



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2020 – 10:25 pm BST

PDB ID : 1LS3
Title : Crystal Structure of the Complex between Rabbit Cytosolic Serine Hydroxymethyltransferase and TriGlu-5-formyl-tetrahydrofolate
Authors : Fu, T.F.; Scarsdale, J.N.; Kazanina, G.; Schirch, V.; Wright, H.T.
Deposited on : 2002-05-16
Resolution : 2.70 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

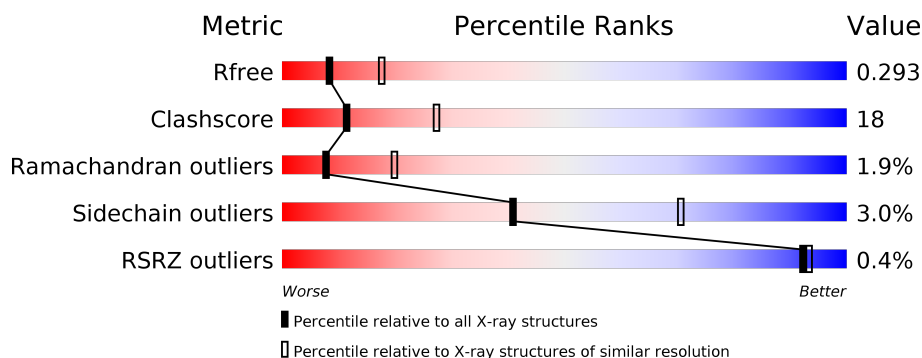
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	483	
1	B	483	
1	C	483	
1	D	483	

2 Entry composition [i](#)

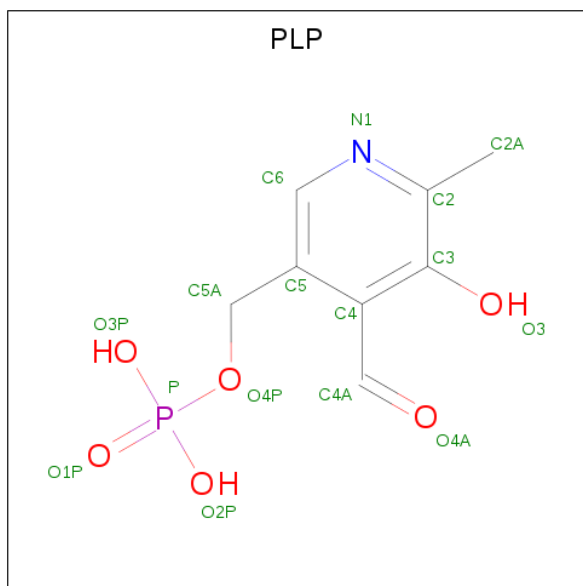
There are 6 unique types of molecules in this entry. The entry contains 14342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine Hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	1	0
			3489	2187	620	664	18			
1	B	455	Total	C	N	O	S	0	3	0
			3404	2132	611	643	18			
1	C	465	Total	C	N	O	S	0	0	0
			3470	2178	616	658	18			
1	D	456	Total	C	N	O	S	0	0	0
			3374	2115	601	640	18			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



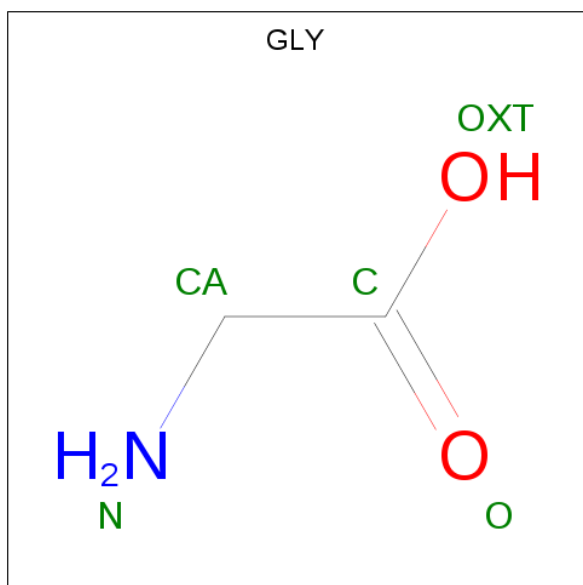
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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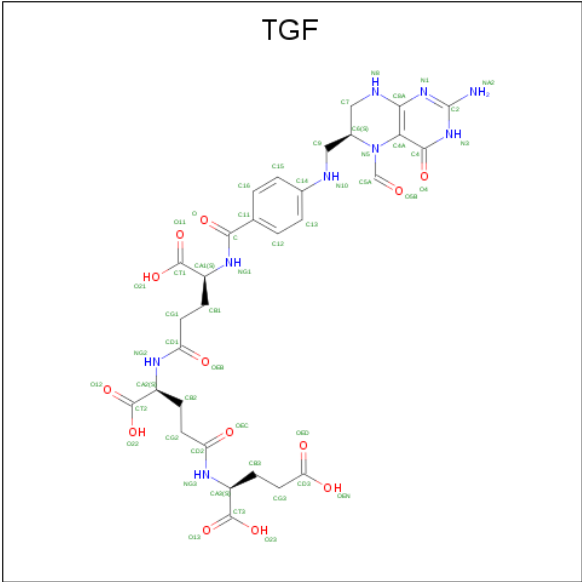
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	2	1	2		
3	C	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is 2-[4-(4-{4-[(2-AMINO-5-FORMYL-4-OXO-3,4,5,6,7,8-HEXAHYDRO-PTERIDIN-6-YLMETHYL)-AMINO]-BENZOYLAMINO}-4-CARBOXY-BUTYRYLAMINO)-4-CARBOXY-BUTYRYLAMINO]-PENTANEDIOIC ACID (three-letter code: TGF) (formula: C₃₀H₃₇N₉O₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	1
			60	34	9	17		
4	D	1	Total	C	N	O	0	1
			73	41	11	21		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	99	Total	O	0	0
			99	99		
6	B	107	Total	O	0	0
			107	107		
6	C	99	Total	O	0	0
			99	99		
6	D	73	Total	O	0	0
			73	73		

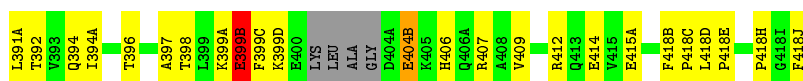
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Chain A:

65% 28%

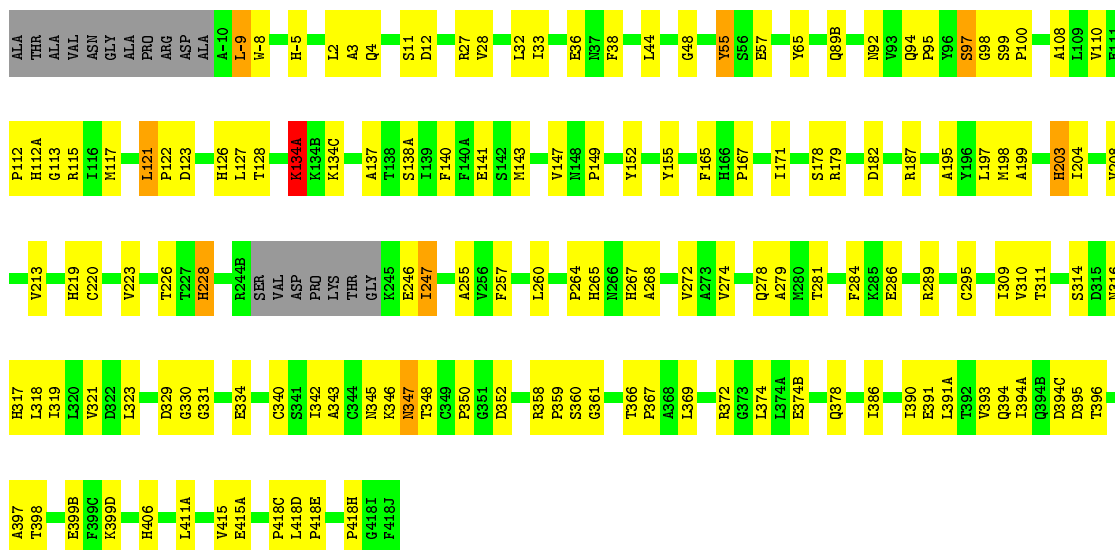
ALA
THR
ALA
VAL
ASN
GLY
PRO
ARG
ASP
ALA
A-10
L-9
W-8
S-7
S-6
H-5
L2
A3
Q4
P6
L6
D12
R25
Q26
R27
V28
E31
L32
E36
A39
S40
V43
L44
G48
Y55
S56
E57
Y86
D89
P89A
Q89B
Q94
Y96
S97
G98
S99
T227
H228
V244A
R244B
S244C
V244D
D244E
PRO
LYS
THR
GLY
LYS
GLU
ILE
L248
Y249
A255
V256
F257
L260
A268
V272
A273
V274
Q278
N294
C295
Y307
R308
I309
V310
T311
S314
D315
N316
H317
L318
I319
L320
V321
D322
L323
D329
G330
G331
R332
A333
E334
A403
G404
D404A
E404C
K405
H406
A408
L411A
R412
E415A
S415B
F416
L418A
L418D
L418G
P418H
G418I
F418J
E418
N347
G351
D352
K354
S355
A356
L357
R358
P359
S360
T366
P367
A368
L369
R372
G373
L374
L374A
E374B
K375
D376
F377
Q378
K380
V382
L386
H387
G388
G389
L390
E391
L391A
Q394
L394A
Q394B
D394C
P396B
R396C
A397
T398
L399
K399A
E399B
F399C
A403
G404
D404A

[illegible]



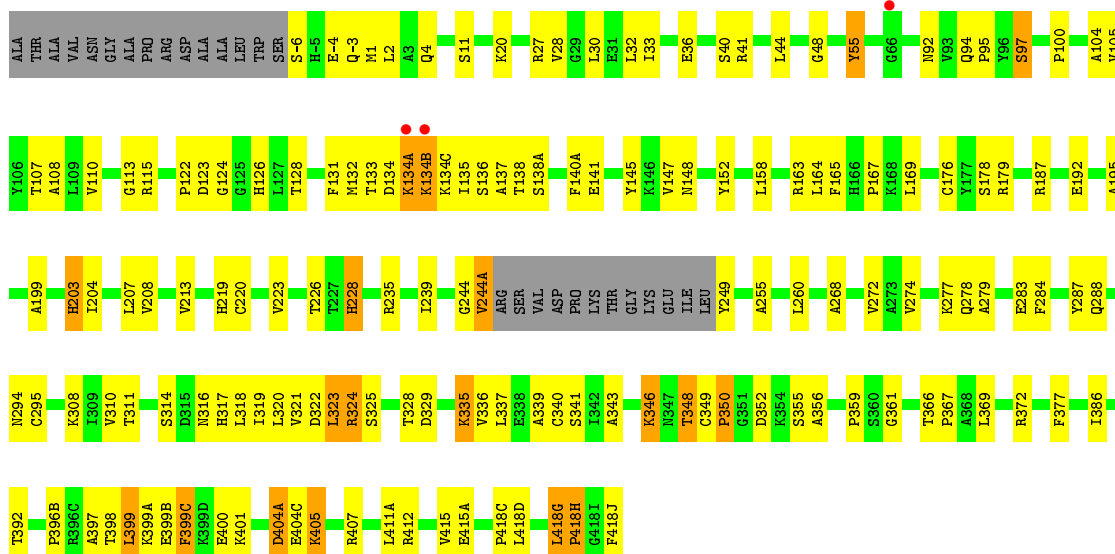
• Molecule 1: Serine Hydroxymethyltransferase

Chain C: 66% 28%



• Molecule 1: Serine Hydroxymethyltransferase

Chain D: 62% 29% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	114.08Å 114.08Å 156.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.79 – 2.70 35.16 – 2.70	Depositor EDS
% Data completeness (in resolution range)	86.7 (19.79-2.70) 86.7 (35.16-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.294 0.221 , 0.293	Depositor DCC
R_{free} test set	4801 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 25.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14342	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: GOL, TGF, PLP

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	0.38	0/3560	0.62	1/4828 (0.0%)
1	B	0.39	0/3471	0.62	1/4706 (0.0%)
1	C	0.38	0/3541	0.62	0/4804
1	D	0.38	0/3442	0.63	0/4671
All	All	0.38	0/14014	0.62	2/19009 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244(F)	PRO	N-CA-CB	5.76	110.21	103.30
1	A	418(H)	PRO	N-CA-CB	5.61	110.03	103.30

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	3489	0	3326	116	0
1	B	3404	0	3204	134	0
1	C	3470	0	3301	115	0
1	D	3374	0	3201	143	0
2	A	15	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	6	0	0
2	C	15	0	6	0	0
2	D	15	0	6	0	0
3	A	5	0	2	0	0
3	C	5	0	2	2	0
4	B	60	0	10	2	0
4	D	73	0	28	4	0
5	B	12	0	16	1	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	99	0	0	5	0
6	B	107	0	0	4	0
6	C	99	0	0	5	0
6	D	73	0	0	3	0
All	All	14342	0	13130	481	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 18.

The worst 5 of 481 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:C:398:THR:HG22	1:C:399(B):GLU:HG3	1.17	1.07
1:C:398:THR:HG22	1:C:399(B):GLU:CG	1.89	1.01
1:C:398:THR:CG2	1:C:399(B):GLU:HG3	1.88	1.01
1:D:418(G):LEU:HD12	1:D:418(J):PHE:HD2	1.36	0.90
1:B:346:LYS:HD2	1:B:359:PRO:HG2	1.55	0.85

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	462/483 (96%)	412 (89%)	39 (8%)	11 (2%)	6	15
1	B	447/483 (92%)	404 (90%)	34 (8%)	9 (2%)	7	19
1	C	461/483 (95%)	427 (93%)	31 (7%)	3 (1%)	22	46
1	D	452/483 (94%)	404 (89%)	36 (8%)	12 (3%)	5	12
All	All	1822/1932 (94%)	1647 (90%)	140 (8%)	35 (2%)	8	20

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244(C)	SER
1	A	244(D)	VAL
1	A	355	SER
1	A	356	ALA
1	A	396(B)	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/391 (90%)	340 (97%)	10 (3%)	42	71
1	B	335/391 (86%)	324 (97%)	11 (3%)	38	67
1	C	345/391 (88%)	335 (97%)	10 (3%)	42	71
1	D	333/391 (85%)	322 (97%)	11 (3%)	38	67
All	All	1363/1564 (87%)	1321 (97%)	42 (3%)	41	69

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	228	HIS
1	C	89(B)	GLN
1	D	324	ARG
1	B	399(B)	GLU
1	C	-9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	228	HIS
1	C	4	GLN
1	D	-3	GLN
1	B	203	HIS
1	D	4	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 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	$\# Z > 2$
2	PLP	D	419(A)	1	15,15,16	1.45	3 (20%)	20,22,23	2.69	10 (50%)
5	GOL	C	421	-	5,5,5	0.94	0	5,5,5	0.20	0
2	PLP	A	419(A)	1,3	15,15,16	1.58	3 (20%)	20,22,23	2.54	8 (40%)
2	PLP	C	419(A)	1,3	15,15,16	1.42	3 (20%)	20,22,23	2.60	8 (40%)
2	PLP	B	419(A)	1	15,15,16	1.59	4 (26%)	20,22,23	2.69	10 (50%)
4	TGF	B	420(C)[B]	-	40,54,54	2.72	11 (27%)	42,74,74	3.15	17 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TGF	B	420(C)[A]	-	40,54,54	2.72	11 (27%)	42,74,74	3.17	18 (42%)
4	TGF	D	420(F)[A]	-	40,54,54	2.66	14 (35%)	42,74,74	3.31	16 (38%)
5	GOL	B	421	-	5,5,5	0.59	0	5,5,5	0.25	0
4	TGF	D	420(F)[B]	-	40,54,54	2.65	14 (35%)	42,74,74	3.29	15 (35%)
5	GOL	D	421	-	5,5,5	0.66	0	5,5,5	0.26	0
5	GOL	B	422	-	5,5,5	0.82	0	5,5,5	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	D	419(A)	1	-	3/6/6/8	0/1/1/1
5	GOL	C	421	-	-	0/4/4/4	-
2	PLP	A	419(A)	1,3	-	0/6/6/8	0/1/1/1
2	PLP	C	419(A)	1,3	-	0/6/6/8	0/1/1/1
2	PLP	B	419(A)	1	-	3/6/6/8	0/1/1/1
4	TGF	B	420(C)[B]	-	-	14/36/63/63	0/2/3/3
4	TGF	B	420(C)[A]	-	-	14/36/63/63	0/2/3/3
4	TGF	D	420(F)[A]	-	-	15/36/63/63	0/2/3/3
5	GOL	B	421	-	-	0/4/4/4	-
4	TGF	D	420(F)[B]	-	-	18/36/63/63	0/2/3/3
5	GOL	D	421	-	-	0/4/4/4	-
5	GOL	B	422	-	-	0/4/4/4	-

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	420(C)[B]	TGF	C4A-N5	7.86	1.52	1.41
4	B	420(C)[A]	TGF	C4A-N5	7.86	1.52	1.41
4	D	420(F)[B]	TGF	C4A-N5	7.47	1.51	1.41
4	D	420(F)[A]	TGF	C4A-N5	7.47	1.51	1.41
4	D	420(F)[B]	TGF	C4-C4A	7.17	1.51	1.41

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	420(C)[B]	TGF	NA2-C2-N1	9.62	132.21	117.25
4	B	420(C)[A]	TGF	NA2-C2-N1	9.62	132.21	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	420(F)[B]	TGF	NA2-C2-N1	9.37	131.82	117.25
4	D	420(F)[A]	TGF	NA2-C2-N1	9.37	131.82	117.25
4	B	420(C)[B]	TGF	C4-N3-C2	7.74	128.23	115.93

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	420(F)[B]	TGF	O5B-C5A-N5-C4A
4	D	420(F)[B]	TGF	O5B-C5A-N5-C6
4	D	420(F)[B]	TGF	CB1-CA1-NG1-C
4	D	420(F)[B]	TGF	CB2-CA2-NG2-CD1
4	D	420(F)[B]	TGF	CT2-CA2-NG2-CD1

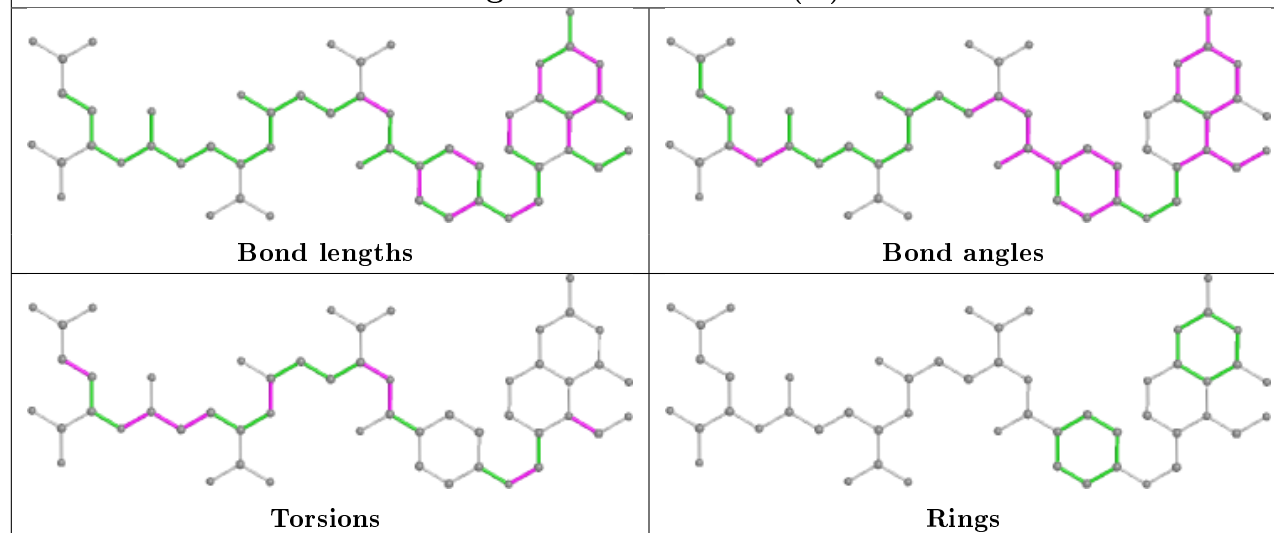
There are no ring outliers.

4 monomers are involved in 7 short contacts:

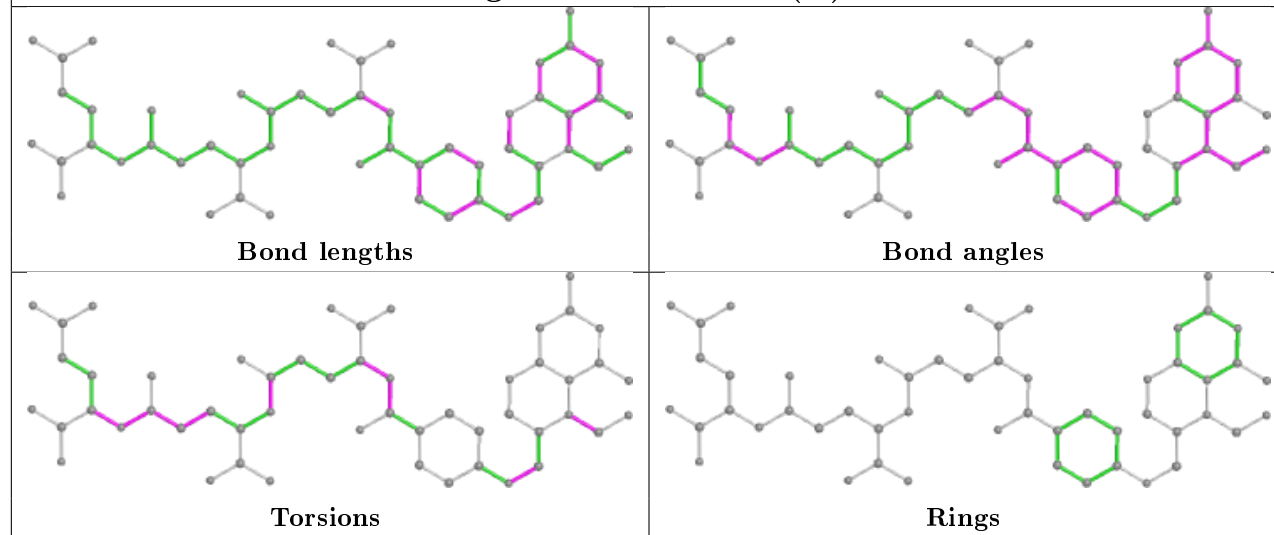
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	420(C)[A]	TGF	2	0
4	D	420(F)[A]	TGF	2	0
4	D	420(F)[B]	TGF	2	0
5	B	422	GOL	1	0

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

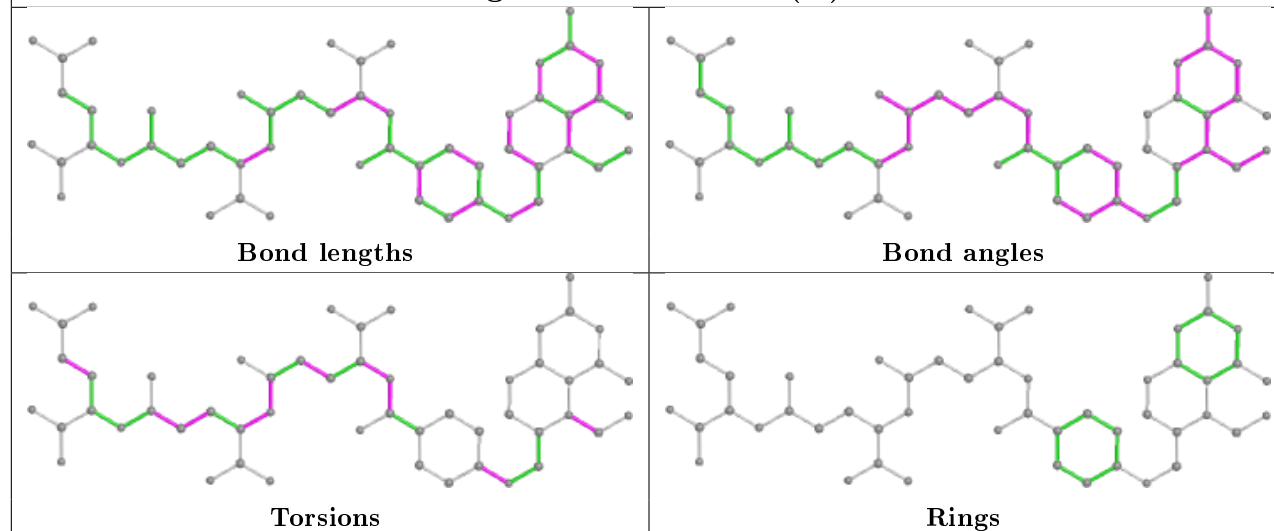
Ligand TGF B 420C (B)

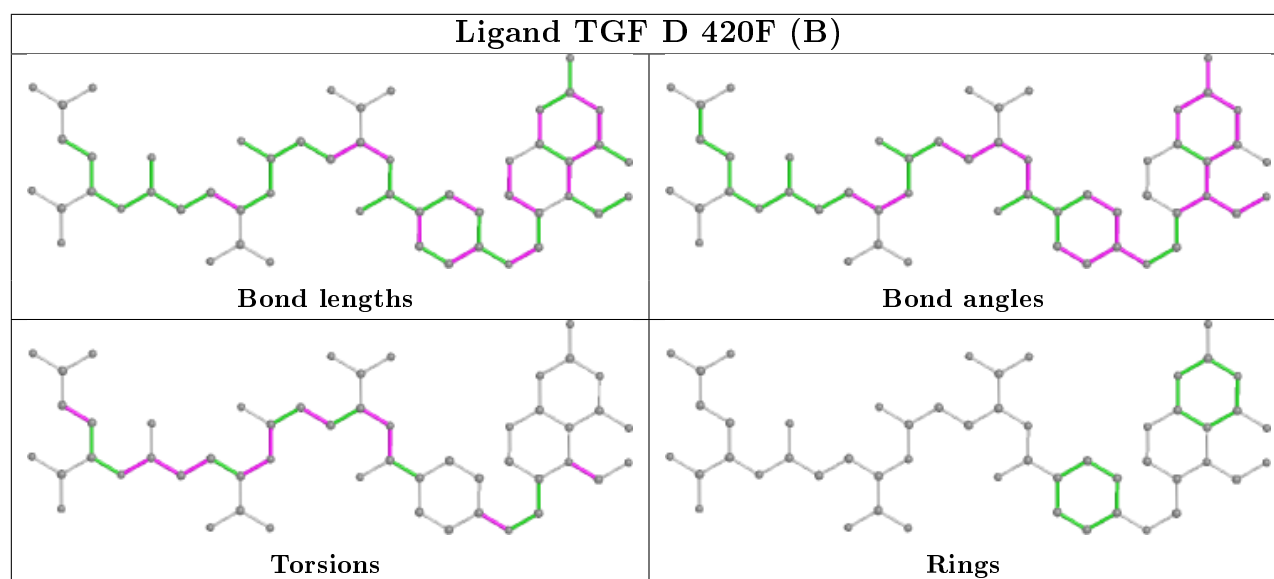


Ligand TGF B 420C (A)



Ligand TGF D 420F (A)





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	465/483 (96%)	-0.51	2 (0%) 92 93	24, 44, 78, 153	0
1	B	455/483 (94%)	-0.46	3 (0%) 87 89	21, 45, 92, 155	1 (0%)
1	C	465/483 (96%)	-0.54	0 100 100	22, 43, 73, 125	0
1	D	456/483 (94%)	-0.45	3 (0%) 87 89	20, 46, 94, 156	0
All	All	1841/1932 (95%)	-0.49	8 (0%) 92 93	20, 44, 83, 156	1 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	134(B)	LYS	3.8
1	A	355	SER	3.1
1	B	357	LEU	2.8
1	D	66	GLY	2.7
1	D	134(A)	LYS	2.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

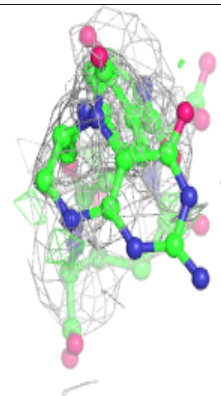
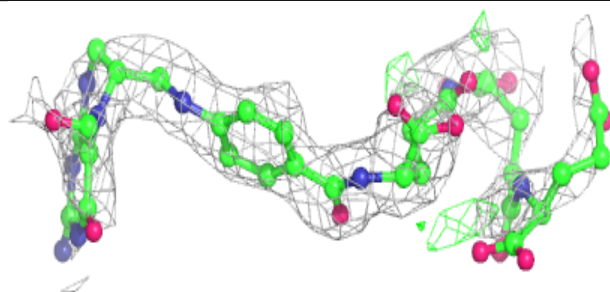
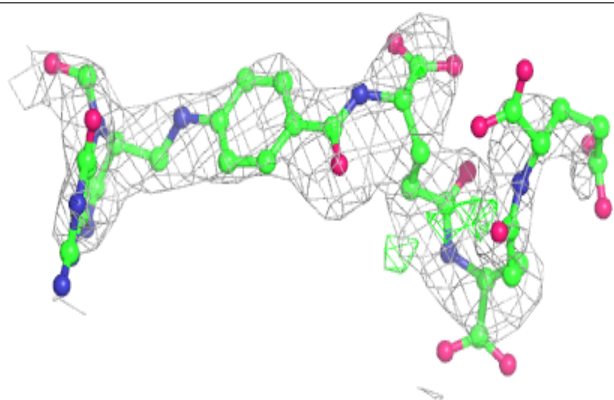
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	C	421	6/6	0.76	0.40	75,75,75,75	0
4	TGF	D	420(F)[B]	52/52	0.79	0.36	20,59,94,99	52
4	TGF	D	420(F)[A]	52/52	0.79	0.36	8,54,92,99	52
4	TGF	B	420(C)[A]	52/52	0.83	0.28	20,58,107,122	52
4	TGF	B	420(C)[B]	52/52	0.83	0.28	24,61,107,122	52
5	GOL	B	422	6/6	0.83	0.25	77,77,77,77	0
3	GLY	A	420(B)	5/5	0.90	0.20	67,67,67,67	0
5	GOL	D	421	6/6	0.95	0.12	56,56,56,56	0
5	GOL	B	421	6/6	0.95	0.17	58,58,58,58	0
2	PLP	B	419(A)	15/16	0.96	0.17	45,45,45,45	0
3	GLY	C	420(B)	5/5	0.96	0.13	51,51,51,51	0
2	PLP	C	419(A)	15/16	0.97	0.12	36,36,36,36	0
2	PLP	D	419(A)	15/16	0.97	0.15	37,37,37,37	0
2	PLP	A	419(A)	15/16	0.98	0.12	37,37,37,37	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.

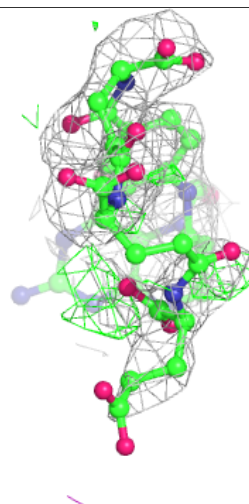
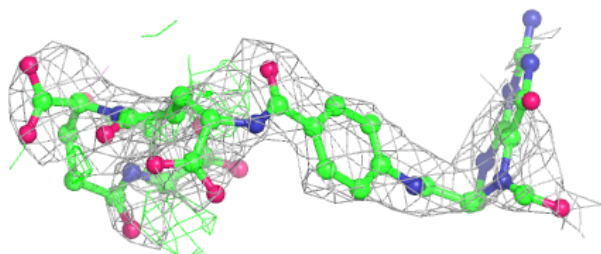
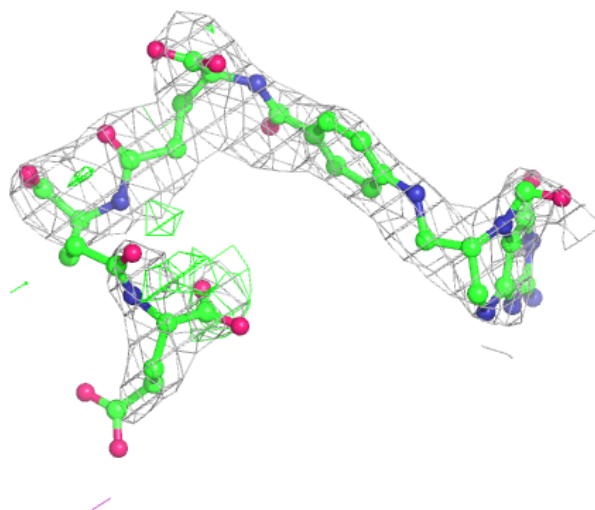
Electron density around TGF D 420F (B):

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



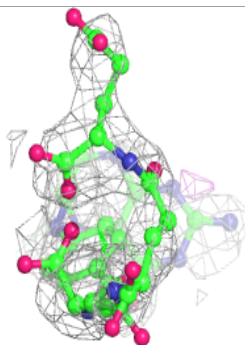
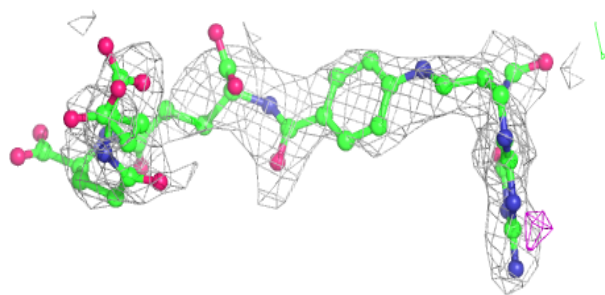
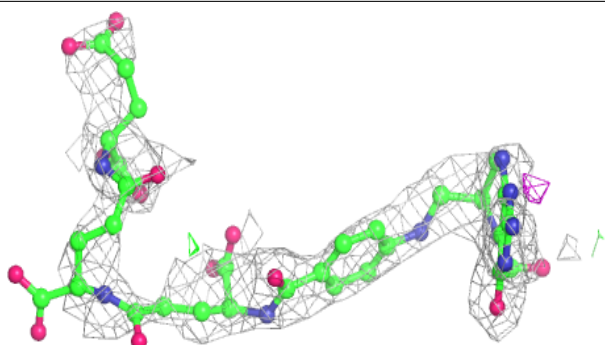
Electron density around TGF D 420F (A):

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

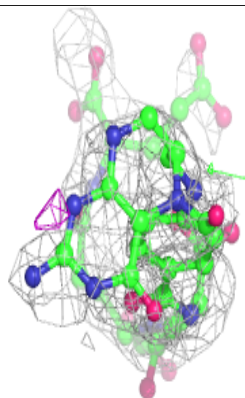
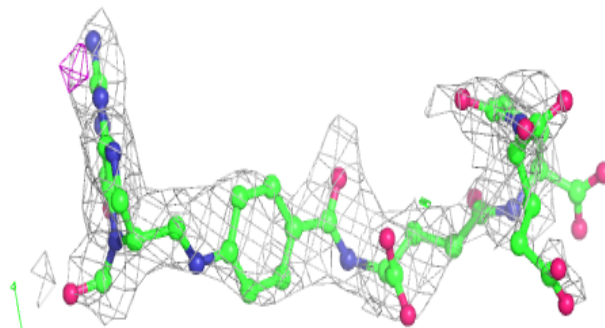
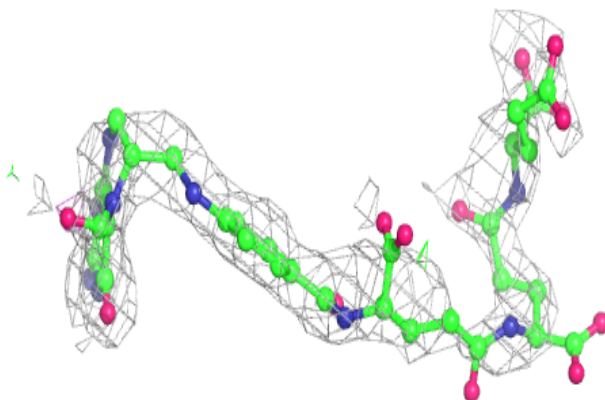


Electron density around TGF B 420C (A):

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

**Electron density around TGF B 420C (B):**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.