



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:09 AM UTC

PDB ID : 8QVU / pdb_00008qvu
Title : Crystal Structure of ligand ACBI3 in complex with KRAS G12D C118S GDP and pVHL:ElonginC:ElonginB complex
Authors : Wijaya, A.J.; Zollman, D.; Farnaby, W.; Ciulli, A.
Deposited on : 2023-10-18
Resolution : 2.24 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

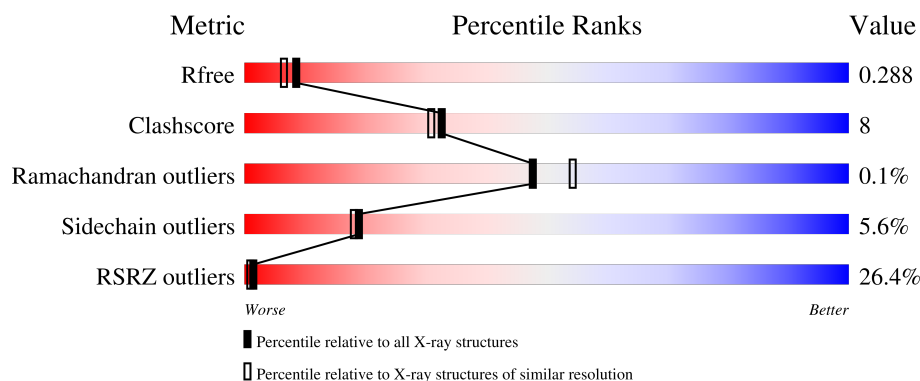
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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 $\leq 5\%$. 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	D	104	
1	H	104	
2	C	97	
2	G	97	
3	B	213	

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Mol	Chain	Length	Quality of chain
3	F	213	2% 54% 12% • 32%
4	A	188	52% 61% 19% • 18%
4	E	188	54% 65% 16% • 15%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7887 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 Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	103	Total	C	N	O	S	0	0	0
			799	506	132	156	5			
1	D	102	Total	C	N	O	S	0	0	0
			805	510	135	155	5			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	88	Total	C	N	O	S	0	0	0
			693	446	110	130	7			
2	C	88	Total	C	N	O	S	0	0	0
			693	447	109	131	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	16	MET	-	initiating methionine	UNP Q15369
C	16	MET	-	initiating methionine	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	144	Total	C	N	O	S	0	0	0
			1171	745	212	212	2			
3	B	147	Total	C	N	O	S	0	0	0
			1198	762	220	214	2			

- Molecule 4 is a protein called Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	159	Total	C	N	O	S	0	0	0
			1132	711	191	225	5			

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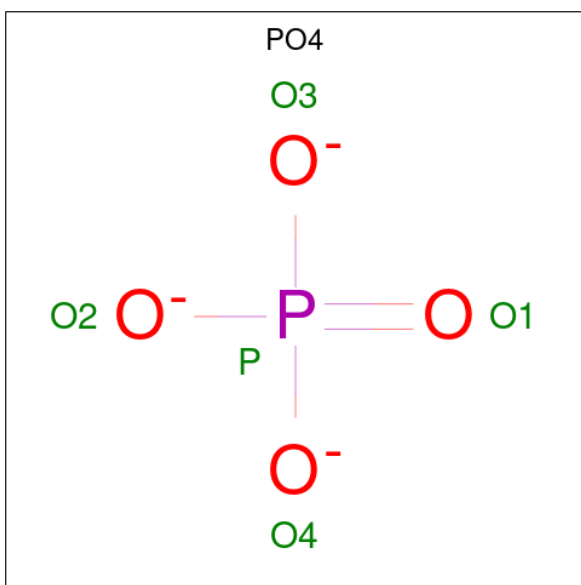
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	155	Total	C	N	O	S	0	0	0
			1123	705	193	221	4			

There are 4 discrepancies between the modelled and reference sequences:

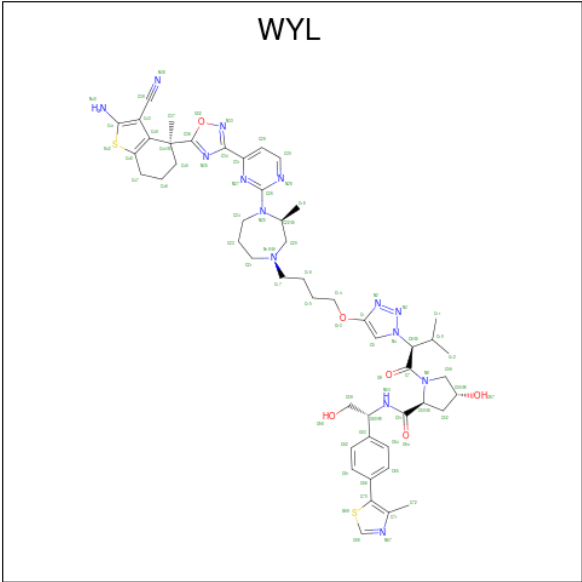
Chain	Residue	Modelled	Actual	Comment	Reference
E	12	ASP	GLY	engineered mutation	UNP P01116
E	118	SER	CYS	engineered mutation	UNP P01116
A	12	ASP	GLY	engineered mutation	UNP P01116
A	118	SER	CYS	engineered mutation	UNP P01116

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



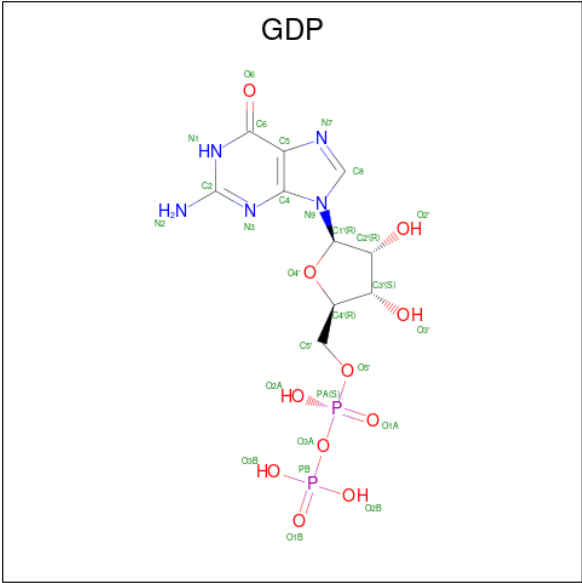
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is (2S,4R)-1-[(2S)-2-[4-[4-[(3S)-4-[4-[5-[(4S)-2-azanyl-3-cyano-4-methyl-6,7-dihydro-5H-1-benzothiophen-4-yl]-1,2,4-oxadiazol-3-yl]pyrimidin-2-yl]-3-methyl-1,4-diazepan-1-yl]butoxy]-1,2,3-triazol-1-yl]-3-methyl-butanoyl]-N-[(1R)-1-[4-(4-methyl-1,3-thiazol-5-yl)phenyl]-2-oxidanyl-ethyl]-4-oxidanyl-pyrrolidine-2-carboxamide (CCD ID: WYL) (formula: C₅₀H₆₂N₁₄O₆S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			72	50	14	6	2		
6	E	1	Total	C	N	O	S	0	0
			72	50	14	6	2		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	1	Total	Mg	0	0
			1	1		
8	A	1	Total	Mg	0	0
			1	1		

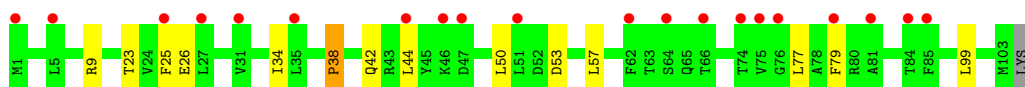
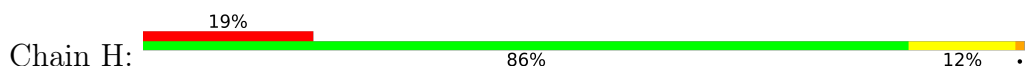
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	1	Total	O	0	0
			1	1		
9	G	8	Total	O	0	0
			8	8		
9	F	19	Total	O	0	0
			19	19		
9	D	3	Total	O	0	0
			3	3		
9	C	8	Total	O	0	0
			8	8		
9	B	14	Total	O	0	0
			14	14		
9	E	10	Total	O	0	0
			10	10		
9	A	3	Total	O	0	0
			3	3		

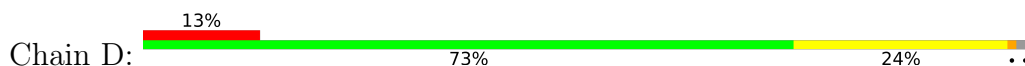
3 Residue-property plots [i](#)

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.

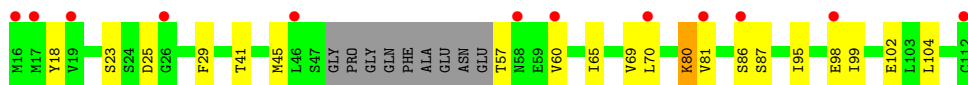
- Molecule 1: Elongin-B



- Molecule 1: Elongin-B



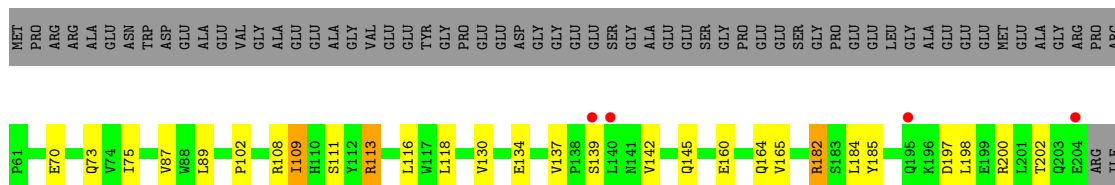
- Molecule 2: Elongin-C



- Molecule 2: Elongin-C



- Molecule 3: von Hippel-Lindau disease tumor suppressor



ALA
HIS
GLN
ARG
MET
GLY
ASP

- Molecule 3: von Hippel-Lindau disease tumor suppressor



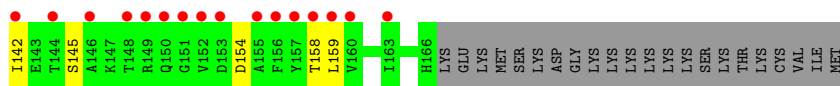
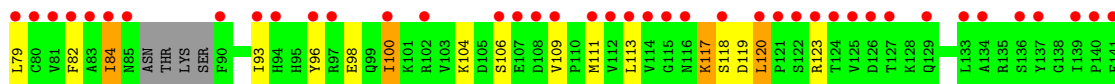
MET PRO ARG ARG ALA GLU ASN TRP ASP GLU VAL VAL GLY GLU ALA GLU ALA ALA GLY VAL GLU TYR GLY PRO GLU GLU ASP GLY GLY GLU SER GLY ALA GLU SER GLY PRO GLN GLU GLU SER ARG MET GLY PRO GLU LEU GLY ALA GLU GLU MET MET GLY ARG PRO ARG



- Molecule 4: Isoform 2B of GTPase KRas



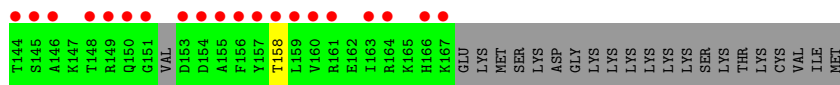
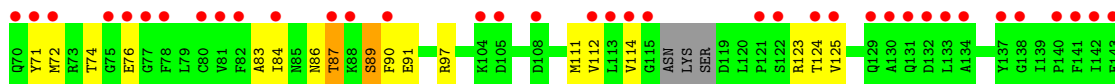
MET THR E3 Y4 K5 L6 V7 V8 V9 G10 G13 G14 G15 G16 S17 S18 A18 L19 L20 L21 Q22 L23 L24 Q25 Q26 H27 F28 V29 V30 E31 V32 D33 P34 T35 Y40 V44 V45 I46 D47 GLY E49 E50 G51 L52 L53 D54 L55 L56 D57 T58 A59 Q70 G75 E76 G77 F78



- Molecule 4: Isoform 2B of GTPase KRas



MET T2 E3 K5 L6 V7 V8 V9 D12 K16 S17 A18 L19 T20 T21 Q22 L23 L24 Q25 Q26 H27 F28 V29 D30 E31 D33 P34 T35 I36 E37 D38 S39 Y40 E41 K42 Q43 VAL VAL ILE D47 G48 E49 T50 CYS LEU LEU D54 L55 L56 D57 T58 G60 Y64



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.25Å 120.90Å 81.02Å 90.00° 111.67° 90.00°	Depositor
Resolution (Å)	55.86 – 2.24 55.86 – 2.24	Depositor EDS
% Data completeness (in resolution range)	58.9 (55.86-2.24) 58.8 (55.86-2.24)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.248 , 0.287 0.251 , 0.288	Depositor DCC
R_{free} test set	1885 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7887	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.57% 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: MG, WYL, GDP, PO4

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	D	0.43	0/820	0.69	0/1107
1	H	0.48	1/815 (0.1%)	0.70	0/1105
2	C	0.38	0/707	0.63	0/955
2	G	0.50	0/707	0.77	2/957 (0.2%)
3	B	0.64	0/1229	0.84	0/1677
3	F	0.62	1/1202 (0.1%)	0.85	0/1642
4	A	0.61	0/1137	0.93	3/1538 (0.2%)
4	E	0.65	0/1151	0.94	1/1568 (0.1%)
All	All	0.57	2/7768 (0.0%)	0.82	6/10549 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	38	PRO	C-O	-5.62	1.20	1.24
3	F	102	PRO	C-O	-5.01	1.20	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	119	ASP	N-CA-C	-7.03	105.24	114.31
4	A	60	GLY	CA-C-O	-5.90	118.20	122.45
2	G	80	LYS	N-CA-C	-5.38	103.42	110.53
4	A	64	TYR	CB-CA-C	5.15	119.05	111.06
2	G	80	LYS	CA-C-O	-5.13	115.92	121.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	D	805	0	806	21	0
1	H	799	0	785	10	0
2	C	693	0	686	15	0
2	G	693	0	682	12	0
3	B	1198	0	1201	8	0
3	F	1171	0	1161	21	0
4	A	1123	0	1000	23	0
4	E	1132	0	956	17	0
5	B	5	0	0	0	0
6	B	72	0	0	0	0
6	E	72	0	0	1	0
7	A	28	0	12	1	0
7	E	28	0	12	1	0
8	A	1	0	0	0	0
8	E	1	0	0	0	0
9	A	3	0	0	0	0
9	B	14	0	0	0	0
9	C	8	0	0	2	0
9	D	3	0	0	1	0
9	E	10	0	0	0	0
9	F	19	0	0	1	0
9	G	8	0	0	0	0
9	H	1	0	0	0	0
All	All	7887	0	7301	119	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 8.

The worst 5 of 119 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:43:ARG:HD2	1:D:85:PHE:CD2	2.23	0.73
4:A:29:VAL:HG12	4:A:31:GLU:H	1.54	0.72
3:F:134:GLU:HG3	9:F:303:HOH:O	1.94	0.68
3:B:87:VAL:HB	3:B:118:LEU:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:86:ASN:HB3	4:A:89:SER:HB3	1.77	0.67

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	D	98/104 (94%)	93 (95%)	5 (5%)	0	100	100
1	H	101/104 (97%)	98 (97%)	3 (3%)	0	100	100
2	C	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
2	G	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
3	B	145/213 (68%)	141 (97%)	4 (3%)	0	100	100
3	F	142/213 (67%)	137 (96%)	5 (4%)	0	100	100
4	A	143/188 (76%)	136 (95%)	7 (5%)	0	100	100
4	E	153/188 (81%)	145 (95%)	7 (5%)	1 (1%)	18	16
All	All	950/1204 (79%)	914 (96%)	35 (4%)	1 (0%)	48	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	84	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	D	90/92 (98%)	86 (96%)	4 (4%)	25	27
1	H	88/92 (96%)	86 (98%)	2 (2%)	44	53
2	C	78/86 (91%)	76 (97%)	2 (3%)	40	48
2	G	78/86 (91%)	74 (95%)	4 (5%)	21	21
3	B	136/185 (74%)	130 (96%)	6 (4%)	25	27
3	F	133/185 (72%)	129 (97%)	4 (3%)	36	43
4	A	105/168 (62%)	94 (90%)	11 (10%)	6	3
4	E	100/168 (60%)	88 (88%)	12 (12%)	5	2
All	All	808/1062 (76%)	763 (94%)	45 (6%)	19	18

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	100	ILE
4	A	16	LYS
4	E	113	LEU
4	E	120	LEU
4	A	38	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	164	GLN
4	E	61	GLN
4	A	70	GLN
2	C	27	HIS
2	C	85	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
6	WYL	B	302	-	75,80,80	0.49	0	91,116,116	0.53	1 (1%)
7	GDP	A	201	8	29,30,30	1.17	2 (6%)	45,47,47	1.76	7 (15%)
6	WYL	E	201	-	75,80,80	0.60	2 (2%)	91,116,116	0.48	1 (1%)
7	GDP	E	202	8	29,30,30	1.21	4 (13%)	45,47,47	1.70	6 (13%)
5	PO4	B	301	-	4,4,4	0.80	0	6,6,6	0.44	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
6	WYL	E	201	-	-	4/53/97/97	0/9/9/9
7	GDP	E	202	8	-	4/16/32/32	0/3/3/3
6	WYL	B	302	-	-	5/53/97/97	0/9/9/9
7	GDP	A	201	8	-	1/16/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	201	GDP	C5-C4	3.16	1.47	1.38
7	E	202	GDP	C5-C4	2.94	1.46	1.38
7	E	202	GDP	C6-N1	-2.80	1.33	1.38
6	E	201	WYL	C20-N19	2.62	1.49	1.46
7	A	201	GDP	C6-N1	-2.45	1.34	1.38

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	201	GDP	C5-C4-N3	-5.99	118.86	128.39
7	E	202	GDP	C5-C4-N3	-5.61	119.47	128.39
7	A	201	GDP	C2-N3-C4	4.89	120.73	112.30
7	E	202	GDP	C2-N3-C4	4.69	120.38	112.30
7	A	201	GDP	N9-C4-N3	4.43	134.82	125.95

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

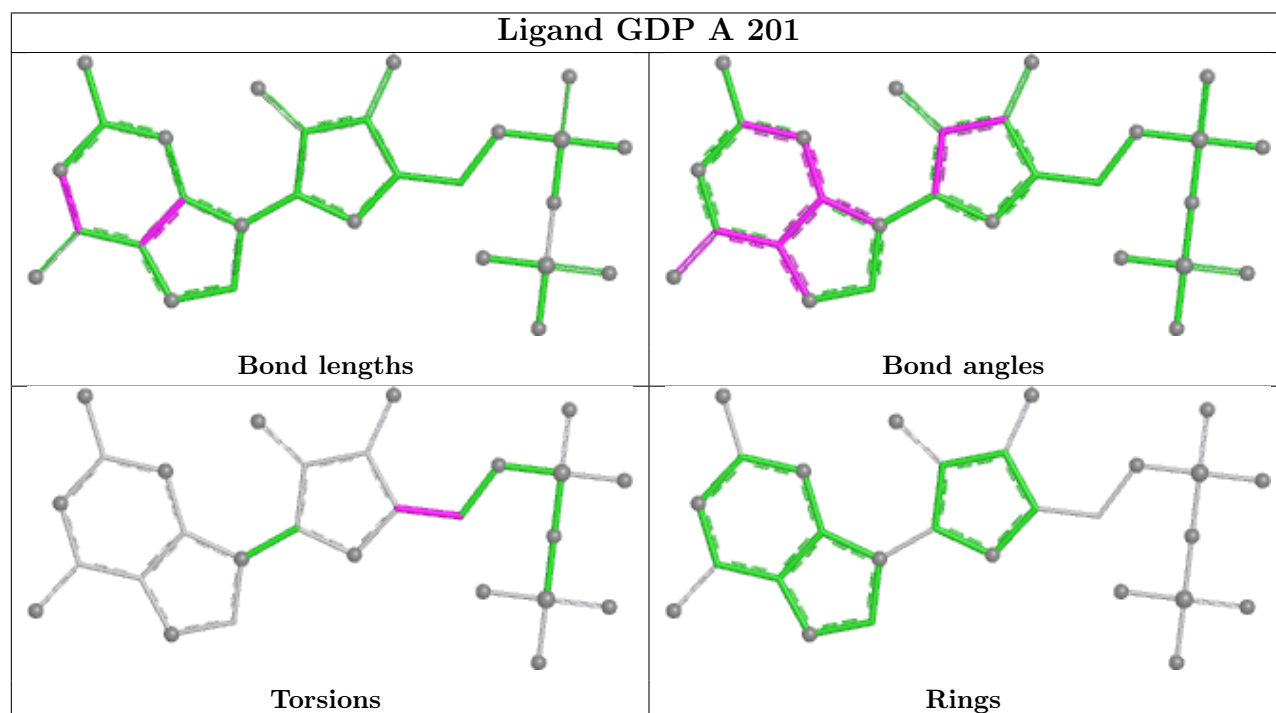
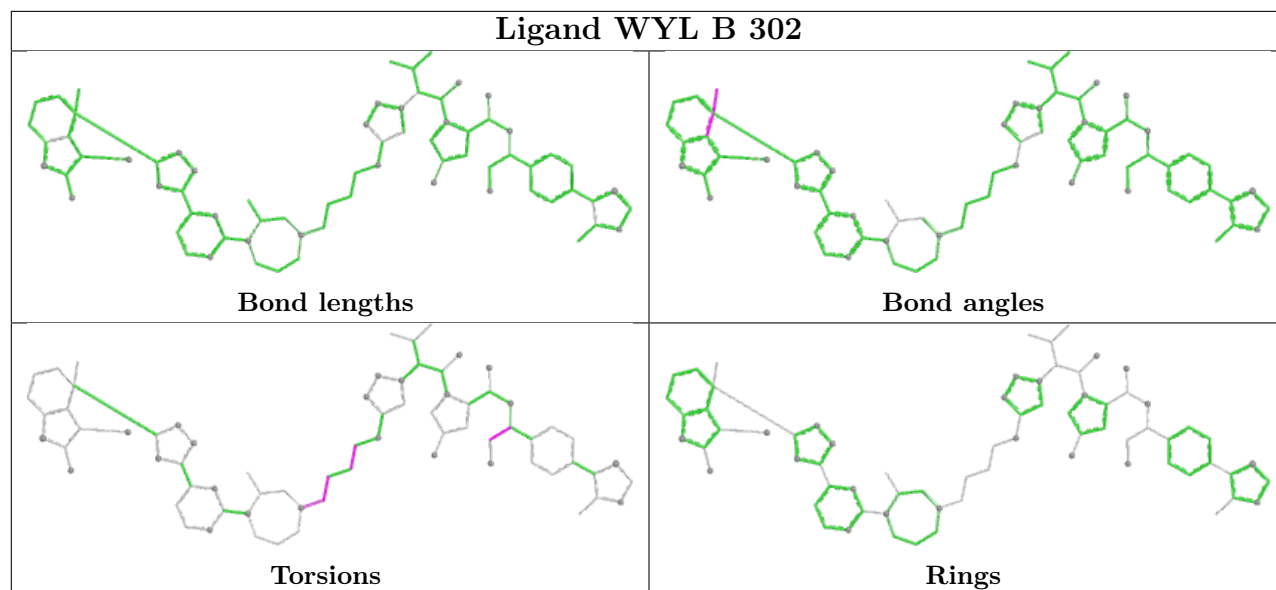
Mol	Chain	Res	Type	Atoms
6	B	302	WYL	O58-C59-C60-C63
6	B	302	WYL	O58-C59-C60-N53
6	E	201	WYL	O58-C59-C60-C63
6	E	201	WYL	O58-C59-C60-N53
7	E	202	GDP	C5'-O5'-PA-O3A

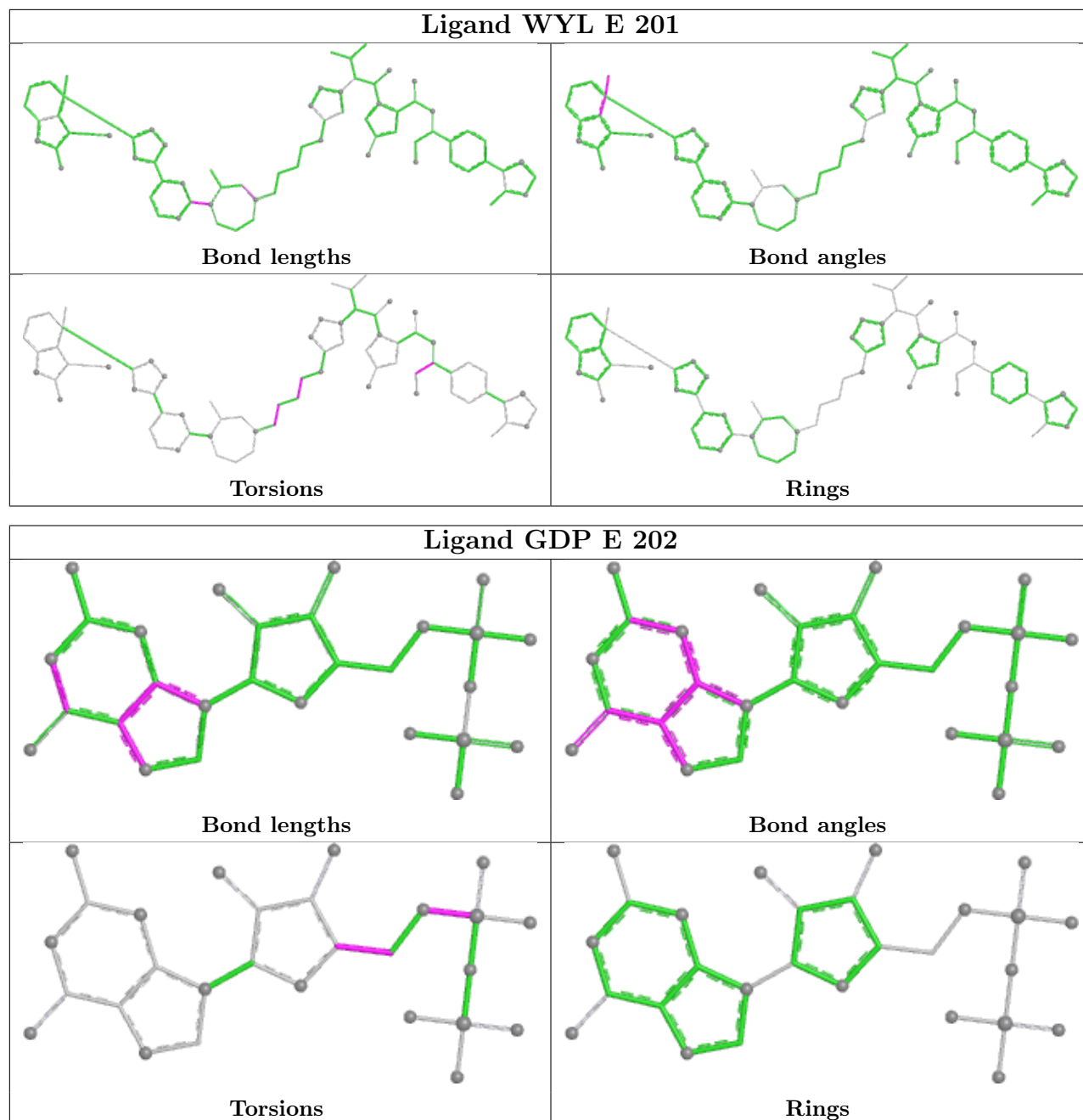
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	201	GDP	1	0
6	E	201	WYL	1	0
7	E	202	GDP	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.





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	D	102/104 (98%)	1.01	14 (13%)	6 6	26, 58, 86, 117	0
1	H	103/104 (99%)	1.21	20 (19%)	3 2	31, 70, 107, 149	0
2	C	88/97 (90%)	0.50	7 (7%)	18 16	19, 40, 70, 88	0
2	G	88/97 (90%)	0.93	12 (13%)	7 6	24, 50, 87, 122	0
3	B	147/213 (69%)	0.36	5 (3%)	48 48	16, 36, 72, 92	0
3	F	144/213 (67%)	0.41	4 (2%)	55 55	16, 37, 66, 104	0
4	A	155/188 (82%)	2.64	97 (62%)	0 0	40, 92, 134, 170	0
4	E	159/188 (84%)	2.56	101 (63%)	0 0	36, 79, 119, 145	0
All	All	986/1204 (81%)	1.30	260 (26%)	1 1	16, 57, 111, 170	0

The worst 5 of 260 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	156	PHE	9.1
4	A	155	ALA	8.3
4	E	20	THR	8.0
3	F	140	LEU	8.0
4	A	6	LEU	7.4

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](#)

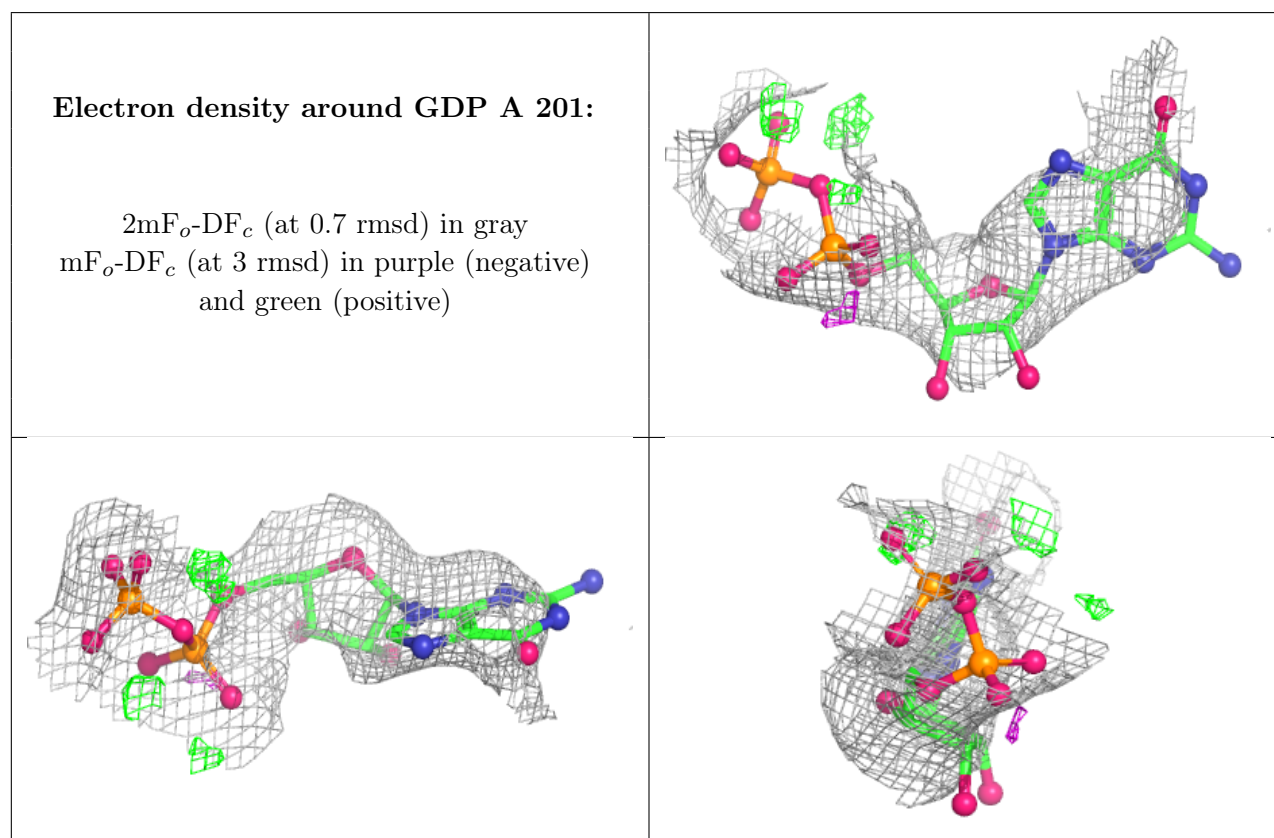
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

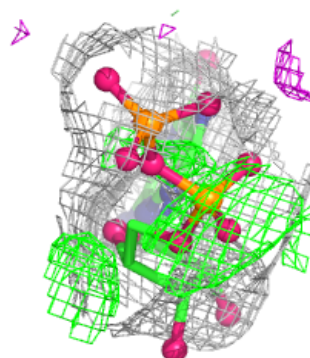
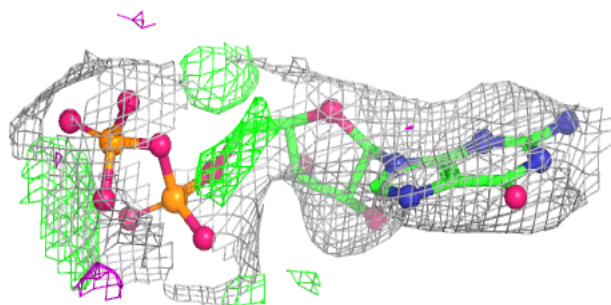
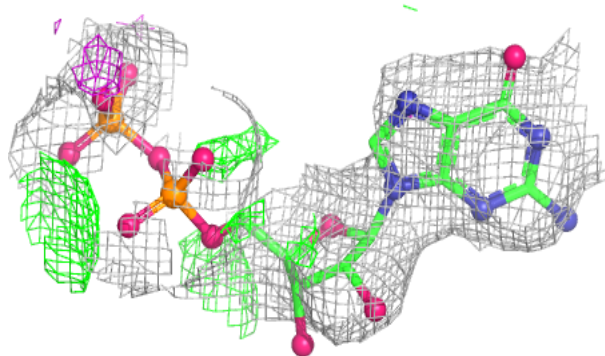
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GDP	A	201	28/28	0.73	0.14	89,105,114,119	0
7	GDP	E	202	28/28	0.75	0.16	63,88,99,104	0
8	MG	E	203	1/1	0.76	0.12	59,59,59,59	0
5	PO4	B	301	5/5	0.86	0.30	27,27,27,27	0
8	MG	A	202	1/1	0.91	0.13	65,65,65,65	0
6	WYL	E	201	72/72	0.92	0.10	20,39,59,72	0
6	WYL	B	302	72/72	0.95	0.09	14,36,64,72	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.



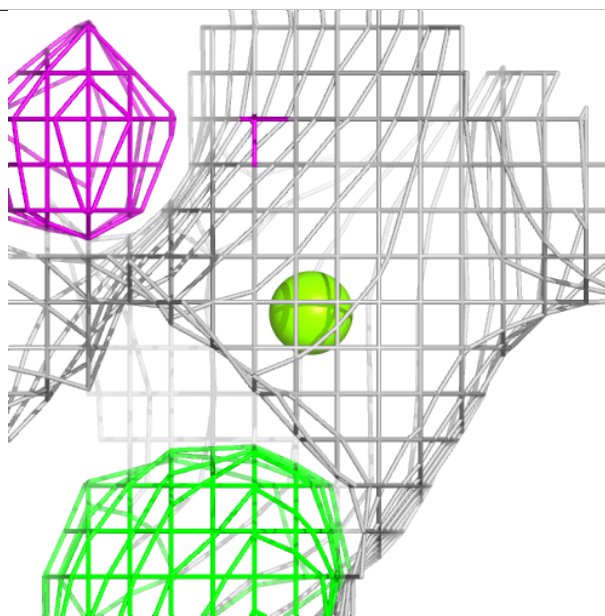
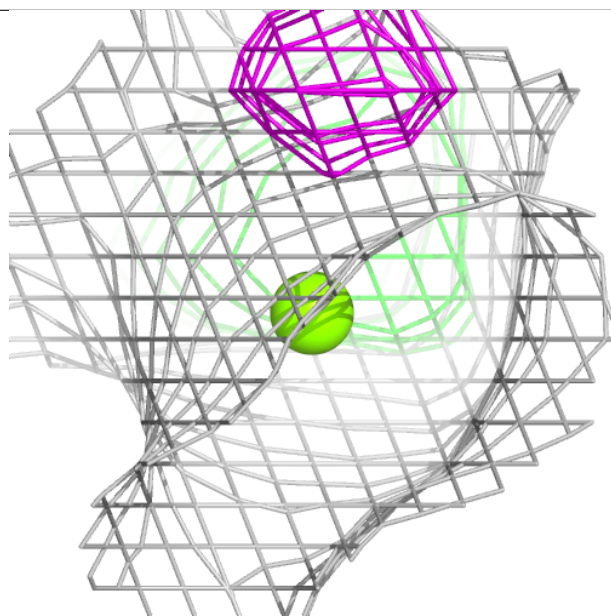
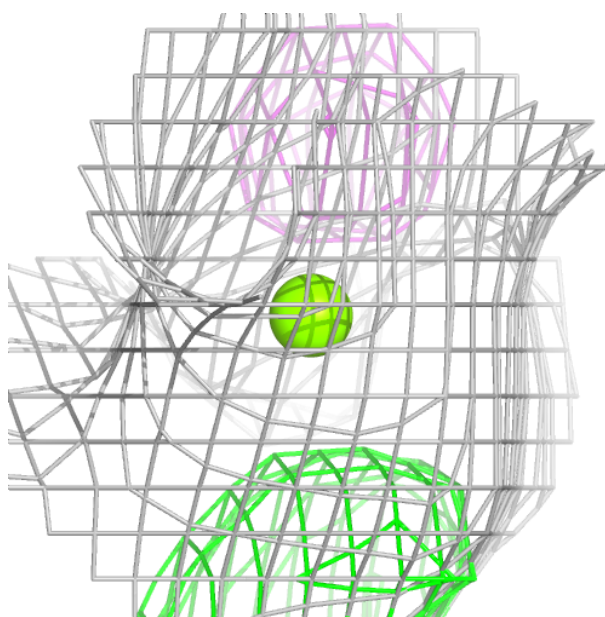
Electron density around GDP E 202:

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



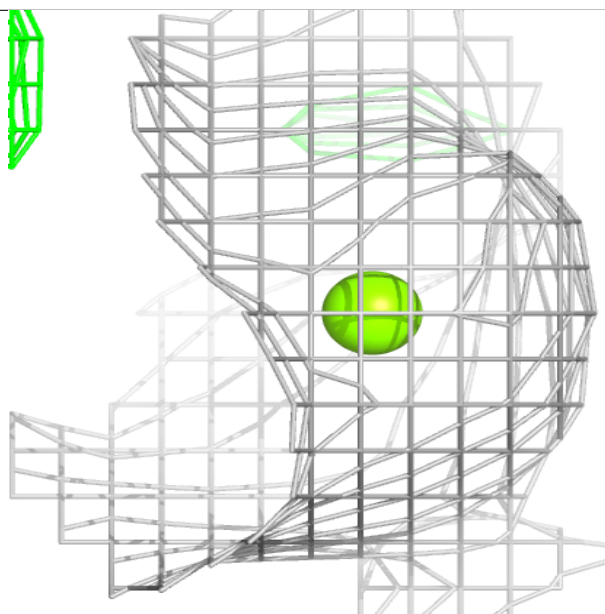
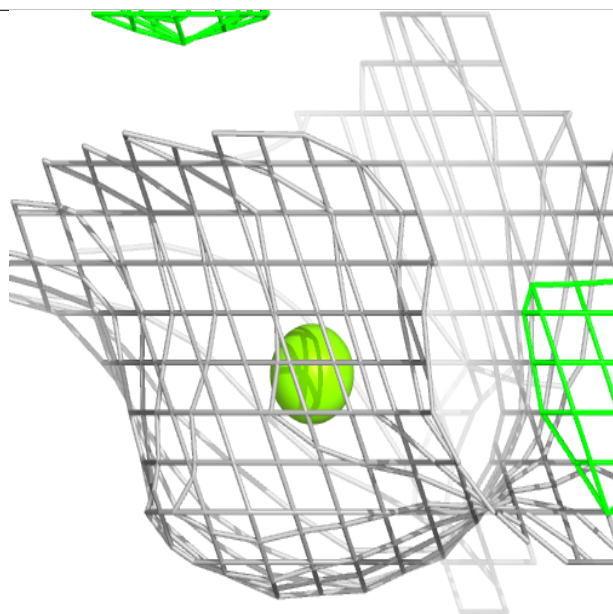
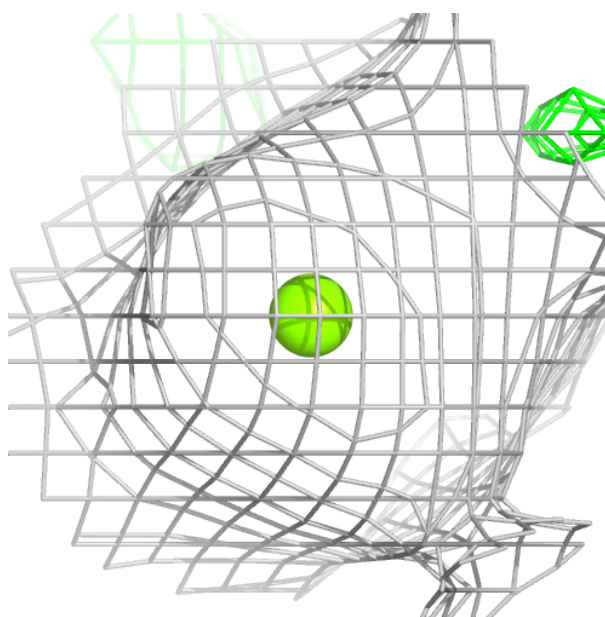
Electron density around MG E 203:

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



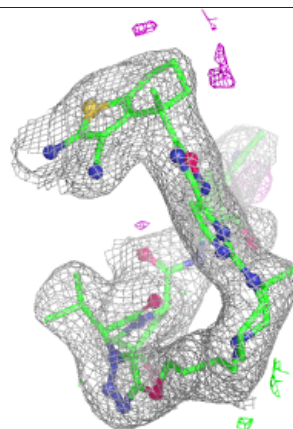
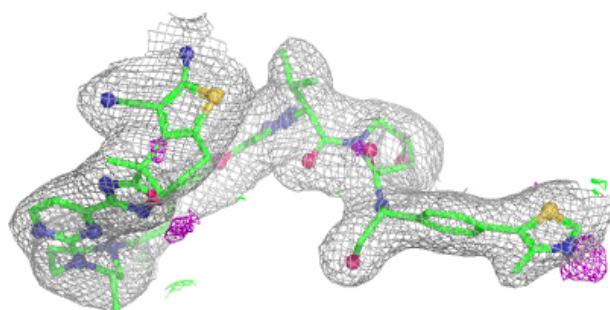
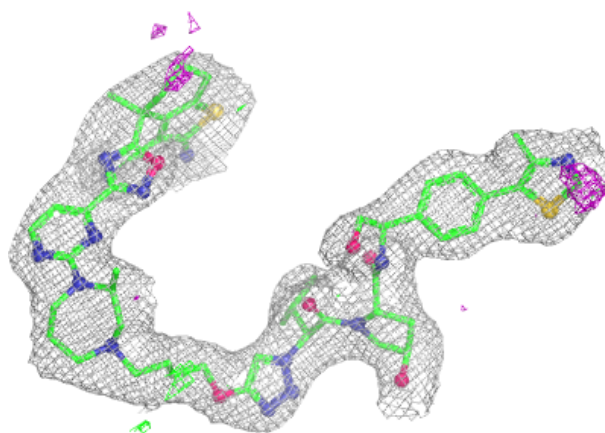
Electron density around MG A 202:

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

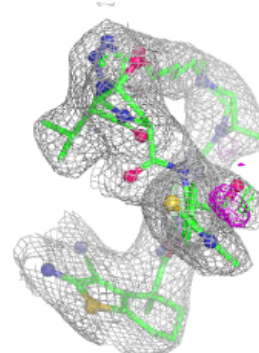
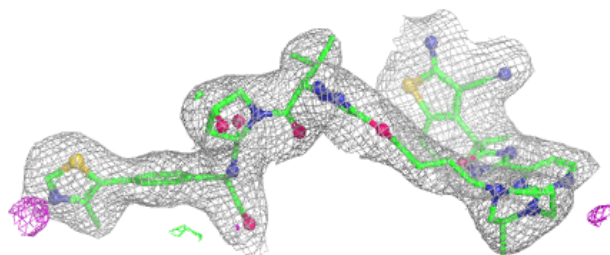
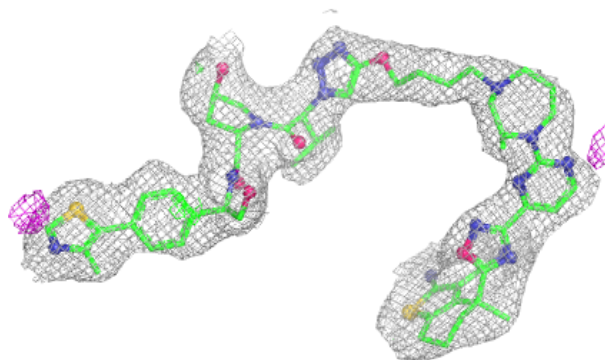


Electron density around WYL E 201:

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

**Electron density around WYL B 302:**

$2mF_o-DF_c$ (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.