

# wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 02:37 pm GMT

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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

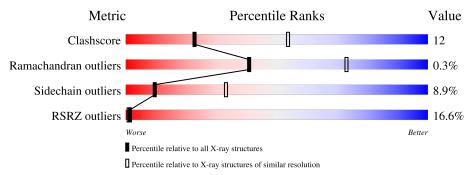
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
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 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					
			16%					
1	A	482	63%	27%	• 7%			
			15%					
1	В	482	65%	27%	• 5%			
			4%					
1	С	482	73%	22%	• •			
			29%					
1	D	482	65%	28%	• •			

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	В	371	-	-	X	-
2	SO4	В	1471	-	-	-	X
2	SO4	С	1474	-	-	=	X
2	SO4	С	1481	-	-	-	X



# 2 Entry composition (i)

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	С	Hg	N	О	S	0	0	0
1	Λ	440	3475	2220	4	593	644	14	U	0	
1	В	456	Total	С	Hg	N	О	S	0	0	0
1	Ъ	450	3533	2257	4	603	655	14	0		
1	С	471	Total	С	Hg	N	О	S	0	0	0
1		411	3651	2327	4	627	679	14	U	0	
1	D	467	Total	С	Hg	N	О	S	0	0	0
1	ע	407	3615	2305	4	618	675	13	U	0	

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
В	-13	MET	_	expression tag	UNP Q8J307
В	-12	HIS	-	expression tag	UNP Q8J307
В	-11	HIS	-	expression tag	UNP Q8J307
В	-10	HIS	-	expression tag	UNP Q8J307
В	-9	HIS	-	expression tag	UNP Q8J307
В	-8	HIS		expression tag	UNP Q8J307
В	-7	HIS	_	expression tag	UNP Q8J307

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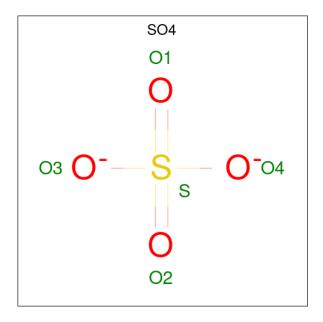


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Chain	Residue	Modelled	Actual	Comment	Reference
В	-6	SER	-	expression tag	UNP Q8J307
В	-5	ILE	-	expression tag	UNP Q8J307
В	-4	GLU	-	expression tag	UNP Q8J307
В	-3	GLY	-	expression tag	UNP Q8J307
В	-2	ARG	-	expression tag	UNP Q8J307
В	-1	PRO	-	expression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

 $\bullet$  Molecule 2 is SULFATE ION (three-letter code: SO4) (formula:  $\mathrm{O_4S}).$ 

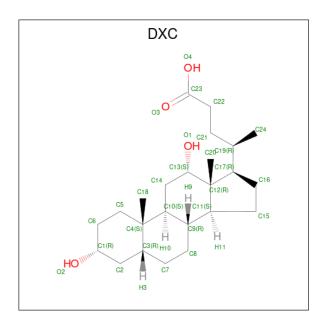




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total O S 5 4 1	0	0
2	В	1	Total O S 5 4 1	0	0
2	С	1	Total O S 5 4 1	0	0
2	С	1	Total O S 5 4 1	0	0
2	С	1	Total O S 5 4 1	0	0
2	С	1	Total O S 5 4 1	0	0
2	С	1	Total O S 5 4 1	0	0

• Molecule 3 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula:  $C_{24}H_{40}O_4$ ).

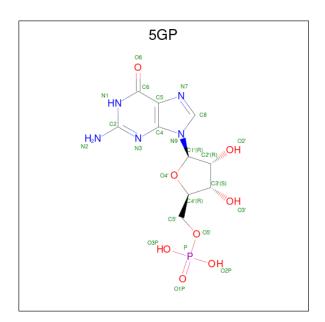




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total C O 28 24 4	0	0
3	С	1	Total C O 28 24 4	0	0
3	С	1	Total C O 28 24 4	0	0
3	С	1	Total C O 28 24 4	0	0
3	С	1	Total C O 28 24 4	0	0
3	С	1	Total C O 28 24 4	0	0
3	С	1	Total C O 28 24 4	0	0

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





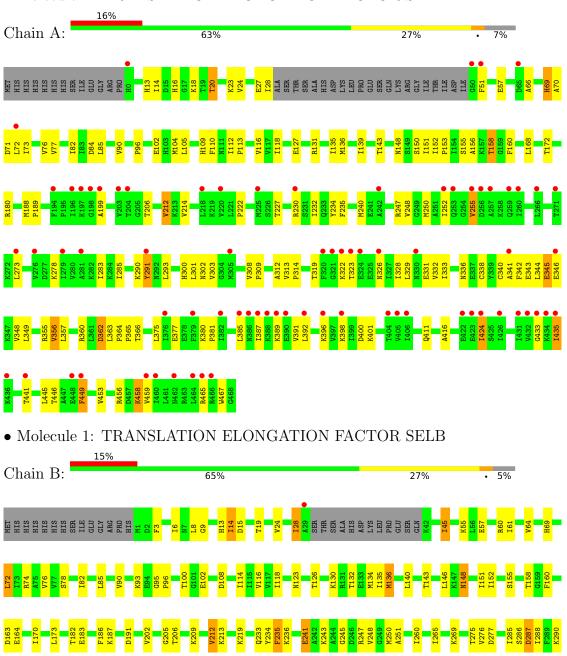
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
1	D	1	Total	С	N	О	Р	0	0
4	Б	1	24	10	5	8	1	U	U



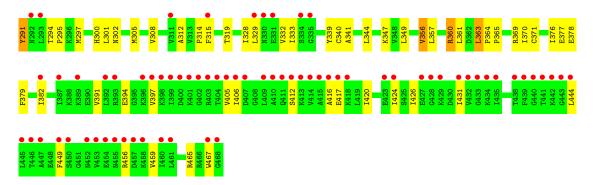
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

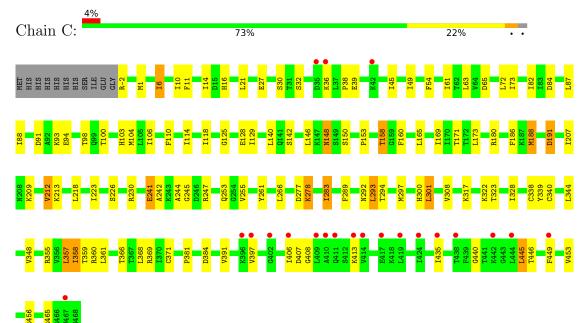
• Molecule 1: TRANSLATION ELONGATION FACTOR SELB



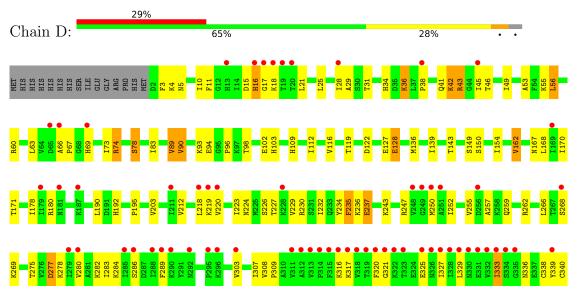




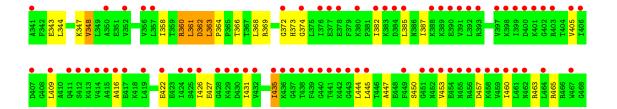
• Molecule 1: TRANSLATION ELONGATION FACTOR SELB



• Molecule 1: TRANSLATION ELONGATION FACTOR SELB









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants	146.86Å 146.86Å 297.83Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	19.97 - 3.15	Depositor
Resolution (A)	48.07 - 3.15	EDS
% Data completeness	86.9 (19.97-3.15)	Depositor
(in resolution range)	90.3 (48.07-3.15)	EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.25 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
D.D.	0.172 , $0.215$	Depositor
$R, R_{free}$	0.193 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	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 <sup>2</sup>	$< L > = 0.49, < L^2> = 0.32$	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 <sup>2</sup> )	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.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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, CMH, SO4, DXC

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 $\mid \# Z  > 5$		
MIOI	Moi Chain		RMSZ   #  Z  > 5		# Z  > 5	
1	A	0.31	0/3484	0.54	0/4684	
1	В	0.34	0/3541	0.57	0/4760	
1	С	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	В	3533	0	3728	91	0
1	С	3651	0	3838	70	0
1	D	3615	0	3799	101	0
2	В	10	0	0	1	0
2	С	25	0	0	1	0
3	В	28	0	39	2	0
3	С	168	0	234	11	0
4	В	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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$	
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	Perce	ntiles
1	A	440/482 (91%)	420 (96%)	19 (4%)	1 (0%)	47	78
1	В	448/482 (93%)	430 (96%)	18 (4%)	0	100	100
1	С	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	В	388/412 (94%)	359 (92%)	29 (8%)	13	42	
1	С	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	D	128	GLU
1	D	154	ILE
1	D	348	VAL
1	В	235	PHE
1	В	212	VAL

Sometimes 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	В	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	В	ond leng	$\operatorname{gths}$	В	ond ang	gles
IVIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CMH	С	371	1	5,7,8	0.69	0	1,7,9	1.01	0
1	CMH	D	340	1	5,7,8	0.71	0	1,7,9	0.56	0
1	CMH	A	264	1	5,7,8	0.58	0	1,7,9	0.47	0
1	CMH	A	338	1	5,7,8	0.65	0	1,7,9	0.18	0
1	CMH	С	338	1	5,7,8	0.73	0	1,7,9	0.35	0
1	CMH	D	264	1	5,7,8	0.62	0	1,7,9	0.58	0
1	CMH	С	264	1	5,7,8	0.73	0	1,7,9	1.91	0
1	CMH	В	340	1	5,7,8	0.57	0	1,7,9	0.35	0
1	CMH	С	340	1	5,7,8	0.88	0	1,7,9	1.05	0
1	CMH	D	338	1	5,7,8	0.70	0	1,7,9	0.53	0
1	CMH	D	371	1	5,7,8	0.58	0	1,7,9	0.36	0
1	CMH	A	371	1	5,7,8	0.63	0	1,7,9	1.54	0
1	CMH	A	340	1	5,7,8	0.72	0	1,7,9	0.80	0
1	CMH	В	338	1	5,7,8	0.65	0	1,7,9	0.47	0
1	CMH	В	371	1	5,7,8	0.54	0	1,7,9	1.76	0
1	СМН	В	264	1	5,7,8	0.88	0	1,7,9	1.55	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	СМН	С	371	1	-	0/0/6/8	-
1	СМН	D	340	1	-	0/0/6/8	-
1	СМН	A	264	1	-	0/0/6/8	-
1	СМН	A	338	1	-	0/0/6/8	-
1	СМН	С	338	1	-	0/0/6/8	-
1	СМН	D	264	1	-	0/0/6/8	-
1	СМН	С	264	1	-	0/0/6/8	-
1	СМН	В	340	1	-	0/0/6/8	-
1	СМН	С	340	1	-	0/0/6/8	-
1	СМН	D	338	1	-	0/0/6/8	-
1	СМН	D	371	1	-	0/0/6/8	-
1	СМН	A	371	1	-	0/0/6/8	
1	СМН	A	340	1	-	0/0/6/8	_

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	СМН	В	338	1	-	0/0/6/8	-
1	СМН	В	371	1	-	0/0/6/8	-
1	СМН	В	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	С	371	СМН	3	0
1	D	340	СМН	1	0
1	A	338	CMH	2	0
1	С	338	CMH	1	0
1	В	340	СМН	1	0
1	С	340	СМН	2	0
1	D	338	СМН	2	0
1	A	340	CMH	4	0
1	В	371	СМН	4	0

# 5.5 Carbohydrates (i)

There are no monosaccharides 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).



Mal	Trimo	Chain	Res	Link	Во	ond leng	ths	В	ond ang	gles
Mol	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	5GP	В	1474	-	22,26,26	1.24	2 (9%)	26,40,40	1.32	5 (19%)
3	DXC	С	1479	-	31,31,31	1.52	7 (22%)	49,49,49	1.92	14 (28%)
2	SO4	С	1474	-	4,4,4	0.18	0	6,6,6	0.19	0
3	DXC	С	1480	-	31,31,31	1.84	8 (25%)	49,49,49	1.73	10 (20%)
2	SO4	С	1471	-	4,4,4	0.12	0	6,6,6	0.34	0
2	SO4	С	1473	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	В	1471	-	4,4,4	0.14	0	6,6,6	0.07	0
3	DXC	С	1476	-	31,31,31	1.65	5 (16%)	49,49,49	1.61	9 (18%)
3	DXC	С	1477	-	31,31,31	1.61	6 (19%)	49,49,49	1.57	12 (24%)
3	DXC	С	1475	-	31,31,31	1.76	6 (19%)	49,49,49	1.80	16 (32%)
2	SO4	В	1472	-	4,4,4	0.14	0	6,6,6	0.20	0
3	DXC	В	1473	-	31,31,31	1.45	5 (16%)	49,49,49	1.66	13 (26%)
3	DXC	С	1478	-	31,31,31	1.51	7 (22%)	49,49,49	1.89	16 (32%)
2	SO4	С	1472	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	С	1481	-	4,4,4	0.15	0	6,6,6	0.06	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	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
4	5GP	В	1474	-	-	2/6/26/26	0/3/3/3
3	DXC	С	1479	-	-	7/9/71/71	0/4/4/4
3	DXC	С	1480	-	-	0/9/71/71	0/4/4/4
3	DXC	С	1477	-	-	4/9/71/71	0/4/4/4
3	DXC	С	1476	-	-	4/9/71/71	0/4/4/4
3	DXC	С	1475	-	-	2/9/71/71	0/4/4/4
3	DXC	С	1478	-	-	1/9/71/71	0/4/4/4
3	DXC	В	1473	_	-	2/9/71/71	0/4/4/4

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	Ideal(Å)
3	С	1475	DXC	C12-C13	-4.68	1.47	1.54
3	С	1480	DXC	C12-C13	-4.28	1.47	1.54
3	С	1477	DXC	C12-C13	-4.01	1.48	1.54
4	В	1474	5GP	C5-C6	-4.00	1.39	1.47
3	С	1480	DXC	C18-C4	-3.94	1.47	1.54



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

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	С	1478	DXC	C7-C8-C9	-4.79	104.25	112.14
3	С	1480	DXC	C18-C4-C5	-4.75	100.60	108.26
3	С	1478	DXC	C10-C14-C13	-4.60	108.23	114.30
3	С	1476	DXC	C18-C4-C3	-4.55	102.64	110.36
3	С	1479	DXC	C8-C9-C10	4.41	115.97	110.49

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

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

There are no ring outliers.

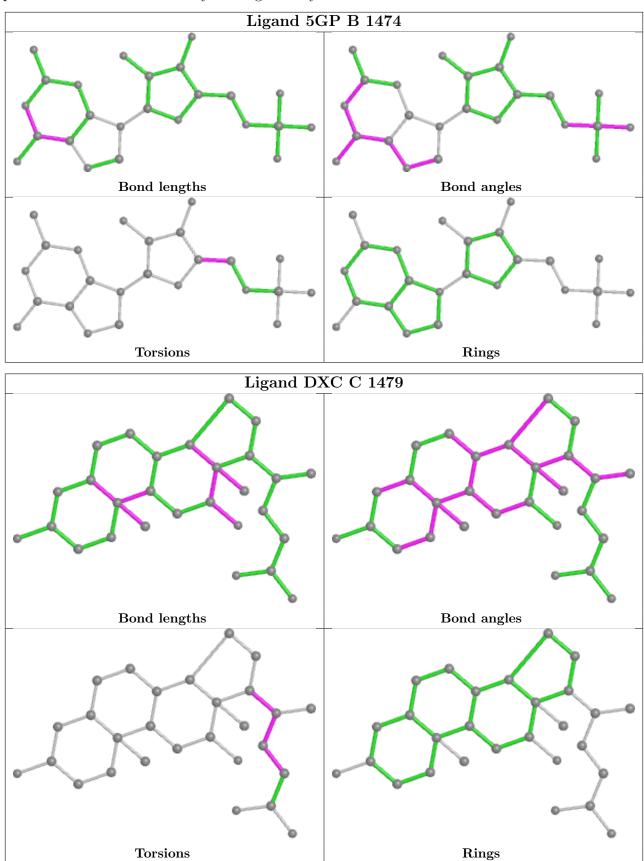
9 monomers are involved in 17 short contacts:

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

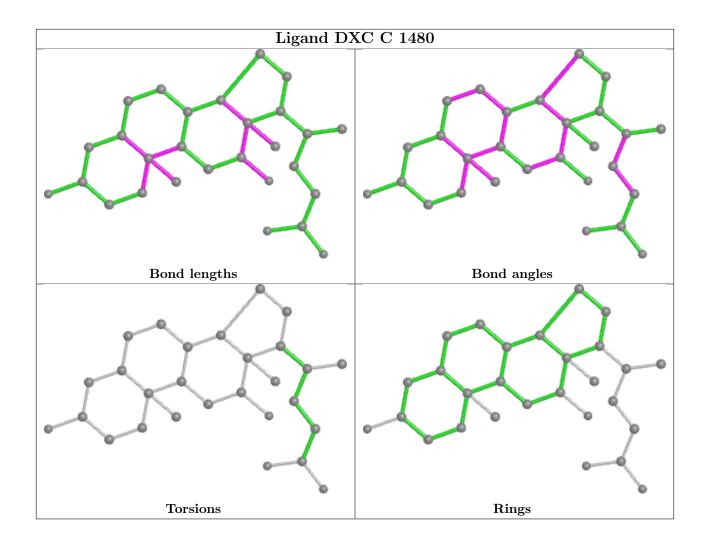
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



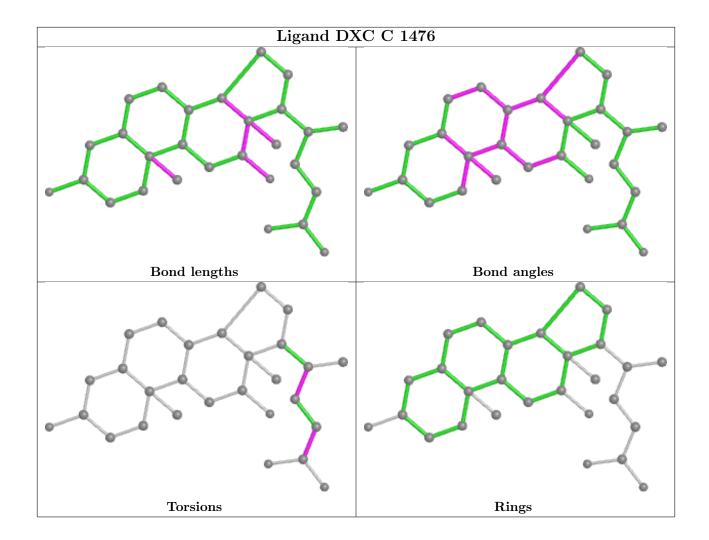
equivalents in the CSD to analyse the geometry.



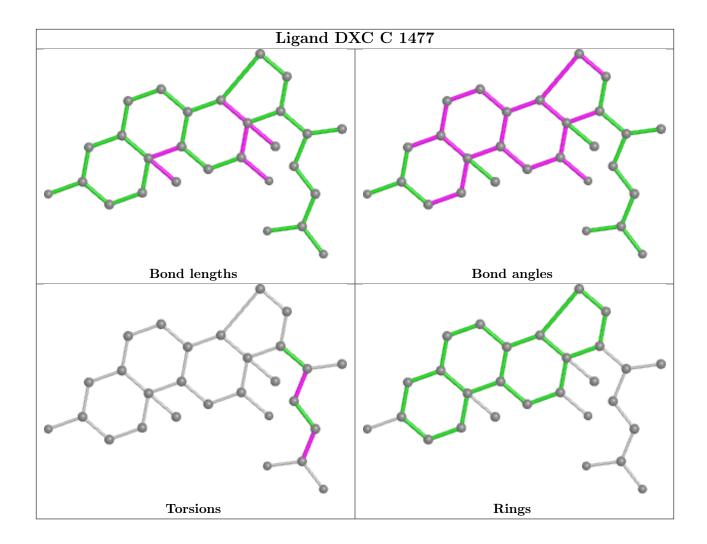




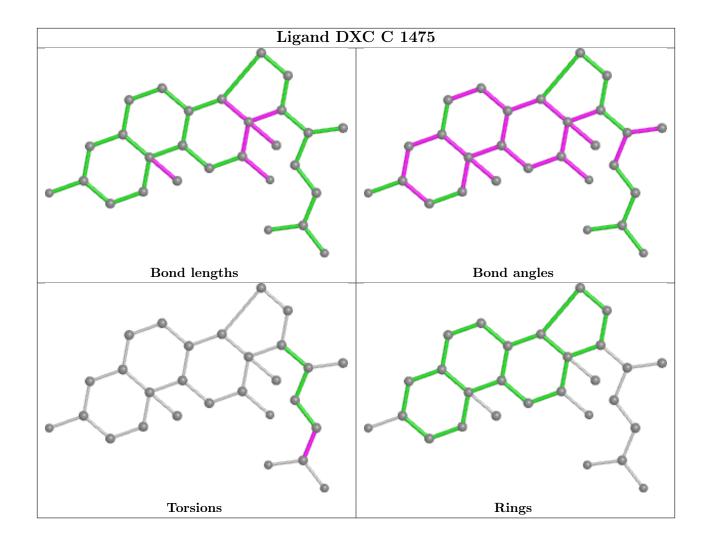




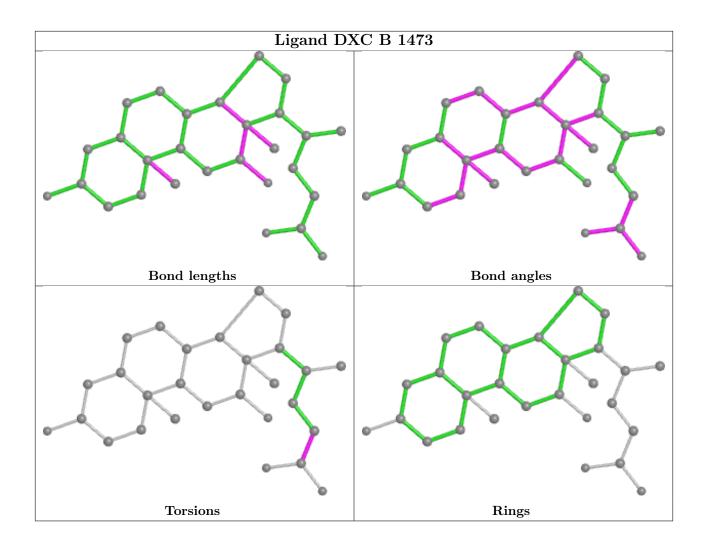




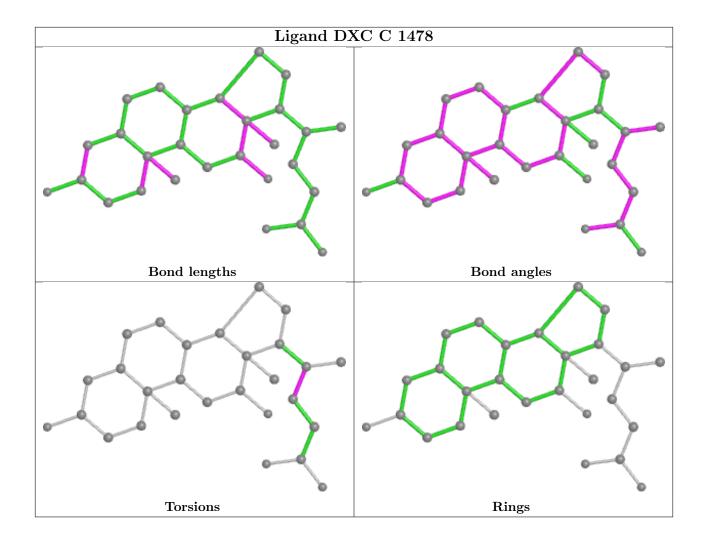












# 5.7 Other polymers (i)

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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	A	444/482 (92%)	0.76	75 (16%) 1 1	89, 172, 246, 330	0
1	В	452/482 (93%)	0.81	70 (15%) 2 1	67, 130, 321, 373	0
1	С	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	В	404	THR	16.5
1	D	442	LYS	12.3
1	D	441	THR	12.2
1	D	453	VAL	11.4
1	В	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,  $95^{th}$  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	$ extbf{B-factors}( extbf{A}^2)$	Q<0.9
1	СМН	D	338	8/9	0.75	0.17	187,264,268,302	2
1	СМН	A	371	8/9	0.91	0.34	154,165,195,202	2
1	СМН	В	371	8/9	0.94	0.13	141,161,218,263	2
1	СМН	A	338	8/9	0.94	0.21	149,179,204,211	2
1	СМН	В	338	8/9	0.95	0.15	157,190,227,235	2
1	СМН	D	340	8/9	0.96	0.24	155,269,276,276	2
1	СМН	D	371	8/9	0.96	0.21	129,151,184,191	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ m \AA}^2)$	Q<0.9
1	CMH	С	338	8/9	0.97	0.19	72,94,152,200	2
1	CMH	С	340	8/9	0.98	0.16	58,87,108,131	2
1	CMH	D	264	8/9	0.98	0.24	164,180,206,220	2
1	CMH	В	340	8/9	0.98	0.17	141,161,259,276	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	С	264	8/9	1.00	0.17	61,95,114,120	0
1	CMH	С	371	8/9	1.00	0.19	55,102,148,154	2
1	CMH	В	264	8/9	1.00	0.23	57,72,95,100	2

## 6.3 Carbohydrates (i)

There are no monosaccharides 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,  $95^{th}$  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	${f B\text{-factors}}({f \AA}^2)$	Q<0.9
2	SO4	С	1474	5/5	0.57	0.62	156,216,245,297	5
2	SO4	С	1481	5/5	0.67	0.85	157,190,196,199	5
2	SO4	В	1471	5/5	0.73	0.41	172,203,237,246	0
4	5GP	В	1474	24/24	0.87	0.41	204,243,284,292	0
2	SO4	С	1473	5/5	0.88	0.11	138,173,210,226	5
3	DXC	С	1476	28/28	0.89	0.34	139,146,204,235	0
2	SO4	В	1472	5/5	0.91	0.42	94,222,224,320	0
3	DXC	С	1479	28/28	0.93	0.34	72,89,173,216	28
3	DXC	С	1477	28/28	0.95	0.30	67,90,157,199	0
3	DXC	С	1478	28/28	0.96	0.31	73,105,138,168	0
2	SO4	С	1472	5/5	0.96	0.17	112,131,153,180	0
2	SO4	С	1471	5/5	0.96	0.24	93,127,147,181	0
3	DXC	С	1475	28/28	0.97	0.26	64,79,119,144	0
3	DXC	С	1480	28/28	0.98	0.23	64,76,98,107	0
3	DXC	В	1473	28/28	0.98	0.26	62,82,119,128	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

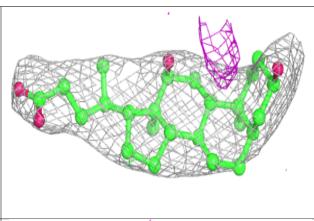


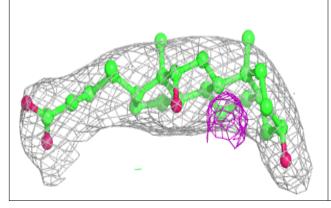
orientation to approximate a three-dimensional view.

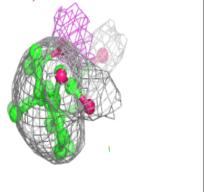
# 

# Electron density around DXC C 1476:

 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



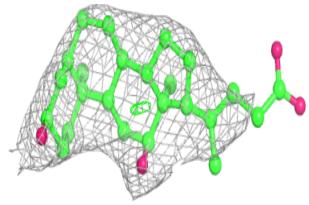


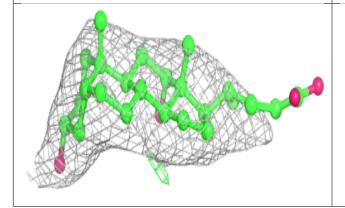


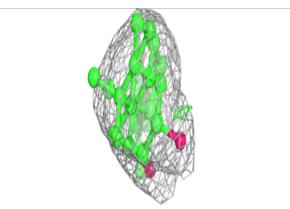


# Electron density around DXC C 1479:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$  (at 0.7 rmsd) in gray  ${\rm mF}_o\text{-}{\rm DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

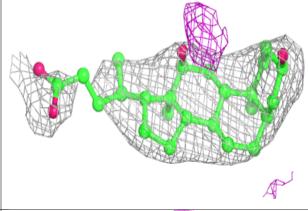


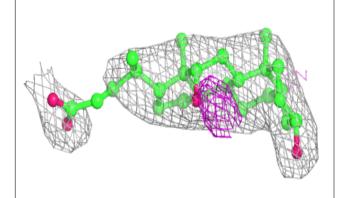


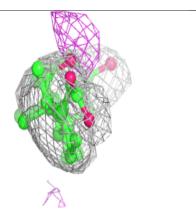


#### Electron density around DXC C 1477:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



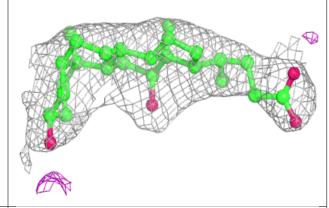


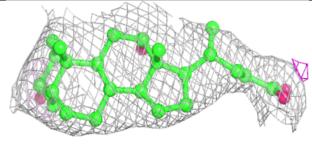


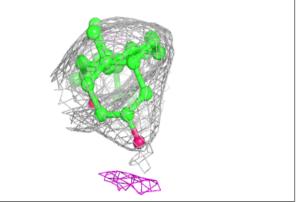


#### Electron density around DXC C 1478:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$  (at 0.7 rmsd) in gray  ${\rm mF}_o\text{-}{\rm DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

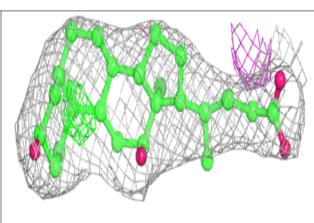


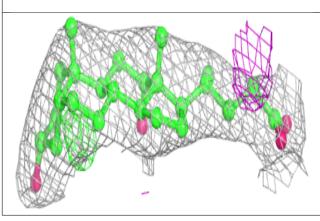


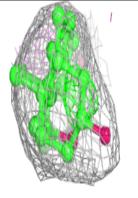


#### Electron density around DXC C 1475:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



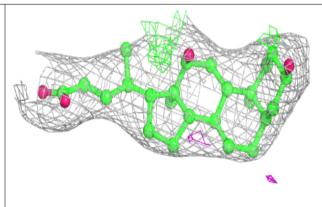


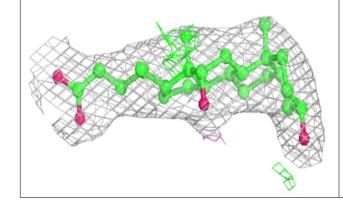


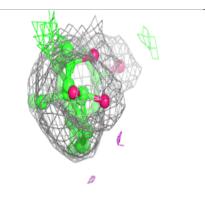


#### Electron density around DXC C 1480:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$  (at 0.7 rmsd) in gray  ${\rm mF}_o\text{-}{\rm DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

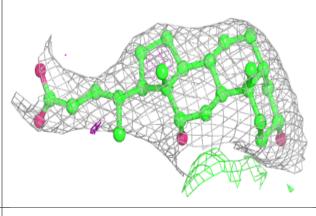


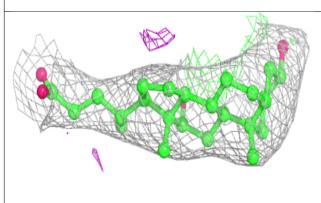


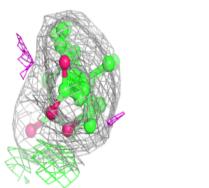


#### Electron density around DXC B 1473:

 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)









# 6.5 Other polymers (i)

There are no such residues in this entry.

