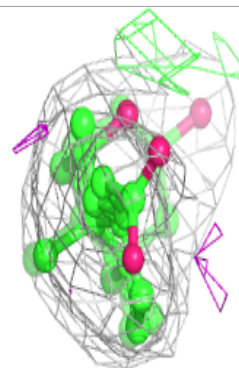
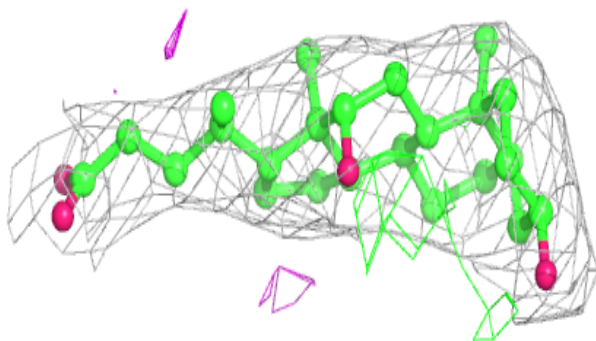
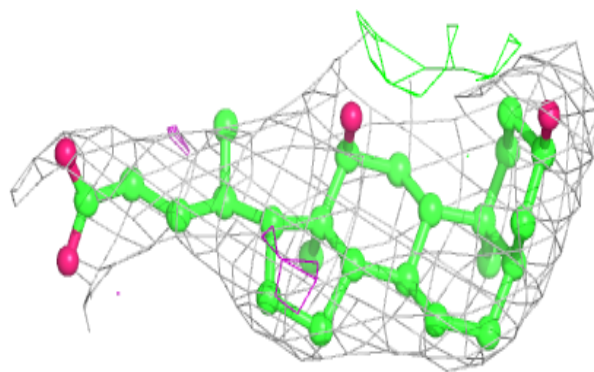
**Electron density around DXC C 1475:**

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

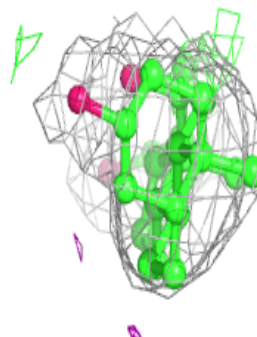
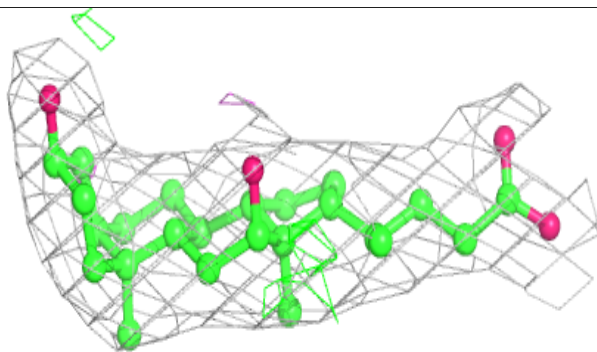
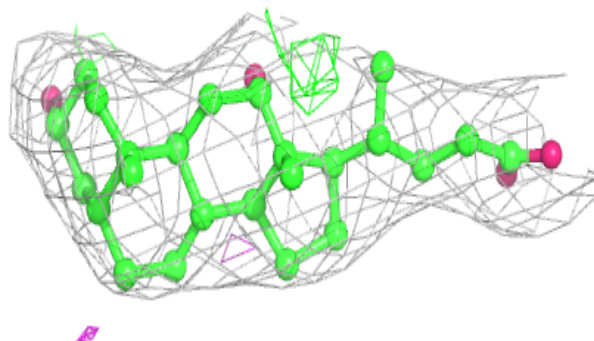


Electron density around DXC B 1473:

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

**Electron density around DXC C 1480:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.