wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 06:38 AM EDT

PDB ID	:	1KV3
Title	:	HUMAN TISSUE TRANSGLUTAMINASE IN GDP BOUND FORM
Authors	:	Liu, S.; Cerione, R.A.; Clardy, J.
Deposited on	:	2002-01-24
Resolution	:	2.80 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 (i)) were used in the production of this report:

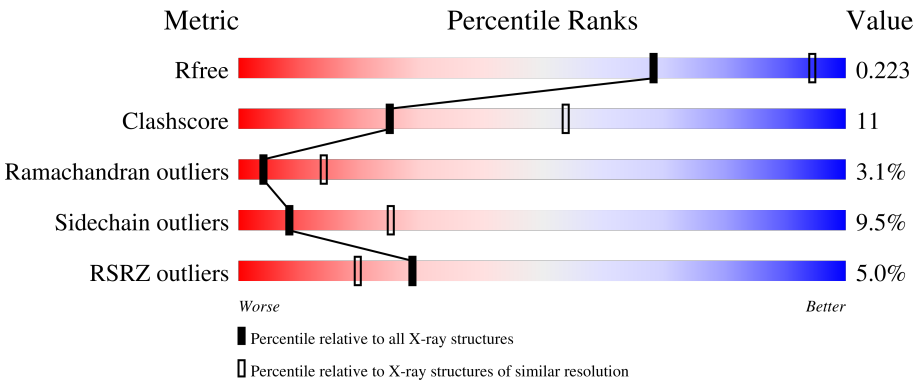
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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
1	A	687	5% 69% 20% 5% • 5%
1	B	687	4% 67% 22% 5% • 5%
1	C	687	4% 67% 22% 5% 5%
1	D	687	5% 65% 24% 5% 5%
1	E	687	5% 67% 22% 5% • 5%

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Mol	Chain	Length	Quality of chain
1	F	687	6% 67% 23% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31466 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 Protein-glutamine gamma-glutamyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	651	5145	3251	889	976	29	0	0	0
1	B	651	5145	3251	889	976	29	0	0	0
1	C	651	5145	3251	889	976	29	0	0	0
1	D	651	5145	3251	889	976	29	0	0	0
1	E	651	5145	3251	889	976	29	0	0	0
1	F	651	5145	3251	889	976	29	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLN	GLU	SEE REMARK 999	UNP P21980
A	186	GLN	GLU	SEE REMARK 999	UNP P21980
A	224	GLY	VAL	SEE REMARK 999	UNP P21980
A	533	THR	ASN	SEE REMARK 999	UNP P21980
A	655	VAL	LEU	SEE REMARK 999	UNP P21980
B	51	GLN	GLU	SEE REMARK 999	UNP P21980
B	186	GLN	GLU	SEE REMARK 999	UNP P21980
B	224	GLY	VAL	SEE REMARK 999	UNP P21980
B	533	THR	ASN	SEE REMARK 999	UNP P21980
B	655	VAL	LEU	SEE REMARK 999	UNP P21980
C	51	GLN	GLU	SEE REMARK 999	UNP P21980
C	186	GLN	GLU	SEE REMARK 999	UNP P21980
C	224	GLY	VAL	SEE REMARK 999	UNP P21980
C	533	THR	ASN	SEE REMARK 999	UNP P21980
C	655	VAL	LEU	SEE REMARK 999	UNP P21980
D	51	GLN	GLU	SEE REMARK 999	UNP P21980
D	186	GLN	GLU	SEE REMARK 999	UNP P21980

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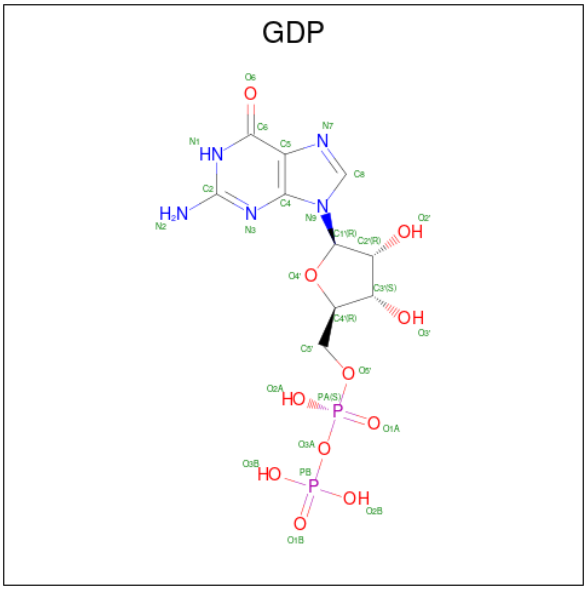
Chain	Residue	Modelled	Actual	Comment	Reference
D	224	GLY	VAL	SEE REMARK 999	UNP P21980
D	533	THR	ASN	SEE REMARK 999	UNP P21980
D	655	VAL	LEU	SEE REMARK 999	UNP P21980
E	51	GLN	GLU	SEE REMARK 999	UNP P21980
E	186	GLN	GLU	SEE REMARK 999	UNP P21980
E	224	GLY	VAL	SEE REMARK 999	UNP P21980
E	533	THR	ASN	SEE REMARK 999	UNP P21980
E	655	VAL	LEU	SEE REMARK 999	UNP P21980
F	51	GLN	GLU	SEE REMARK 999	UNP P21980
F	186	GLN	GLU	SEE REMARK 999	UNP P21980
F	224	GLY	VAL	SEE REMARK 999	UNP P21980
F	533	THR	ASN	SEE REMARK 999	UNP P21980
F	655	VAL	LEU	SEE REMARK 999	UNP P21980

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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		
2	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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

- Molecule 3 is water.

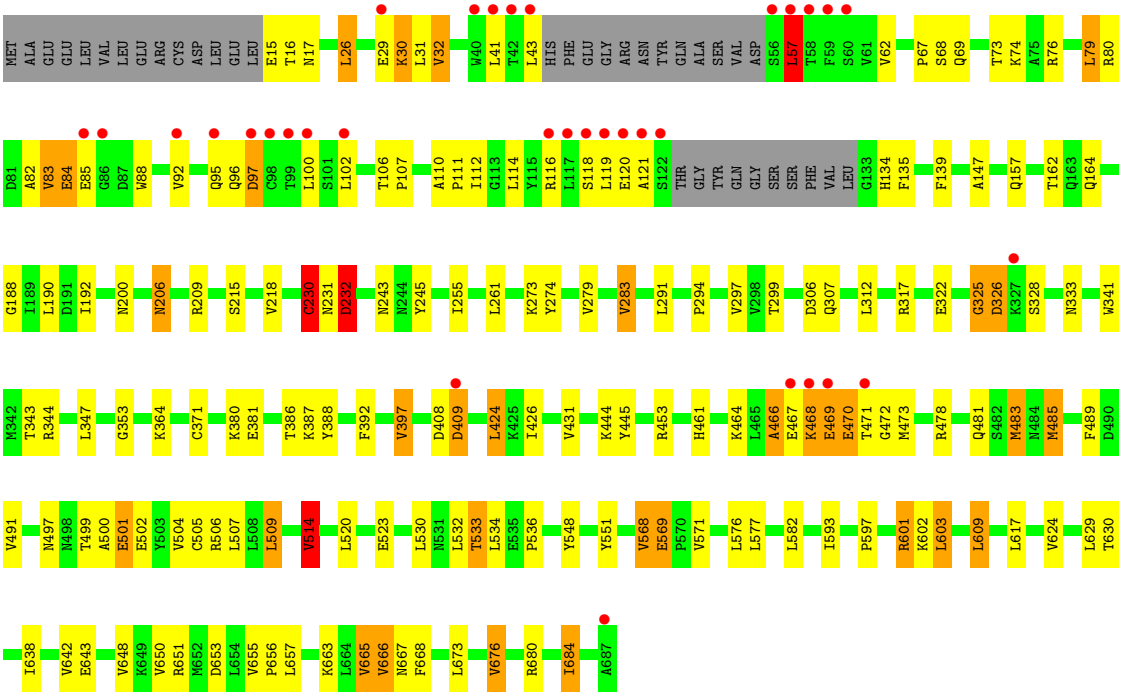
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	64	64	64	0	0
			Total	O		
3	B	68	68	68	0	0
			Total	O		
3	C	104	104	104	0	0
			Total	O		
3	D	66	66	66	0	0
			Total	O		
3	E	72	72	72	0	0
			Total	O		
3	F	54	54	54	0	0

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.

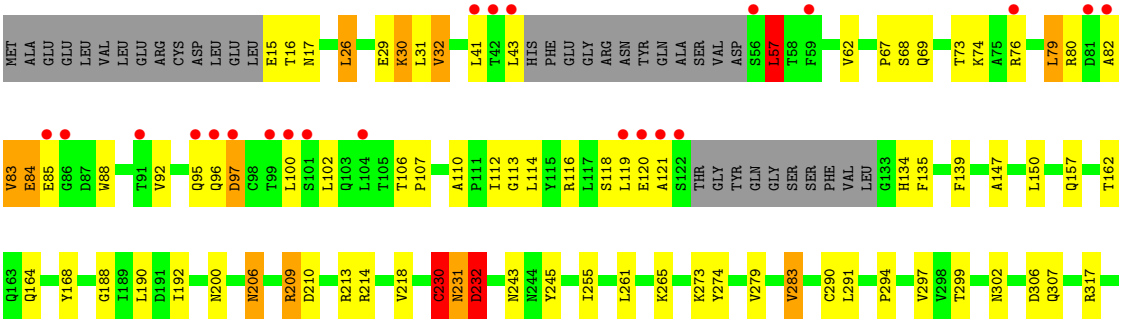
• Molecule 1: Protein-glutamine gamma-glutamyltransferase

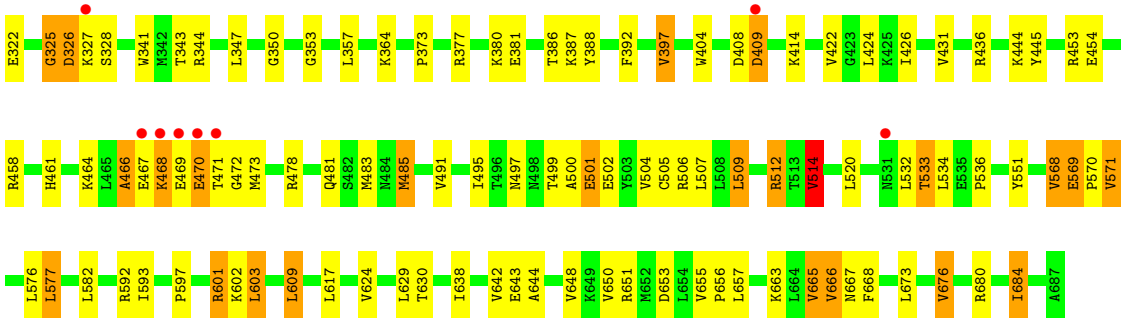
Chain A:



• Molecule 1: Protein-glutamine gamma-glutamyltransferase

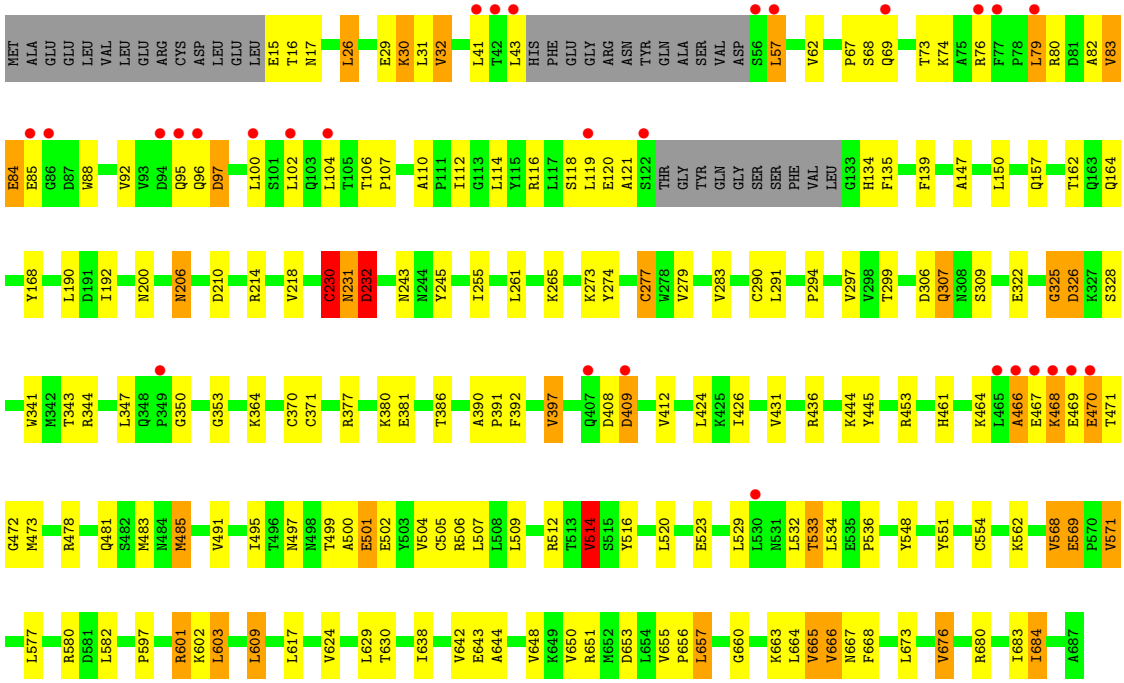
Chain B:





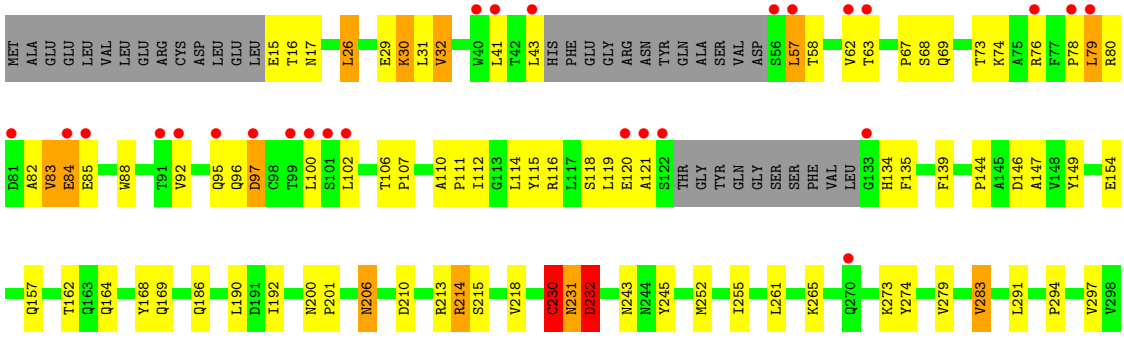
- Molecule 1: Protein-glutamine gamma-glutamyltransferase

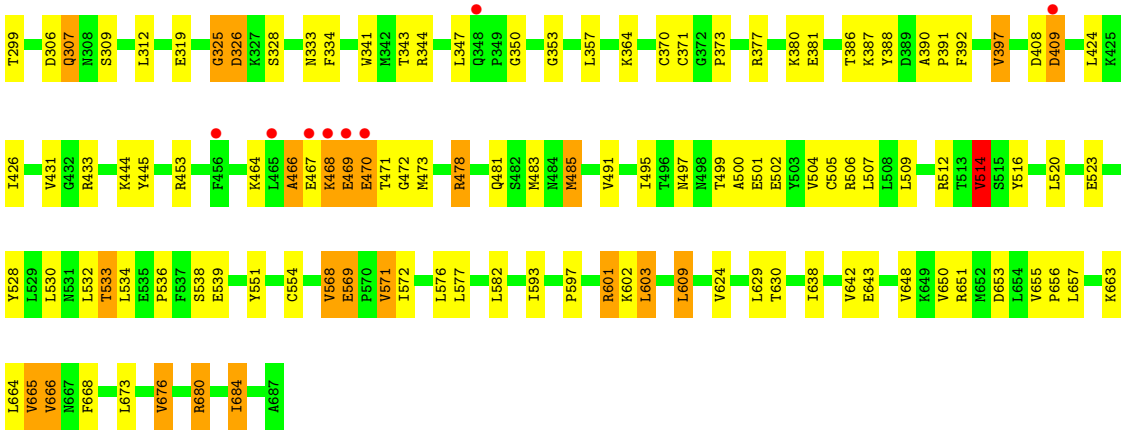
Chain C:



- Molecule 1: Protein-glutamine gamma-glutamyltransferase

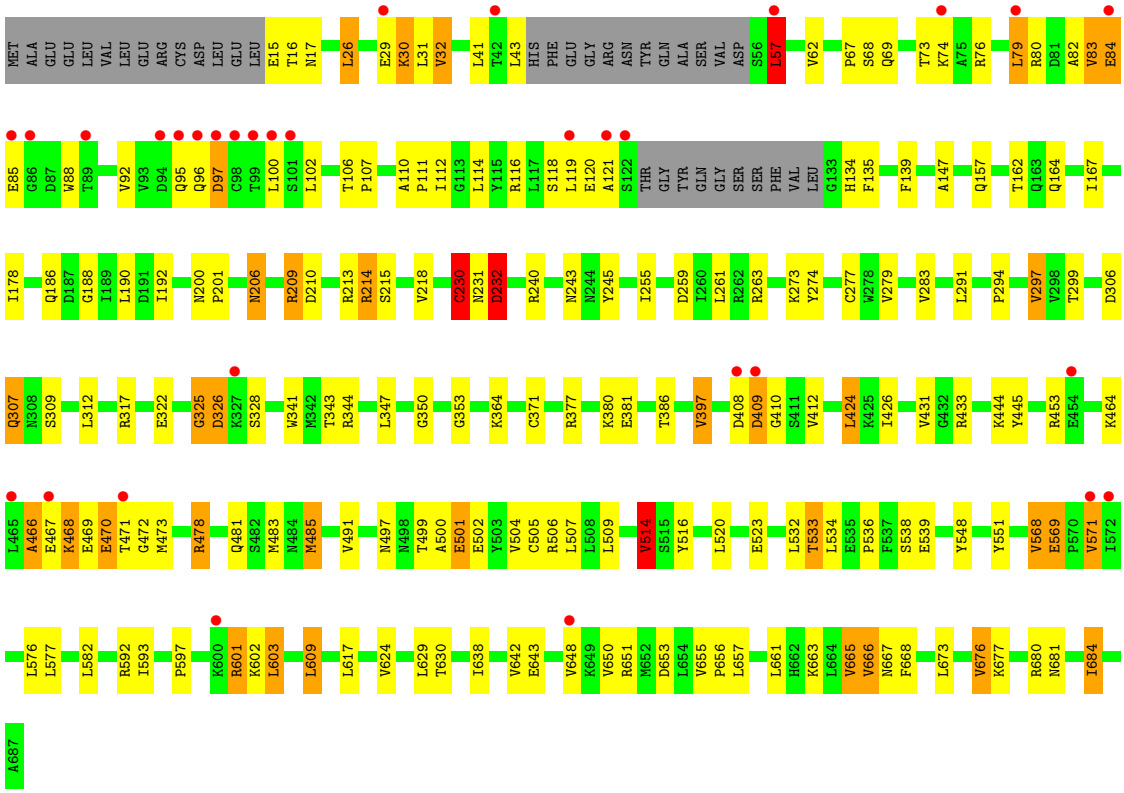
Chain D:





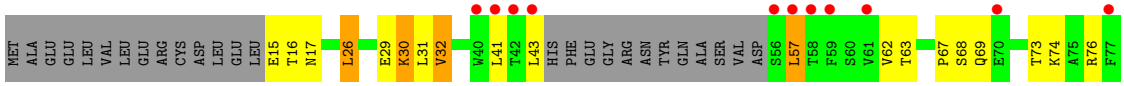
• Molecule 1: Protein-glutamine gamma-glutamyltransferase

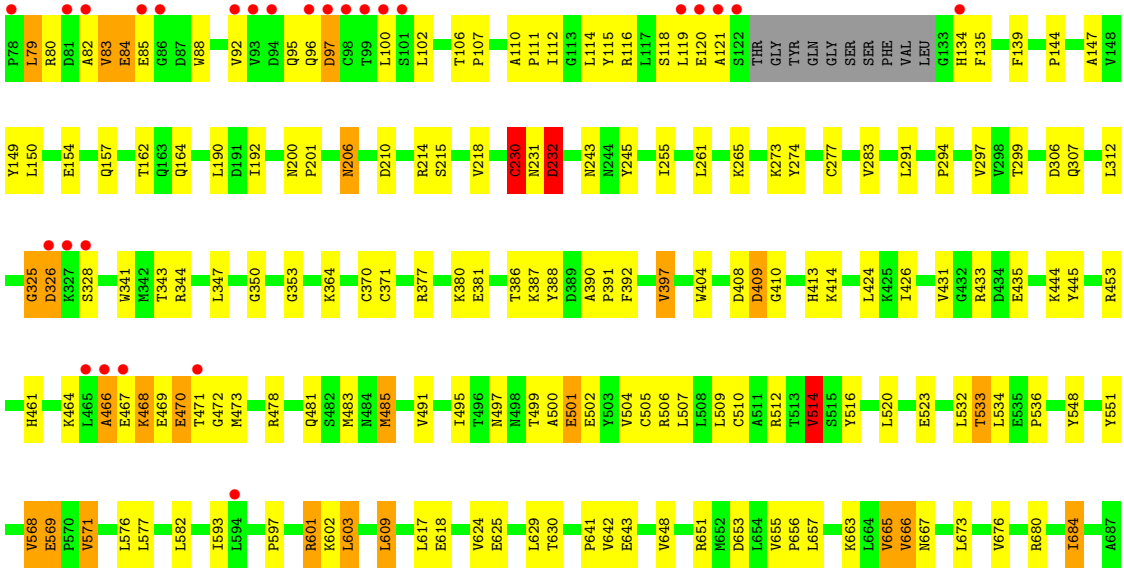
Chain E:



• Molecule 1: Protein-glutamine gamma-glutamyltransferase

Chain F:




P78 L79 R80 D81 A82 V83 E84 E85 G86 D87 W88 V92 V93 D94 Q95 Q96 D97 C98 T99 L100 S101 L102 T106 P107 A110 P111 I112 G113 L114 Y115 R116 L117 S118 L119 E120 A121 S122 THR GLY TYR GLN GLY SER SER PHE VAL LEU G133 H134 F135 F139 P144 A147 V148
Y149 L150 E154 Q157 T162 Q163 Q164 L190 D191 I192 N200 P201 N206 D210 R214 S215 V218 C230 N231 D232 N243 N244 Y245 I255 L261 K265 K273 Y274 C277 V283 L291 P294 V297 V298 T299 D306 Q307 L312
G325 D326 K327 S328 W341 M342 T343 R344 L347 G350 G353 K364 C370 C371 R377 K380 E381 T386 K387 Y388 D389 A390 P391 F392 V397 W404 D408 D409 G410 H413 K414 L424 K425 I426 V431 G432 R433 D434 E435 K444 Y445 R453
H461 K464 L465 A466 E467 K468 E469 E470 T471 G472 M473 R478 Q481 S482 M483 N484 M485 V491 I495 T496 N497 N498 T499 A500 E501 E502 Y503 V504 C505 R506 L507 L508 L509 C510 A511 R512 T513 V514 S515 Y516 L520 E523 L532 T533 L534 E535 P536 Y548 Y551
V568 E569 P570 V571 L576 L577 L582 I593 L594 P597 R601 K602 L603 L609 L617 E618 V624 E625 L629 T630 P641 V642 E643 V648 R651 M652 D653 L654 V655 P656 L657 K663 L664 V665 V666 N667 L673 V676 R680 I684 A687

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.48Å 168.80Å 238.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.79 – 2.80 51.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.6 (51.79-2.80) 94.7 (51.79-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.20 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.272 0.224 , 0.223	Depositor DCC
R_{free} test set	6274 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	58.6	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31466	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.63	0/5256	0.80	5/7131 (0.1%)
1	B	0.65	1/5256 (0.0%)	0.80	5/7131 (0.1%)
1	C	0.69	4/5256 (0.1%)	0.82	4/7131 (0.1%)
1	D	0.66	2/5256 (0.0%)	0.81	4/7131 (0.1%)
1	E	0.63	0/5256	0.80	5/7131 (0.1%)
1	F	0.64	2/5256 (0.0%)	0.81	4/7131 (0.1%)
All	All	0.65	9/31536 (0.0%)	0.81	27/42786 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	290	CYS	CB-SG	-8.31	1.68	1.82
1	C	370	CYS	CB-SG	-7.34	1.69	1.82
1	D	554	CYS	CB-SG	-6.28	1.71	1.82
1	C	277	CYS	CB-SG	-5.95	1.72	1.81
1	F	510	CYS	CB-SG	-5.90	1.72	1.81

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	307	GLN	N-CA-C	-6.58	93.22	111.00
1	A	307	GLN	N-CA-C	-6.55	93.31	111.00
1	B	514	VAL	CB-CA-C	-6.43	99.18	111.40
1	E	307	GLN	N-CA-C	-6.28	94.05	111.00
1	B	307	GLN	N-CA-C	-6.27	94.07	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	168	TYR	Sidechain
1	C	168	TYR	Sidechain
1	D	168	TYR	Sidechain

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	5145	0	5060	104	0
1	B	5145	0	5060	116	0
1	C	5145	0	5060	110	0
1	D	5145	0	5060	122	0
1	E	5145	0	5060	117	0
1	F	5145	0	5060	105	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
2	C	28	0	12	0	0
2	D	28	0	12	0	0
2	E	28	0	12	0	0
2	F	28	0	12	0	0
3	A	64	0	0	1	0
3	B	68	0	0	6	0
3	C	104	0	0	4	0
3	D	66	0	0	5	0
3	E	72	0	0	4	0
3	F	54	0	0	1	0
All	All	31466	0	30432	665	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 11.

The worst 5 of 665 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:83:VAL:HG13	1:D:84:GLU:H	1.32	0.95
1:F:83:VAL:HG13	1:F:84:GLU:H	1.31	0.94
1:E:83:VAL:HG13	1:E:84:GLU:H	1.32	0.94
1:B:83:VAL:HG13	1:B:84:GLU:H	1.31	0.94
1:C:83:VAL:HG13	1:C:84:GLU:H	1.33	0.93

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	645/687 (94%)	584 (90%)	42 (6%)	19 (3%)	4	15
1	B	645/687 (94%)	587 (91%)	38 (6%)	20 (3%)	4	14
1	C	645/687 (94%)	588 (91%)	37 (6%)	20 (3%)	4	14
1	D	645/687 (94%)	585 (91%)	39 (6%)	21 (3%)	4	13
1	E	645/687 (94%)	587 (91%)	37 (6%)	21 (3%)	4	13
1	F	645/687 (94%)	587 (91%)	38 (6%)	20 (3%)	4	14
All	All	3870/4122 (94%)	3518 (91%)	231 (6%)	121 (3%)	4	14

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
1	A	85	GLU
1	A	96	GLN

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Mol	Chain	Res	Type
1	A	121	ALA
1	A	231	ASN

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	565/596 (95%)	512 (91%)	53 (9%)	8 26
1	B	565/596 (95%)	510 (90%)	55 (10%)	8 24
1	C	565/596 (95%)	512 (91%)	53 (9%)	8 26
1	D	565/596 (95%)	511 (90%)	54 (10%)	8 24
1	E	565/596 (95%)	510 (90%)	55 (10%)	8 24
1	F	565/596 (95%)	512 (91%)	53 (9%)	8 26
All	All	3390/3576 (95%)	3067 (90%)	323 (10%)	8 25

5 of 323 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	209	ARG
1	F	218	VAL
1	E	312	LEU
1	E	617	LEU
1	F	481	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	169	GLN
1	F	206	ASN
1	C	103	GLN
1	C	69	GLN
1	F	234	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	GDP	D	703	-	24,30,30	1.45	4 (16%)	30,47,47	0.86	2 (6%)
2	GDP	B	701	-	24,30,30	1.51	4 (16%)	30,47,47	0.84	1 (3%)
2	GDP	E	704	-	24,30,30	1.41	3 (12%)	30,47,47	0.86	1 (3%)
2	GDP	A	700	-	24,30,30	1.47	6 (25%)	30,47,47	0.82	1 (3%)
2	GDP	F	705	-	24,30,30	1.54	5 (20%)	30,47,47	0.82	0
2	GDP	C	702	-	24,30,30	1.62	6 (25%)	30,47,47	0.87	1 (3%)

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	GDP	D	703	-	-	4/12/32/32	0/3/3/3
2	GDP	B	701	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	E	704	-	-	3/12/32/32	0/3/3/3
2	GDP	A	700	-	-	3/12/32/32	0/3/3/3
2	GDP	F	705	-	-	4/12/32/32	0/3/3/3
2	GDP	C	702	-	-	3/12/32/32	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	GDP	C8-N7	-4.17	1.27	1.35
2	C	702	GDP	C8-N7	-4.17	1.27	1.35
2	E	704	GDP	C8-N7	-4.14	1.28	1.35
2	A	700	GDP	C8-N7	-3.88	1.28	1.35
2	F	705	GDP	C8-N7	-3.69	1.28	1.35

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	703	GDP	O6-C6-C5	2.30	128.87	124.37
2	E	704	GDP	O2B-PB-O1B	2.29	119.63	110.68
2	A	700	GDP	O2B-PB-O1B	2.27	119.56	110.68
2	D	703	GDP	O2B-PB-O1B	2.25	119.51	110.68
2	C	702	GDP	O2B-PB-O1B	2.20	119.28	110.68

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	GDP	PA-O3A-PB-O2B
2	B	701	GDP	PA-O3A-PB-O2B
2	C	702	GDP	PA-O3A-PB-O2B
2	D	703	GDP	PA-O3A-PB-O2B
2	D	703	GDP	PB-O3A-PA-O5'

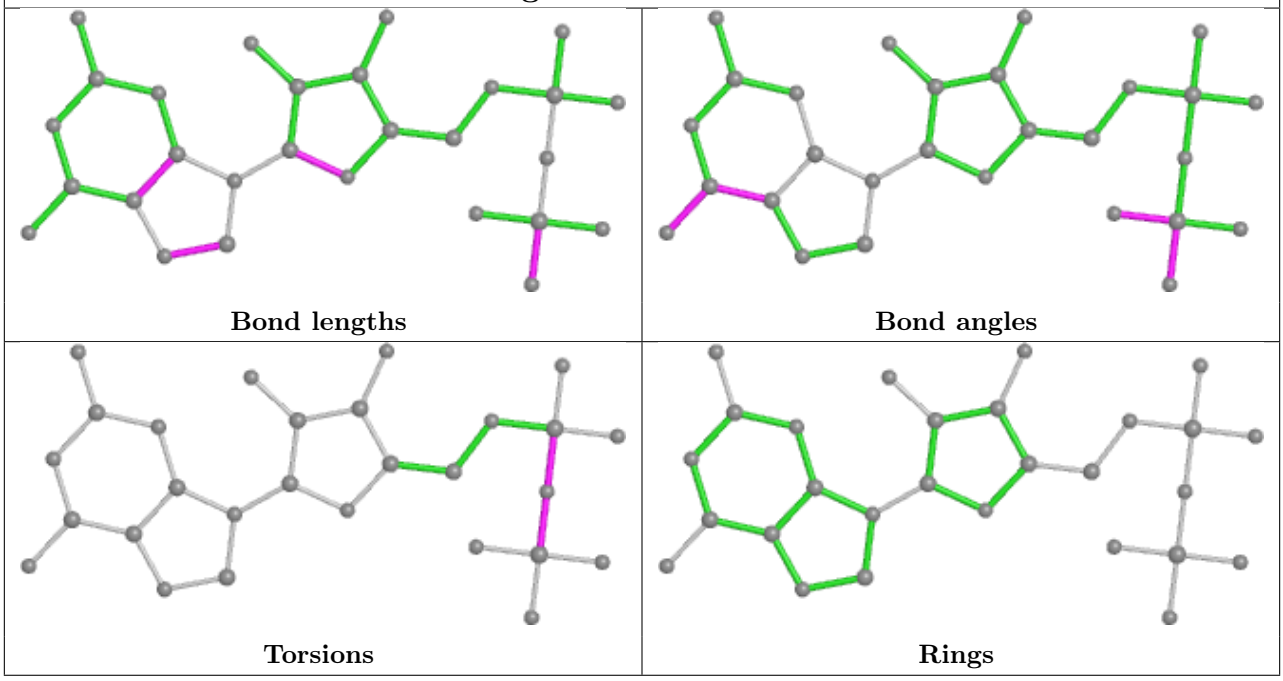
There are no ring outliers.

No monomer is involved in short contacts.

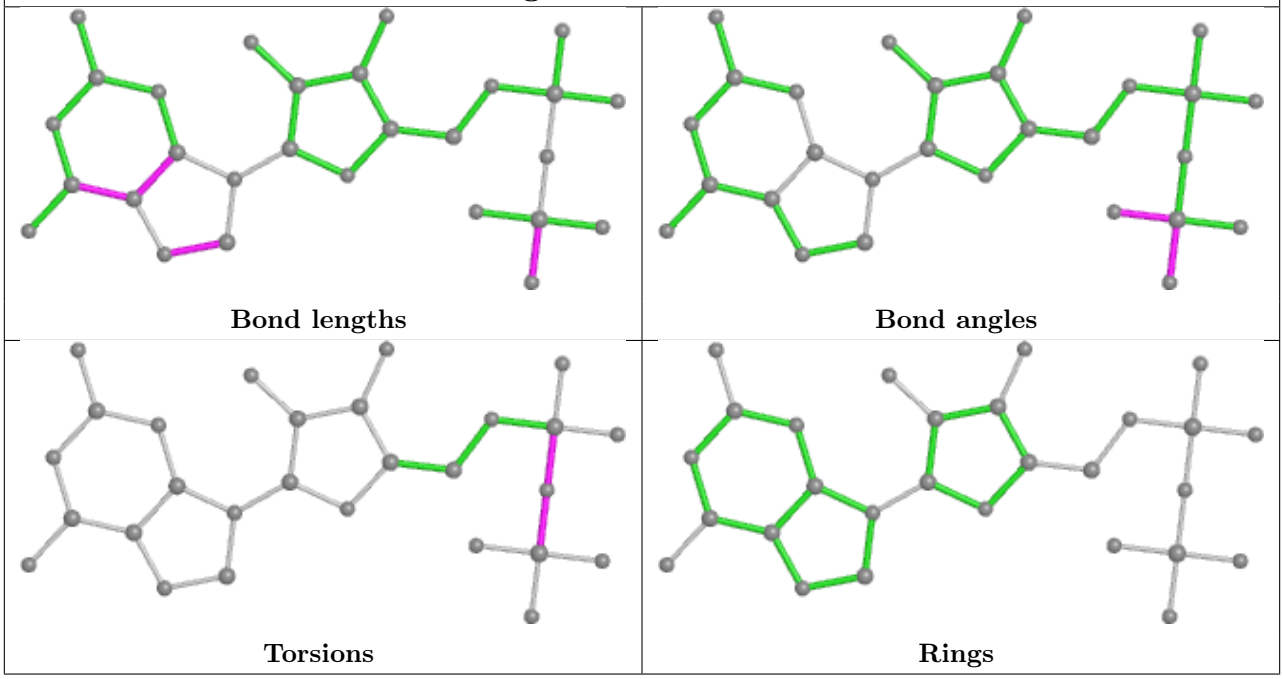
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

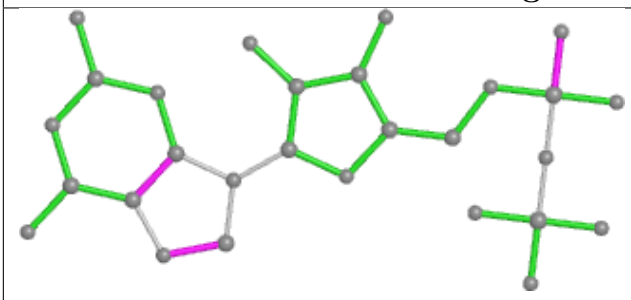
Ligand GDP D 703



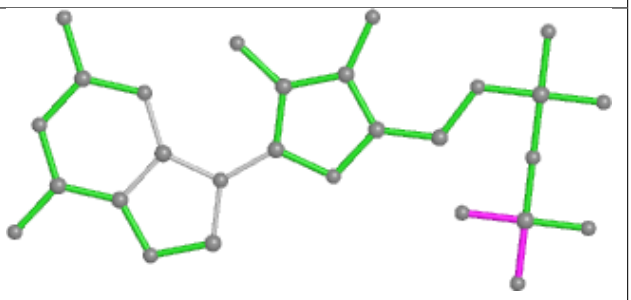
Ligand GDP B 701



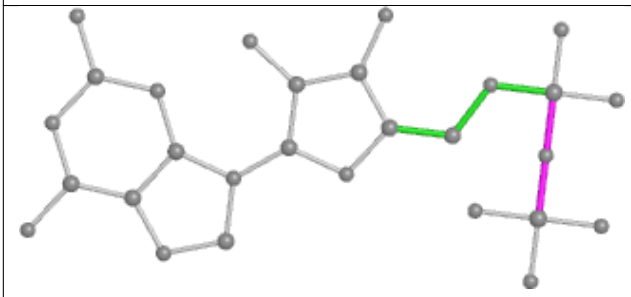
Ligand GDP E 704



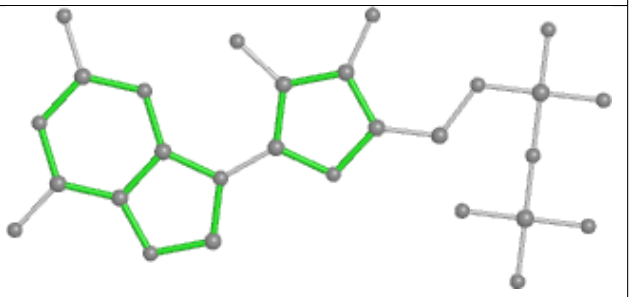
Bond lengths



Bond angles

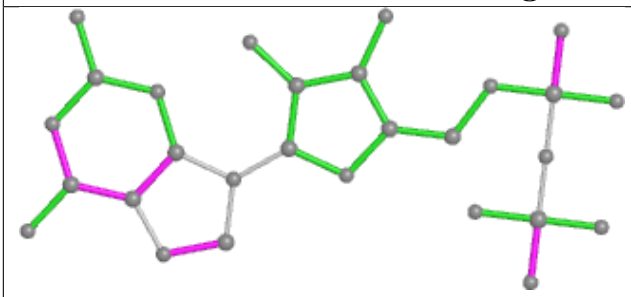


Torsions

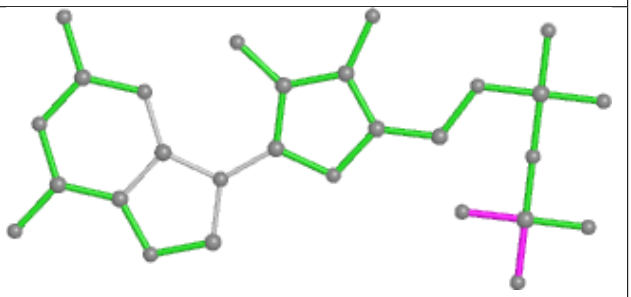


Rings

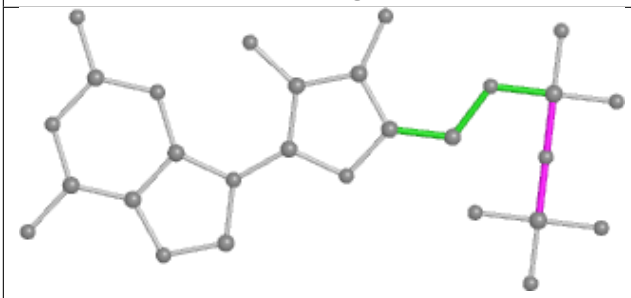
Ligand GDP A 700



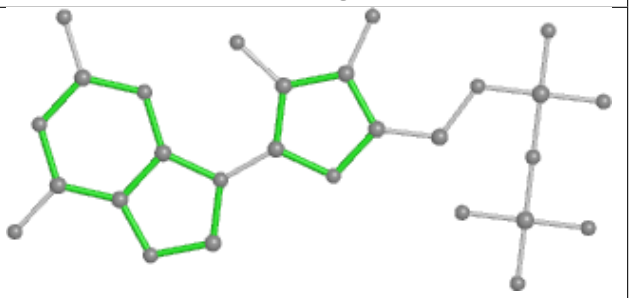
Bond lengths



Bond angles

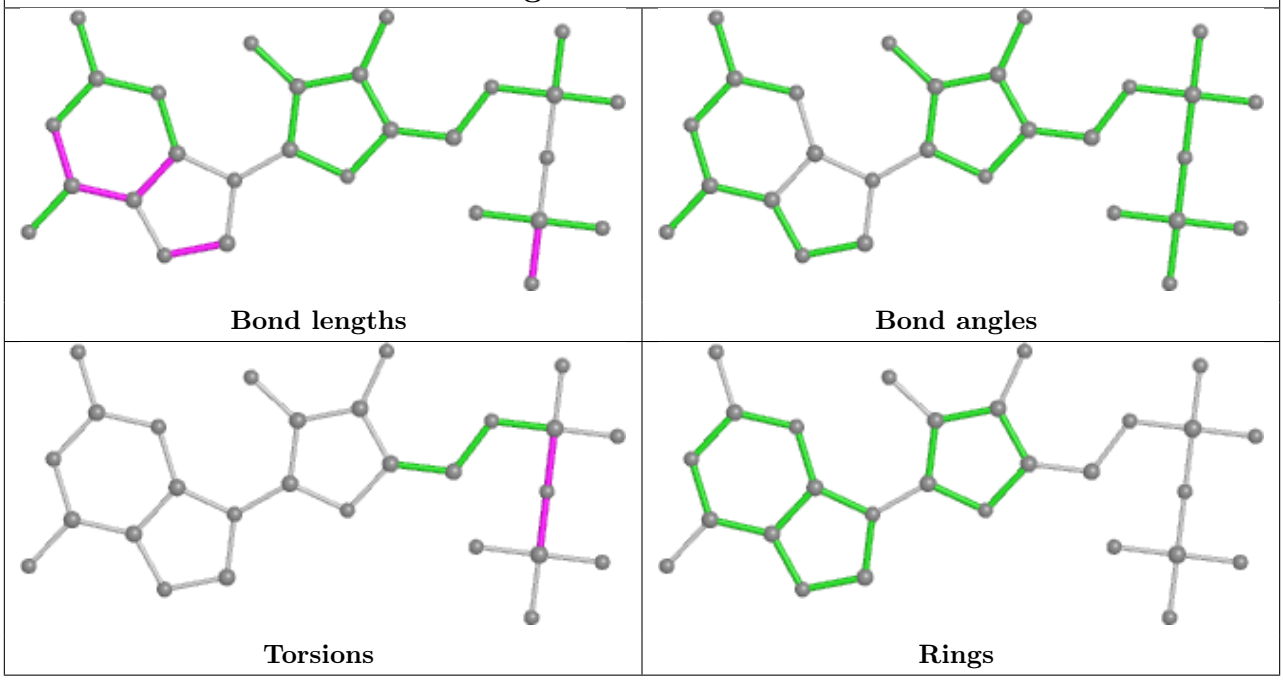


Torsions

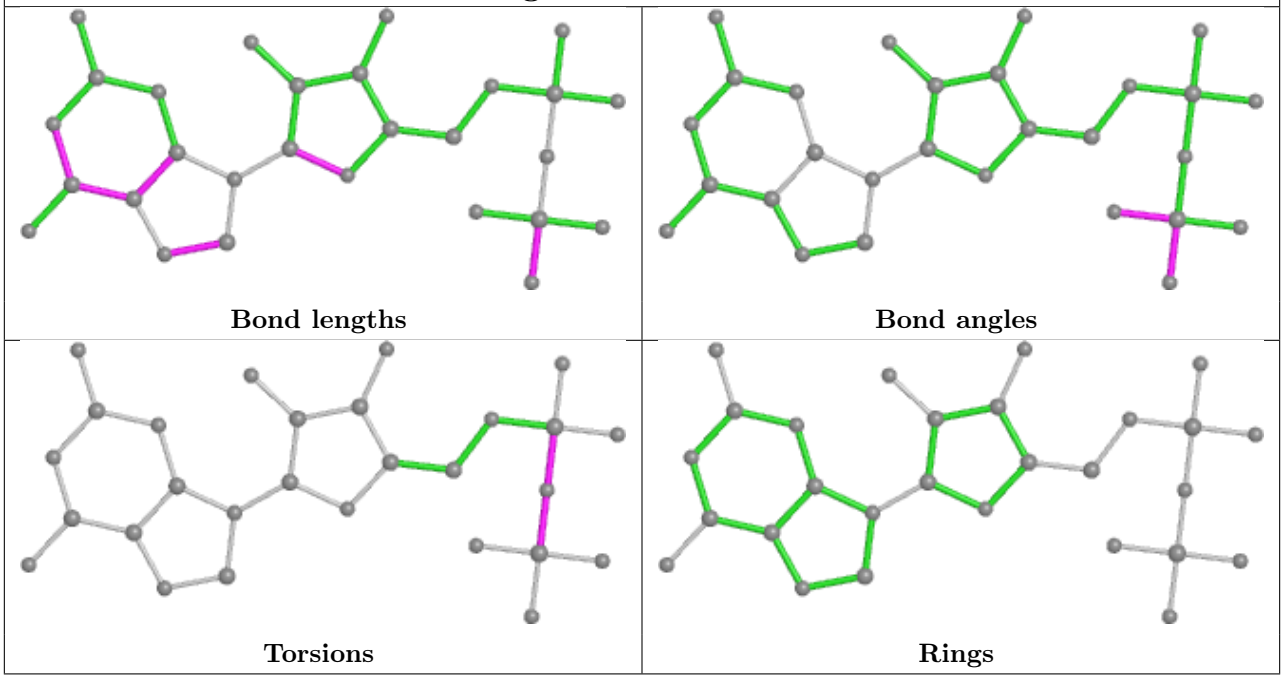


Rings

Ligand GDP F 705



Ligand GDP C 702



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	651/687 (94%)	-0.03	33 (5%)	28	19	22, 53, 108, 141	0
1	B	651/687 (94%)	0.05	30 (4%)	32	22	23, 52, 107, 140	0
1	C	651/687 (94%)	-0.05	29 (4%)	33	23	21, 48, 106, 140	0
1	D	651/687 (94%)	0.05	34 (5%)	27	18	22, 52, 107, 142	0
1	E	651/687 (94%)	0.01	31 (4%)	30	21	28, 53, 106, 141	0
1	F	651/687 (94%)	0.05	38 (5%)	23	15	21, 52, 107, 142	0
All	All	3906/4122 (94%)	0.01	195 (4%)	28	19	21, 52, 107, 142	0

The worst 5 of 195 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	467	GLU	7.0
1	C	85	GLU	6.7
1	B	86	GLY	6.2
1	F	327	LYS	5.4
1	D	467	GLU	5.4

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 monosaccharides in this entry.

6.4 Ligands (i)

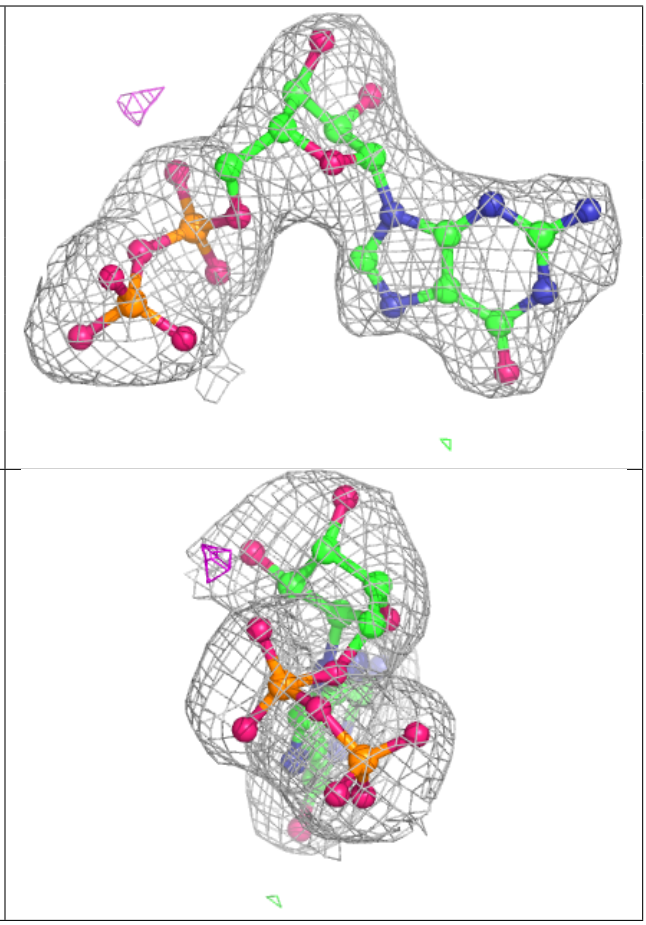
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GDP	E	704	28/28	0.97	0.14	32,42,51,58	0
2	GDP	B	701	28/28	0.98	0.14	20,36,48,53	0
2	GDP	C	702	28/28	0.98	0.15	27,37,50,53	0
2	GDP	D	703	28/28	0.98	0.14	25,34,51,57	0
2	GDP	A	700	28/28	0.98	0.15	29,36,54,55	0
2	GDP	F	705	28/28	0.98	0.14	33,38,45,57	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.

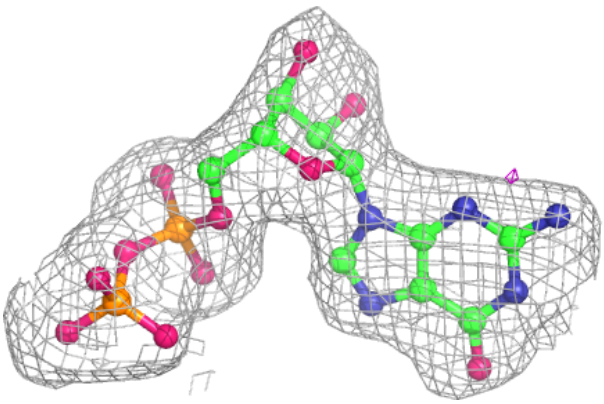
Electron density around GDP E 704:

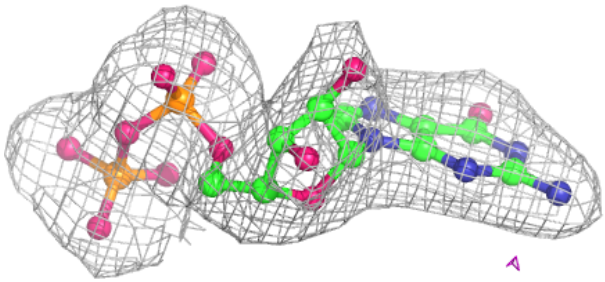
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

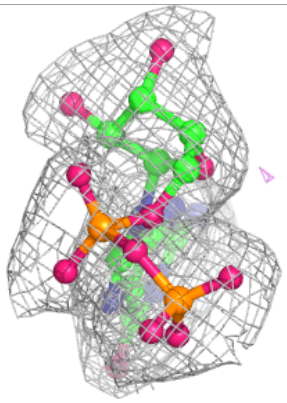


Electron density around GDP B 701:

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

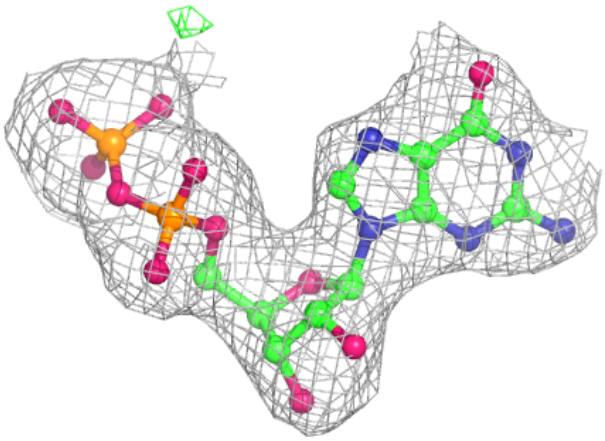


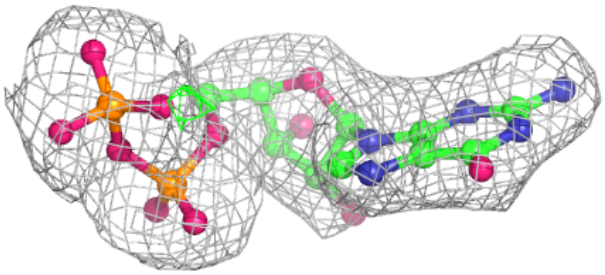


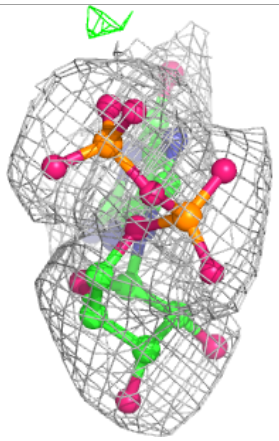


Electron density around GDP C 702:

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

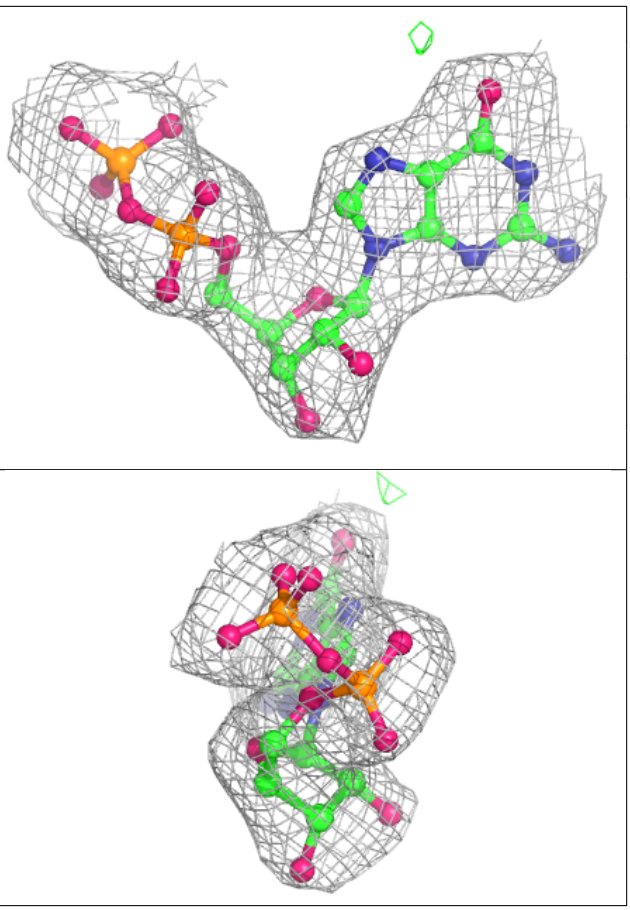






Electron density around GDP D 703:

$2mF_o$-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 A 700:

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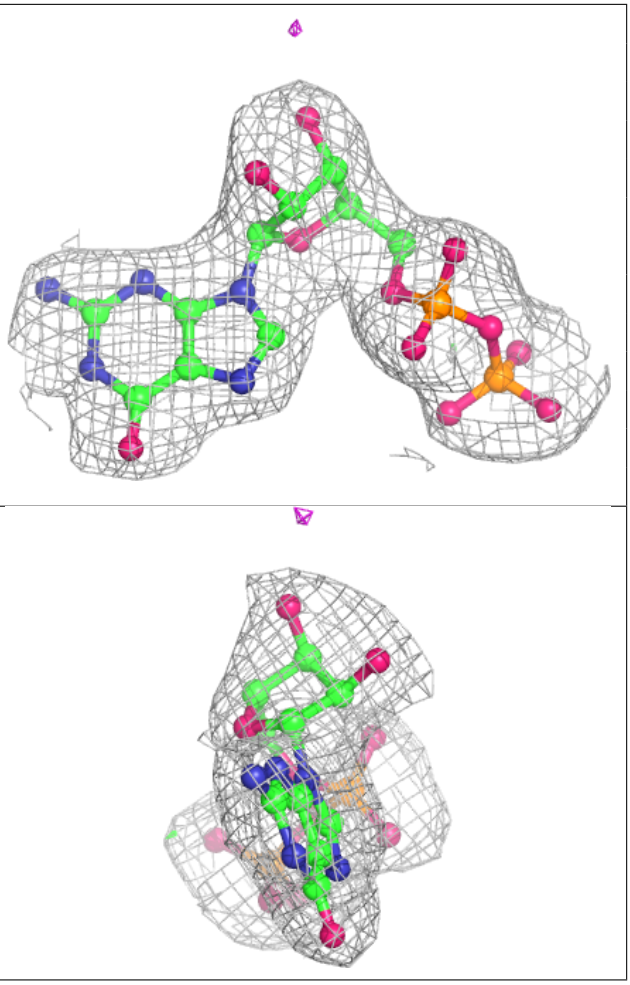
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP F 705:

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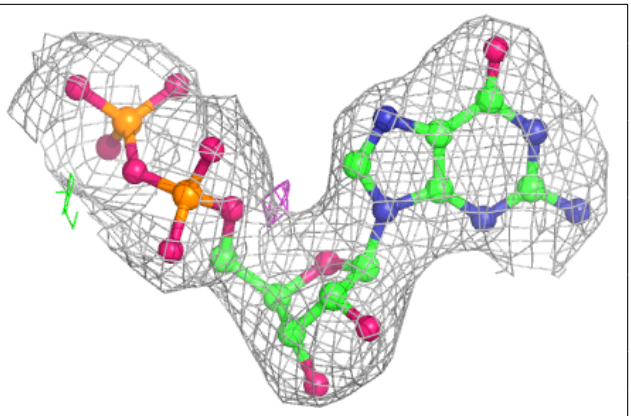
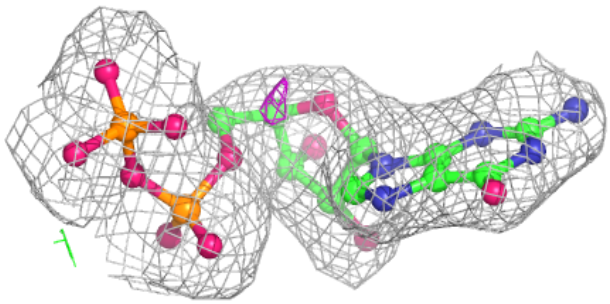
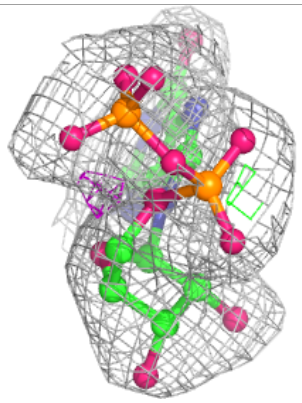
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.