WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 11:49 pm BST

PDB ID	:	4AC9
Title	:	CRYSTAL STRUCTURE OF TRANSLATION ELONGATION FACTOR SELB FROM METHANOCOCCUS MARIPALUDIS IN COMPLEX WITH GDP
Authors	:	Leibundgut, M.; Frick, C.; Thanbichler, M.; Boeck, A.; Ban, N.
Deposited on	:	2011-12-14
Resolution	:	3.03 Å(reported)

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

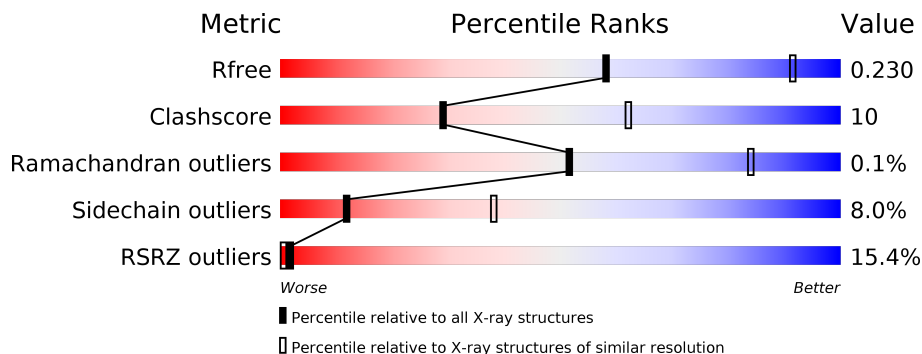|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1   Overall quality at a glance (i)

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

The reported resolution of this entry is 3.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.230
Clashscore		10
Ramachandran outliers		0.1%
Sidechain outliers		8.0%
RSRZ outliers		15.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 <=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	12% / 67% / 24% · 7%
1	B	482	15% / 67% / 25% · 5%
1	C	482	4% / 74% / 23% ··
1	D	482	27% / 68% / 25% · ·

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	C	1474	-	-	-	X
4	SO4	C	1481	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14628 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 MJ0495-LIKE PROTEIN.

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

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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 GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

GDP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 5 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula: $C_{24}H_{40}O_4$).
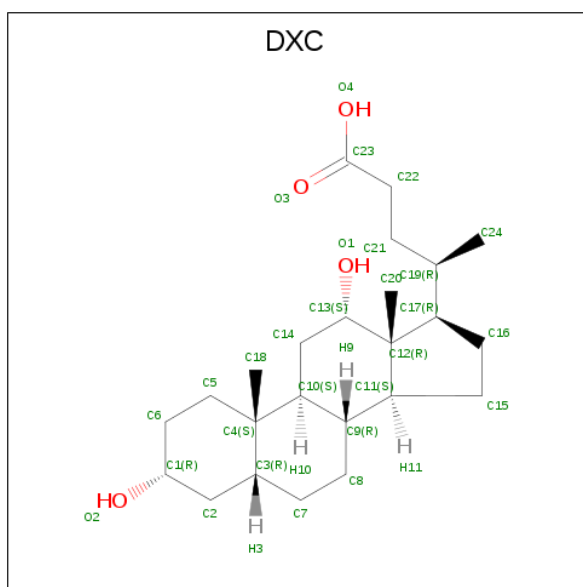
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 28	C 24	O 4	0	0
5	C	1	Total 28	C 24	O 4	0	0
5	C	1	Total 28	C 24	O 4	0	0
5	C	1	Total 28	C 24	O 4	0	0
5	C	1	Total 28	C 24	O 4	0	0
5	C	1	Total 28	C 24	O 4	0	0
5	C	1	Total 28	C 24	O 4	0	0

- Molecule 6 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).

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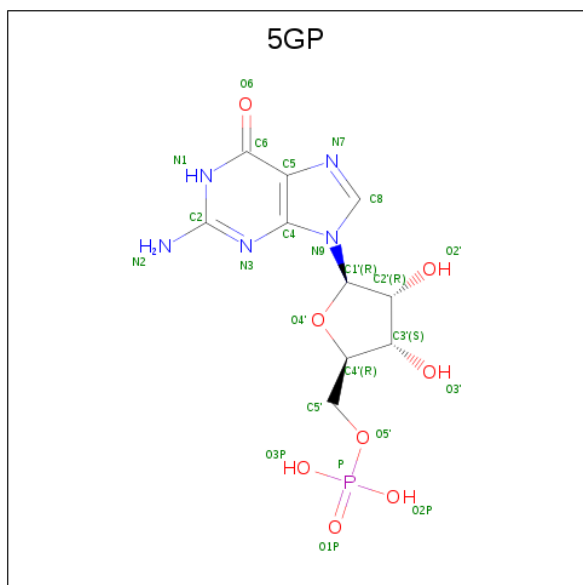
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	B	1	24	10	5	8	1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	O	0	0
			4	4		
7	B	4	Total	O	0	0
			4	4		
7	C	4	Total	O	0	0
			4	4		

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: MJ0495-LIKE PROTEIN
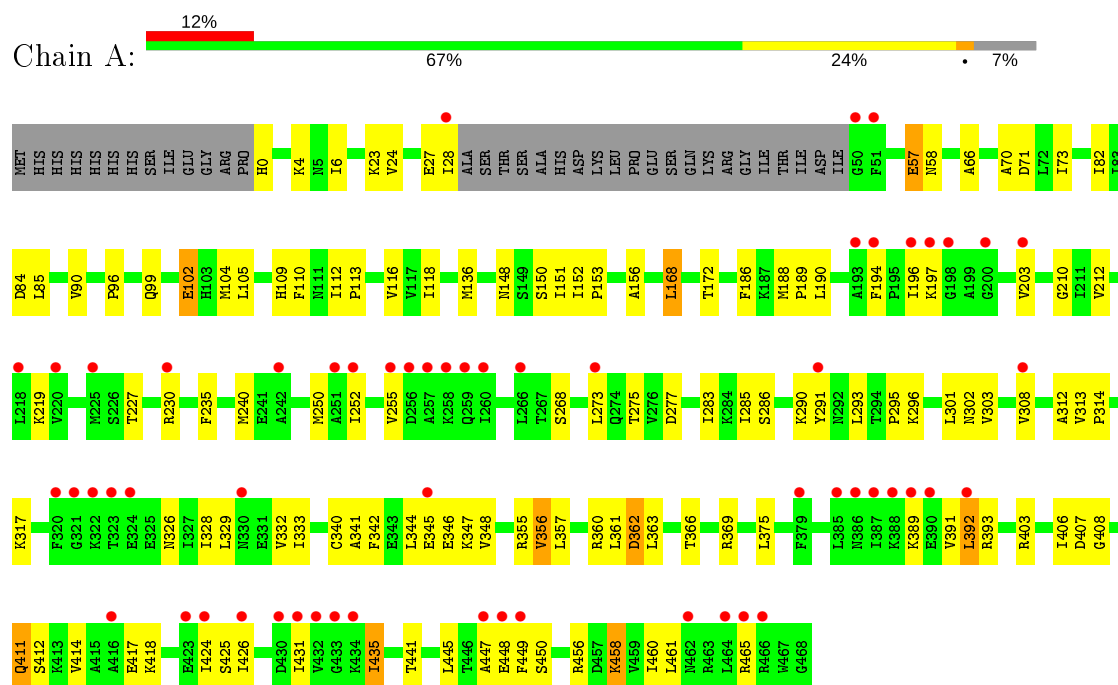
- Molecule 1: MJ0495-LIKE PROTEIN

• Molecule 1: MJ0495-LIKE PROTEIN

Chain C:

• Molecule 1: MJ0495-LIKE PROTEIN

Chain D:
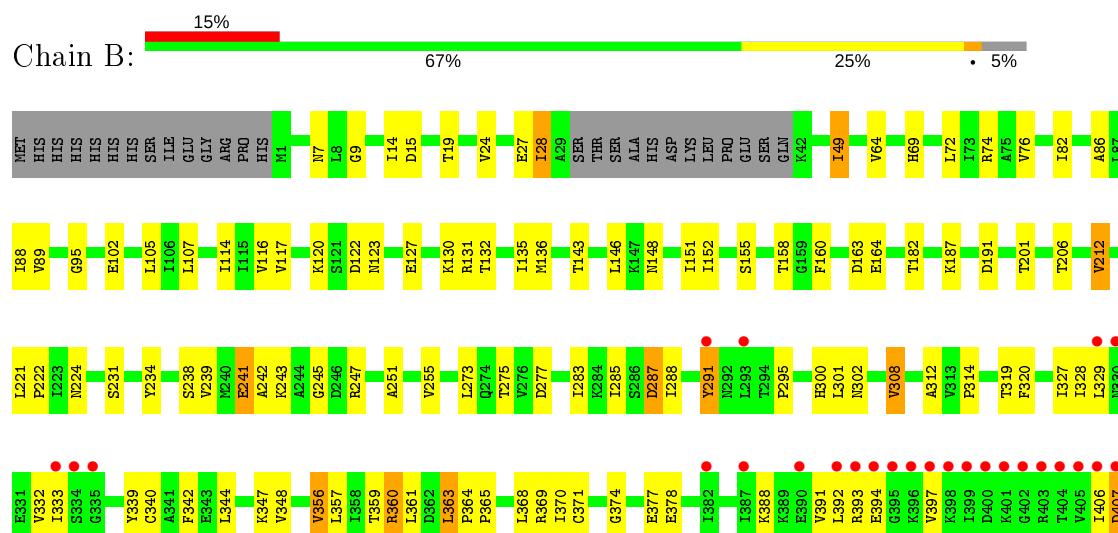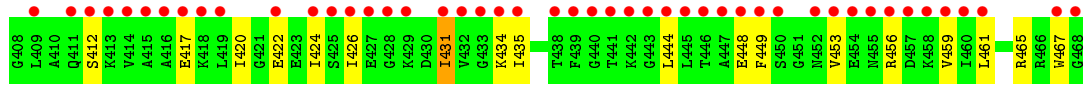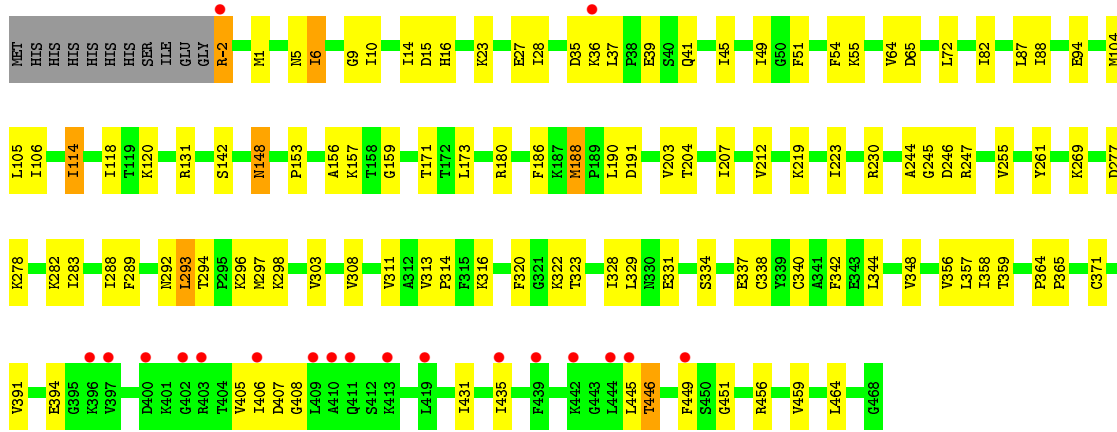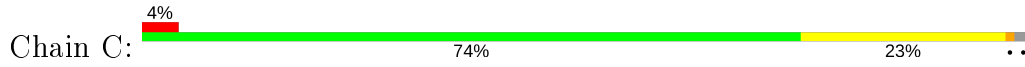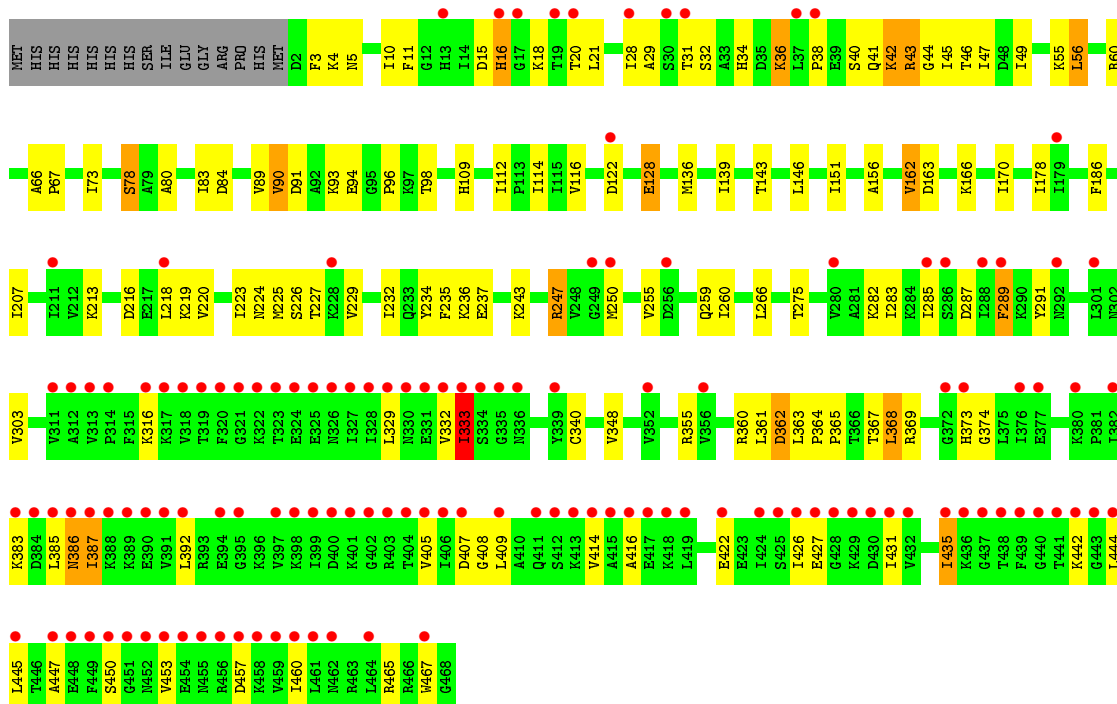
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α, β, γ	146.92Å 146.92Å 297.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.03 48.09 – 3.03	Depositor EDS
% Data completeness (in resolution range)	89.1 (19.98-3.03) 92.3 (48.09-3.03)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.51 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.190 , 0.222 0.198 , 0.230	Depositor DCC
R_{free} test set	2985 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å^2)	84.9	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 101.5	EDS
L-test for twinning [2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14628	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CMH, SO4, 5GP, 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	#$\|Z\|$>5	RMSZ	#$\|Z\|$>5
1	A	0.25	0/3484	0.50	0/4684
1	B	0.25	0/3541	0.49	0/4760
1	C	0.24	0/3664	0.49	0/4929
1	D	0.26	0/3626	0.52	0/4878
All	All	0.25	0/14315	0.50	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	3655	69	0
1	B	3533	0	3727	76	0
1	C	3651	0	3837	65	0
1	D	3615	0	3799	78	0
2	A	28	0	12	0	0
2	B	28	0	12	2	0
2	C	28	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	B	10	0	0	2	0
4	C	25	0	0	0	0
5	B	28	0	39	1	0
5	C	168	0	234	10	0
6	B	24	0	12	2	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
7	C	4	0	0	0	0
All	All	14628	0	15339	288	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 288 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	1.50	0.91
1:C:283:ILE:HG12	1:C:358:ILE:HD11	1.58	0.85
1:D:223:ILE:HG21	1:D:259:GLN:HB3	1.57	0.84
1:C:283:ILE:HD13	1:C:340:CMH:HB3	1.66	0.78
1:C:36:LYS:HB2	1:C:156:ALA:O	1.84	0.77

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%)	428 (97%)	12 (3%)	0	100	100
1	B	448/482 (93%)	433 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	465/482 (96%)	452 (97%)	13 (3%)	0	100	100
1	D	461/482 (96%)	440 (95%)	19 (4%)	2 (0%)	34	69
All	All	1814/1928 (94%)	1753 (97%)	59 (3%)	2 (0%)	51	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	LYS
1	D	333	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%)	350 (92%)	32 (8%)	11	36
1	B	388/412 (94%)	360 (93%)	28 (7%)	14	43
1	C	402/412 (98%)	372 (92%)	30 (8%)	13	41
1	D	398/412 (97%)	362 (91%)	36 (9%)	9	33
All	All	1570/1648 (95%)	1444 (92%)	126 (8%)	12	38

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	407	ASP
1	C	212	VAL
1	D	362	ASP
1	B	431	ILE
1	C	45	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	292	ASN
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	371	1	5,7,8	0.61	0	1,7,9	0.57	0
1	CMH	C	371	1	5,7,8	0.61	0	1,7,9	0.54	0
1	CMH	A	264	1	5,7,8	0.57	0	1,7,9	0.02	0
1	CMH	C	264	1	5,7,8	0.59	0	1,7,9	0.73	0
1	CMH	D	340	1	5,7,8	0.58	0	1,7,9	0.19	0
1	CMH	B	340	1	5,7,8	0.75	0	1,7,9	0.32	0
1	CMH	C	340	1	5,7,8	0.72	0	1,7,9	0.53	0
1	CMH	A	338	1	5,7,8	0.63	0	1,7,9	0.65	0
1	CMH	B	371	1	5,7,8	0.55	0	1,7,9	0.88	0
1	CMH	D	264	1	5,7,8	0.57	0	1,7,9	0.60	0
1	CMH	C	338	1	5,7,8	0.57	0	1,7,9	0.72	0
1	CMH	A	371	1	5,7,8	0.54	0	1,7,9	0.56	0
1	CMH	A	340	1	5,7,8	0.71	0	1,7,9	0.62	0
1	CMH	B	338	1	5,7,8	0.69	0	1,7,9	0.65	0
1	CMH	B	264	1	5,7,8	0.60	0	1,7,9	0.96	0
1	CMH	D	338	1	5,7,8	0.58	0	1,7,9	1.00	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	371	1	-	0/0/6/8	-
1	CMH	C	371	1	-	0/0/6/8	-
1	CMH	A	264	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	-
1	CMH	A	338	1	-	0/0/6/8	-
1	CMH	B	371	1	-	0/0/6/8	-
1	CMH	D	264	1	-	0/0/6/8	-
1	CMH	C	338	1	-	0/0/6/8	-
1	CMH	A	371	1	-	0/0/6/8	-
1	CMH	A	340	1	-	0/0/6/8	-
1	CMH	B	338	1	-	0/0/6/8	-
1	CMH	B	264	1	-	0/0/6/8	-
1	CMH	D	338	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.

7 monomers are involved in 14 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	DXC	C	1479	-	28,31,31	1.71	6 (21%)	46,49,49	1.52	8 (17%)
4	SO4	C	1474	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	1473	-	4,4,4	0.14	0	6,6,6	0.04	0
5	DXC	C	1476	-	28,31,31	1.73	6 (21%)	46,49,49	1.47	8 (17%)
2	GDP	A	1469	3	24,30,30	1.19	2 (8%)	31,47,47	1.98	8 (25%)
5	DXC	C	1480	-	28,31,31	1.75	6 (21%)	46,49,49	1.54	10 (21%)
5	DXC	B	1473	-	28,31,31	1.72	6 (21%)	46,49,49	1.43	8 (17%)
5	DXC	C	1478	-	28,31,31	1.71	6 (21%)	46,49,49	1.66	9 (19%)
5	DXC	C	1475	-	28,31,31	1.76	6 (21%)	46,49,49	1.58	10 (21%)
4	SO4	C	1472	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	1471	-	4,4,4	0.15	0	6,6,6	0.04	0
2	GDP	C	1469	3	24,30,30	1.20	2 (8%)	31,47,47	2.01	8 (25%)
5	DXC	C	1477	-	28,31,31	1.72	6 (21%)	46,49,49	1.47	8 (17%)
2	GDP	B	1469	3	24,30,30	1.19	2 (8%)	31,47,47	1.98	9 (29%)
4	SO4	B	1472	-	4,4,4	0.14	0	6,6,6	0.04	0
6	5GP	B	1474	-	22,26,26	0.58	0	27,40,40	1.75	5 (18%)
4	SO4	C	1471	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	1481	-	4,4,4	0.13	0	6,6,6	0.05	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
5	DXC	C	1479	-	-	6/7/71/71	0/4/4/4
5	DXC	C	1478	-	-	2/7/71/71	0/4/4/4
5	DXC	C	1476	-	-	2/7/71/71	0/4/4/4
2	GDP	A	1469	3	-	6/12/32/32	0/3/3/3
5	DXC	C	1480	-	-	4/7/71/71	0/4/4/4
5	DXC	B	1473	-	-	0/7/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5GP	B	1474	-	-	3/6/26/26	0/3/3/3
5	DXC	C	1475	-	-	0/7/71/71	0/4/4/4
5	DXC	C	1477	-	-	2/7/71/71	0/4/4/4
2	GDP	C	1469	3	-	5/12/32/32	0/3/3/3
2	GDP	B	1469	3	-	6/12/32/32	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1469	GDP	C6-C5	4.29	1.48	1.41
2	B	1469	GDP	C6-C5	4.23	1.48	1.41
2	A	1469	GDP	C6-C5	4.21	1.48	1.41
5	C	1480	DXC	C12-C13	-4.12	1.48	1.54
5	C	1475	DXC	C12-C13	-4.02	1.48	1.54

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1478	DXC	C22-C21-C19	-5.19	107.73	114.72
2	B	1469	GDP	C2-N3-C4	4.99	121.05	115.36
2	A	1469	GDP	C2-N3-C4	4.94	120.99	115.36
2	C	1469	GDP	C2-N3-C4	4.93	120.98	115.36
6	B	1474	5GP	N3-C2-N1	-4.58	121.12	127.22

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1469	GDP	C5'-O5'-PA-O1A
2	A	1469	GDP	C5'-O5'-PA-O2A
2	C	1469	GDP	C5'-O5'-PA-O1A
2	C	1469	GDP	C5'-O5'-PA-O2A
2	C	1469	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1479	DXC	2	0
5	C	1476	DXC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1480	DXC	1	0
5	B	1473	DXC	1	0
5	C	1478	DXC	1	0
5	C	1475	DXC	3	0
4	B	1471	SO4	1	0
2	C	1469	GDP	1	0
5	C	1477	DXC	1	0
2	B	1469	GDP	2	0
4	B	1472	SO4	1	0
6	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DXC C 1479

Bond lengths

Bond angles

Torsions

Rings

Ligand DXC C 1476

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP A 1469

Bond lengths

Bond angles

Torsions

Rings

Ligand DXC C 1480

Bond lengths

Bond angles

Torsions

Rings

Ligand DXC B 1473

Bond lengths

Bond angles

Torsions

Rings

Ligand DXC C 1478

Bond lengths

Bond angles

Torsions

Rings

Ligand DXC C 1475

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP C 1469

Bond lengths

Bond angles

Torsions

Rings

Ligand DXC C 1477

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP B 1469

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP B 1474

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 (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%)	0.67	58 (13%)	3	1	72, 154, 219, 301	0
1	B	452/482 (93%)	0.87	73 (16%)	1	0	54, 109, 284, 316	0
1	C	467/482 (96%)	0.17	19 (4%)	37	15	53, 88, 179, 222	0
1	D	463/482 (96%)	1.44	131 (28%)	0	0	101, 187, 277, 317	0
All	All	1826/1928 (94%)	0.79	281 (15%)	2	0	53, 139, 266, 317	0

The worst 5 of 281 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	THR	16.3
1	D	453	VAL	12.2
1	B	439	PHE	10.9
1	D	441	THR	10.5
1	B	441	THR	10.5

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	0.18	152,222,227,253	2
1	CMH	A	371	8/9	0.82	0.33	133,164,171,190	2
1	CMH	B	338	8/9	0.88	0.14	124,171,196,199	2
1	CMH	D	340	8/9	0.90	0.34	152,216,232,249	2
1	CMH	A	338	8/9	0.93	0.24	137,150,185,236	2
1	CMH	C	338	8/9	0.94	0.15	58,83,145,240	2
1	CMH	B	371	8/9	0.94	0.17	110,130,188,228	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	CMH	C	340	8/9	0.96	0.19	54,75,92,110	2
1	CMH	A	340	8/9	0.97	0.23	136,173,185,199	2
1	CMH	D	371	8/9	0.97	0.17	103,144,150,163	2
1	CMH	D	264	8/9	0.97	0.17	131,162,186,191	2
1	CMH	B	340	8/9	0.98	0.15	120,138,232,238	2
1	CMH	A	264	8/9	0.98	0.13	149,163,190,206	2
1	CMH	C	264	8/9	0.99	0.17	51,90,102,105	0
1	CMH	B	264	8/9	0.99	0.21	49,64,73,84	2
1	CMH	C	371	8/9	0.99	0.20	57,94,131,132	2

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(Å²)	Q<0.9
4	SO4	C	1474	5/5	0.54	0.54	125,199,203,260	5
4	SO4	C	1481	5/5	0.79	0.66	149,157,173,174	5
4	SO4	B	1472	5/5	0.84	0.41	87,206,279,300	0
6	5GP	B	1474	24/24	0.89	0.36	188,232,246,253	0
5	DXC	C	1476	28/28	0.89	0.31	101,121,161,174	0
4	SO4	B	1471	5/5	0.90	0.35	158,172,218,237	0
2	GDP	C	1469	28/28	0.90	0.27	62,99,125,141	28
4	SO4	C	1473	5/5	0.91	0.10	104,155,184,219	5
5	DXC	C	1479	28/28	0.95	0.30	48,73,147,183	28
5	DXC	C	1477	28/28	0.96	0.27	52,78,126,165	0
4	SO4	C	1472	5/5	0.96	0.16	100,129,151,170	0
4	SO4	C	1471	5/5	0.97	0.24	84,115,131,161	0
5	DXC	C	1475	28/28	0.97	0.25	51,65,105,114	0
2	GDP	B	1469	28/28	0.97	0.24	67,86,108,130	0
2	GDP	A	1469	28/28	0.97	0.18	78,92,105,106	28
5	DXC	C	1480	28/28	0.97	0.24	51,64,91,113	0
5	DXC	B	1473	28/28	0.97	0.25	51,71,101,124	0
3	MG	A	1470	1/1	0.98	0.10	147,147,147,147	1
5	DXC	C	1478	28/28	0.98	0.27	60,83,113,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	MG	B	1470	1/1	0.98	0.23	106,106,106,106	0
3	MG	C	1470	1/1	0.98	0.15	152,152,152,152	1

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
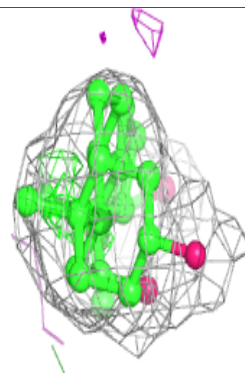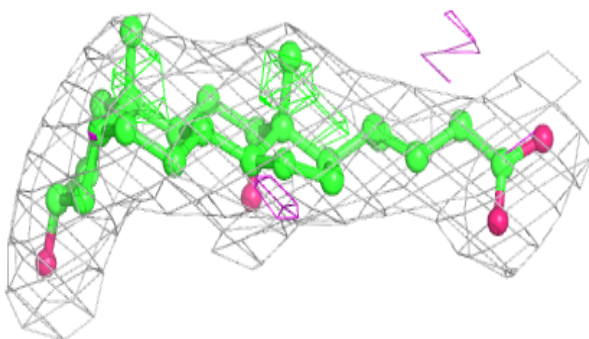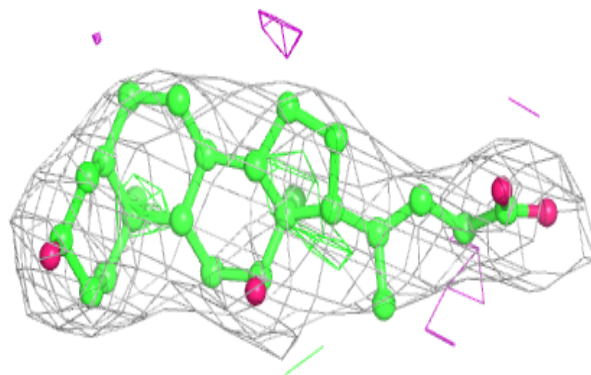mF_o-DF_c (at 3 rmsd) in purple (negative)
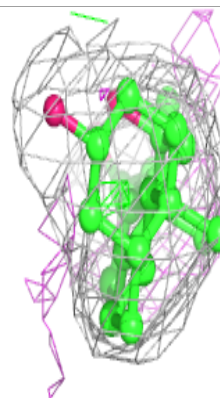and green (positive)
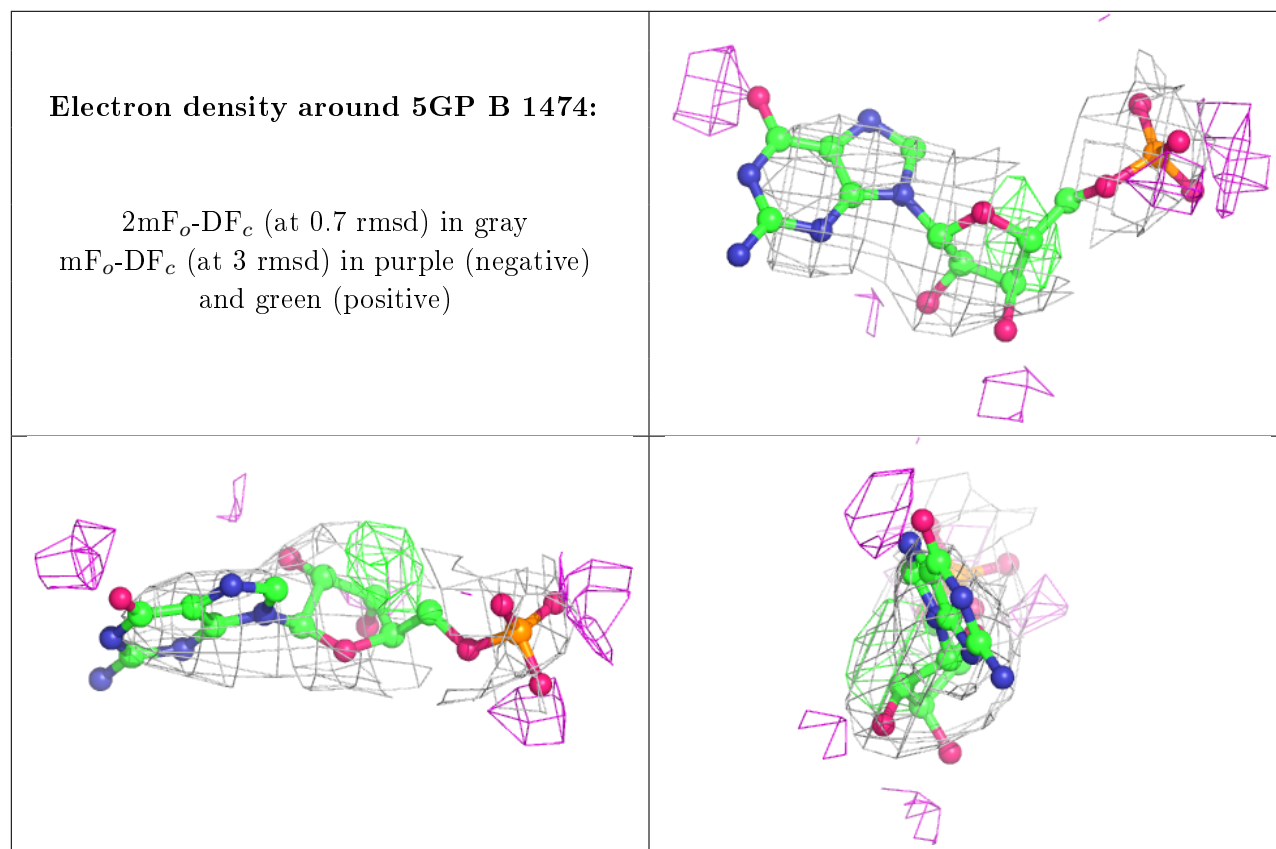
Electron density around DXC C 1476:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
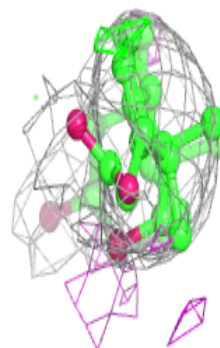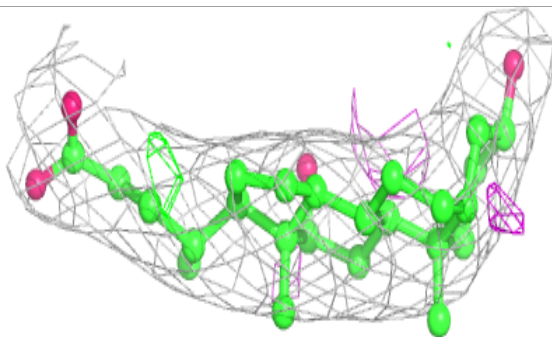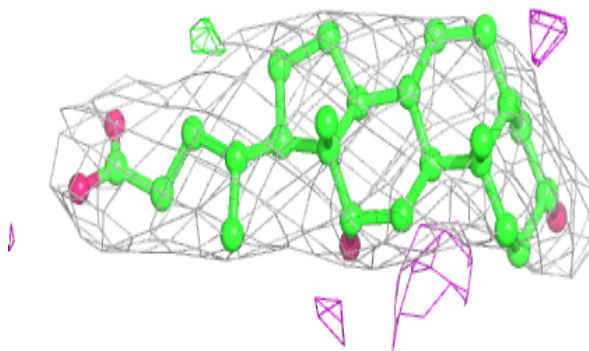
Electron density around GDP C 1469:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
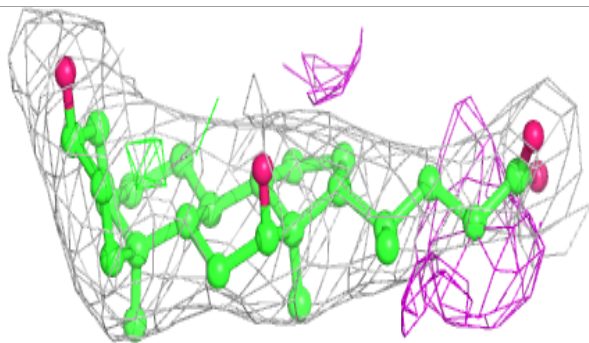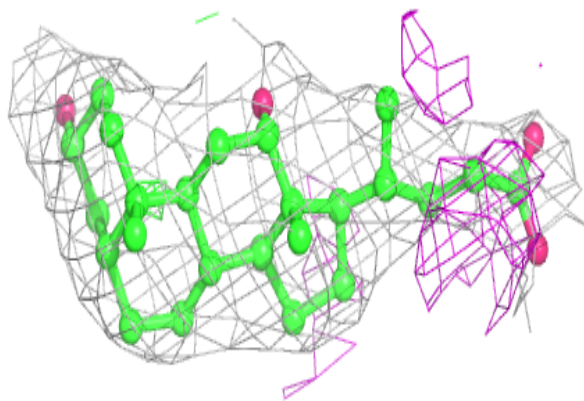and green (positive)
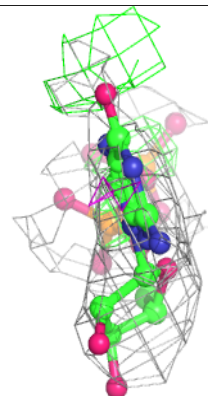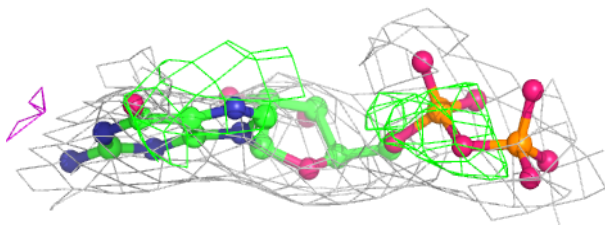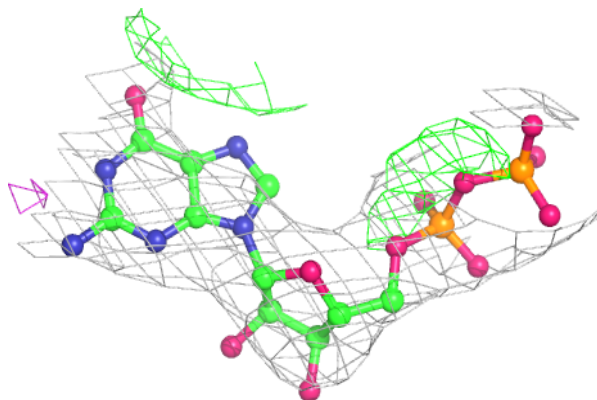
Electron density around DXC C 1479:

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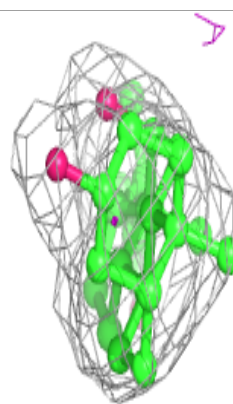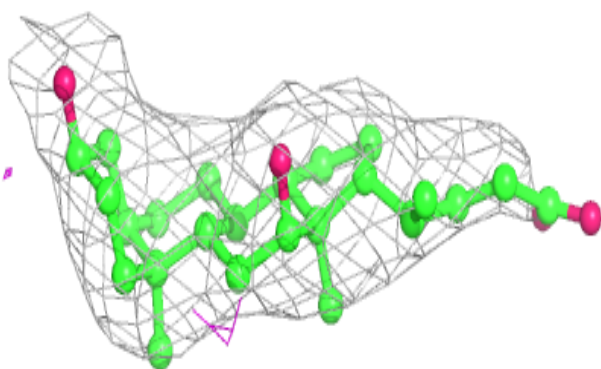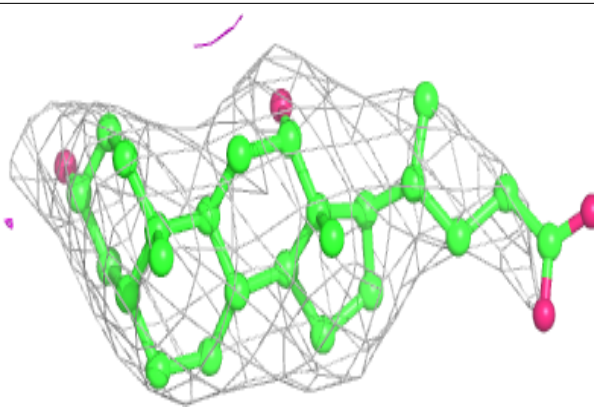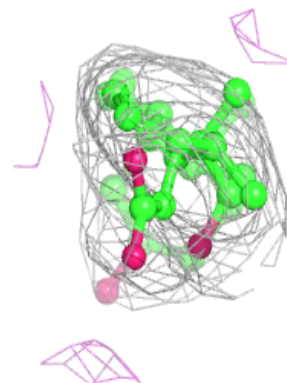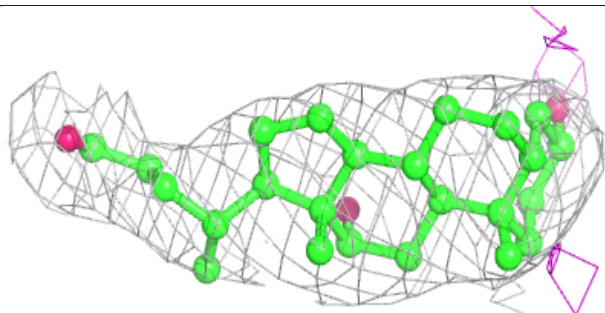

Electron density around DXC C 1477:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
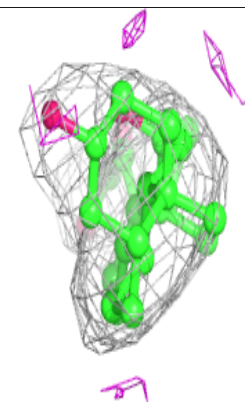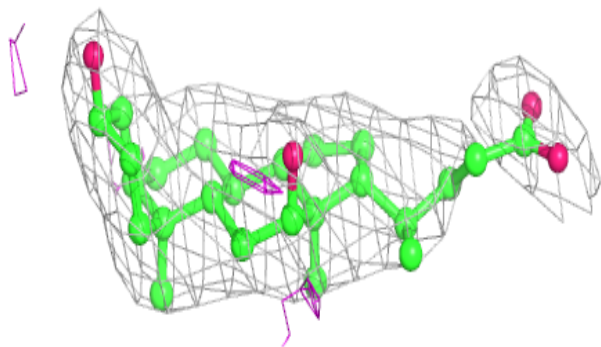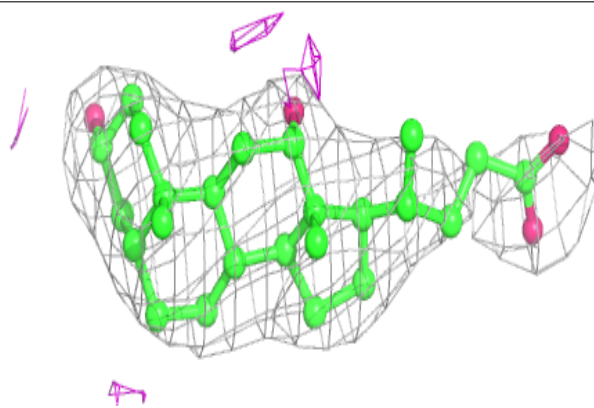
Electron density around DXC C 1475:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
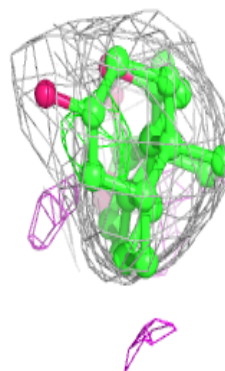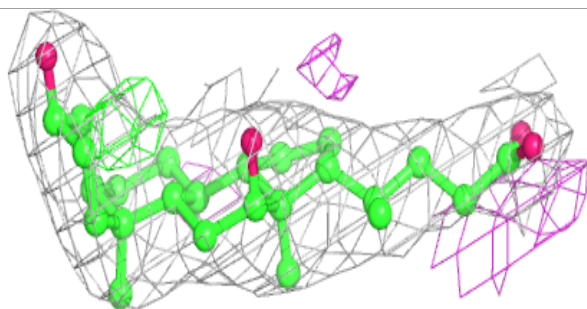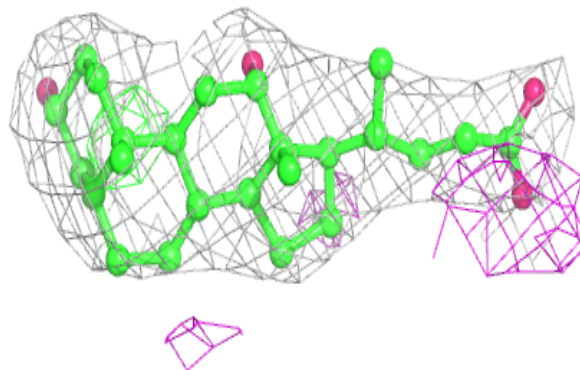
Electron density around GDP B 1469:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
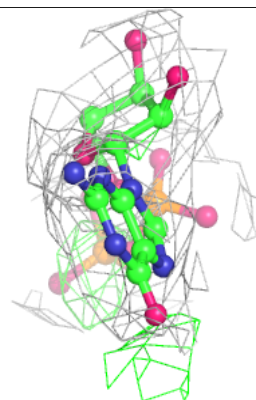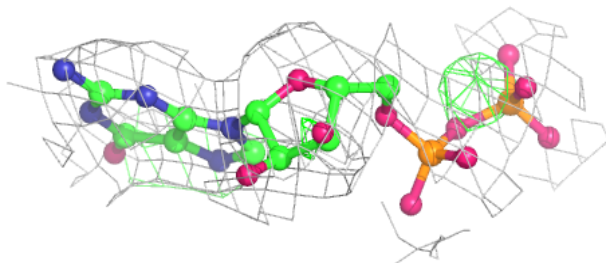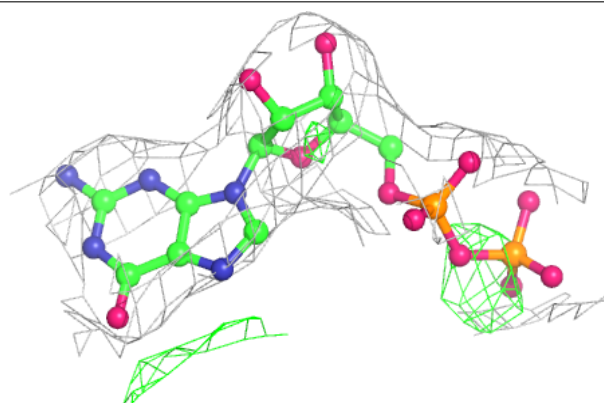
Electron density around GDP A 1469:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
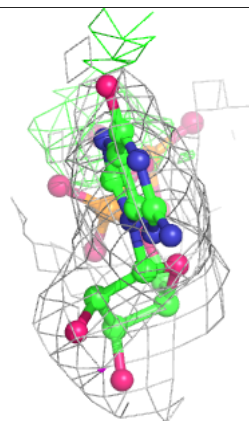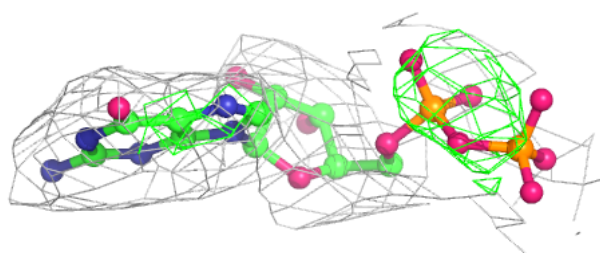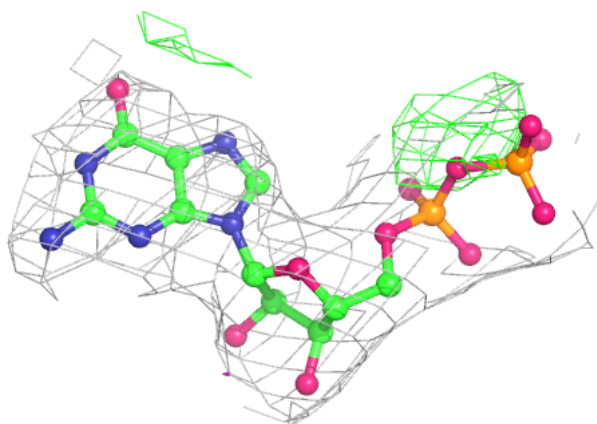
Electron density around DXC C 1480:

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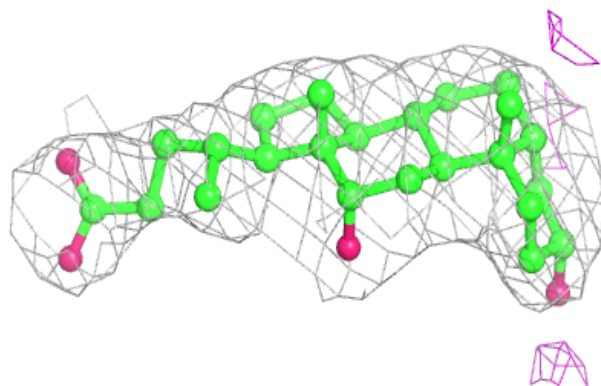$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around DXC B 1473:

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

Electron density around DXC C 1478:

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

6.5 Other polymers (i)

There are no such residues in this entry.