Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2025 – 12:18 pm GMT

PDB ID	:	8QEG
Title	:	Crystal structure of the G11 protein heterotrimer bound to YM-254890 inhibitor
Authors	:	Muehle, J.; Rodrigues, M.J.; Guixa-Gonzalez, R.; Deupi, X.; Schertler, G.F.X.
Deposited on	:	2023-08-31
Resolution	:	1.70 Å(reported)

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

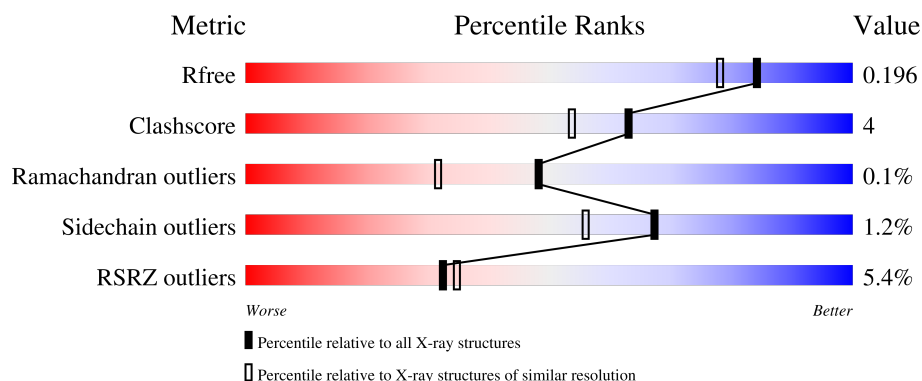|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 1.70 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	Percentile Ranks	Value
Rfree		0.196
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		1.2%
RSRZ outliers		5.4%

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}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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 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	352	4% — 88% — 7% ··
2	B	344	4% — 88% — 8% 5%
3	G	71	17% — 75% — 6% · 18%

2 Entry composition ⓘ

There are 14 unique types of molecules in this entry. The entry contains 6952 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 Guanine nucleotide-binding protein subunit alpha-11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2979	1897	514	556	12	0	24	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	-	expression tag	UNP P29992
A	9	CYS	-	expression tag	UNP P29992
A	10	THR	-	expression tag	UNP P29992
A	11	LEU	-	expression tag	UNP P29992
A	12	SER	-	expression tag	UNP P29992
A	13	ALA	-	expression tag	UNP P29992
A	14	GLU	-	expression tag	UNP P29992
A	15	ASP	-	expression tag	UNP P29992
A	16	LYS	-	expression tag	UNP P29992
A	17	ALA	-	expression tag	UNP P29992
A	18	ALA	-	expression tag	UNP P29992
A	19	VAL	-	expression tag	UNP P29992
A	20	GLU	-	expression tag	UNP P29992
A	21	ARG	-	expression tag	UNP P29992
A	22	SER	-	expression tag	UNP P29992
A	23	LYS	-	expression tag	UNP P29992
A	24	MET	-	expression tag	UNP P29992
A	25	ILE	-	expression tag	UNP P29992
A	26	ASP	-	expression tag	UNP P29992
A	27	ARG	-	expression tag	UNP P29992
A	28	ASN	-	expression tag	UNP P29992
A	29	LEU	-	expression tag	UNP P29992
A	30	ARG	-	expression tag	UNP P29992
A	31	GLU	-	expression tag	UNP P29992
A	32	ASP	-	expression tag	UNP P29992
A	33	GLY	-	expression tag	UNP P29992
A	34	GLU	-	expression tag	UNP P29992

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Chain	Residue	Modelled	Actual	Comment	Reference
A	35	LYS	-	expression tag	UNP P29992

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	328	2593	1600	466	503	24	0	14	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	58	442	282	73	84	3	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	69	SER	CYS	engineered mutation	UNP P59768

- Molecule 4 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
			Total	C	N	O	P		
4	A	1	28	10	5	11	2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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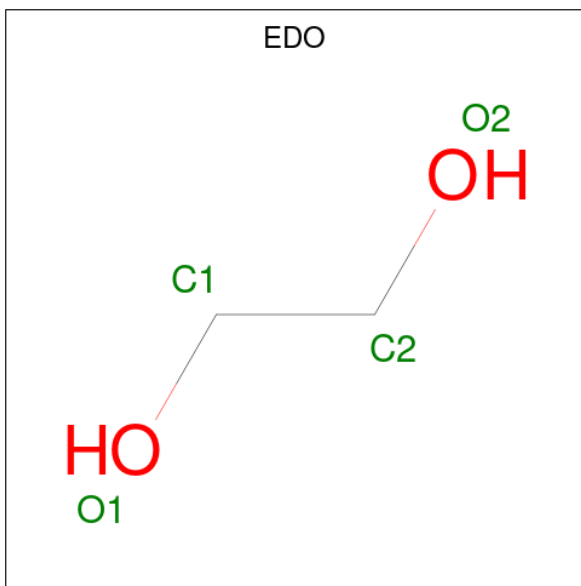
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0

- Molecule 6 is N-METHYL-ALPHA-BETA-DEHYDROALANINE (three-letter code: DAM) (formula: $C_4H_7NO_2$) (labeled as "Ligand of Interest" by depositor).
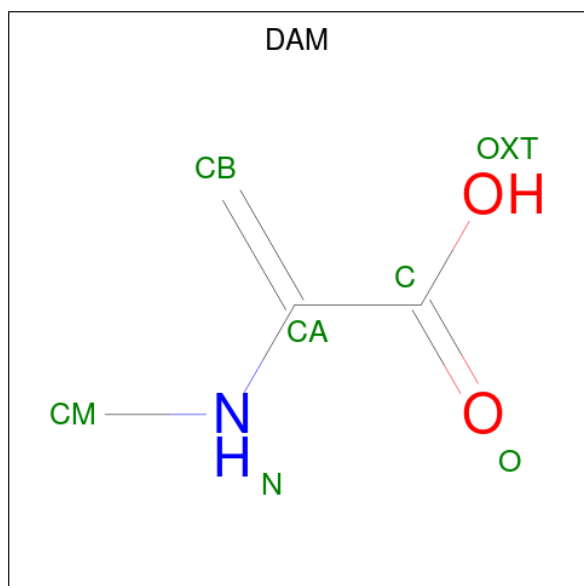
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 6	C 4	N 1	O 1	0	0

- Molecule 7 is (2R)-2-hydroxy-3-phenylpropanoic acid (three-letter code: HF2) (formula: $C_9H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).

HF2
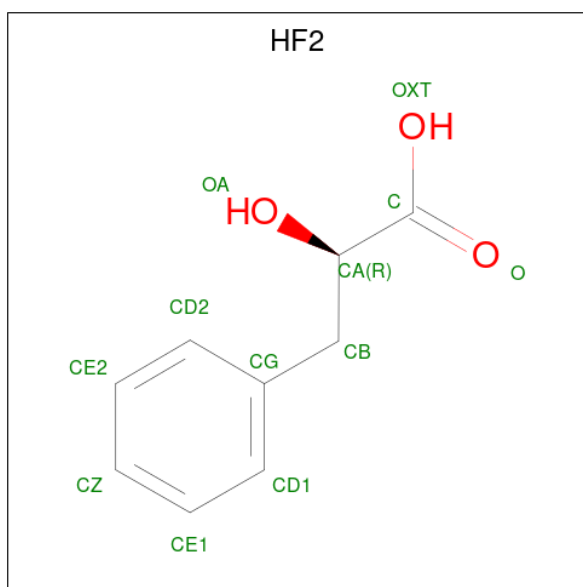
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 11	C 9	O 2	0	0

- Molecule 8 is N-METHYLCARBONYLTHREONINE (three-letter code: THC) (formula: $C_6H_{11}NO_4$) (labeled as "Ligand of Interest" by depositor).


THC
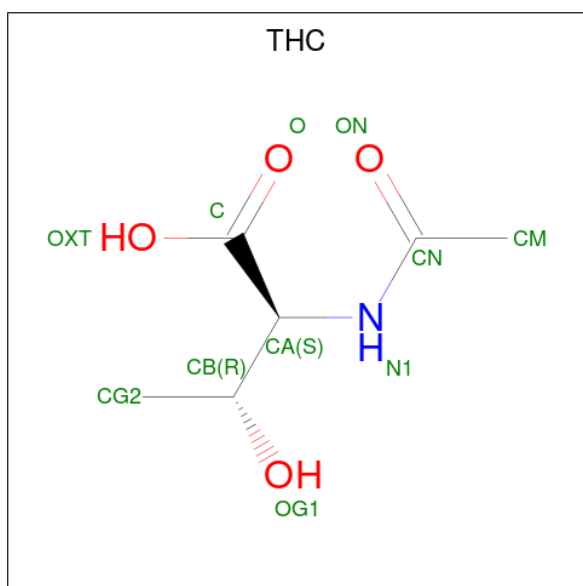
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 10	C 6	N 1	O 3	0	0

- Molecule 9 is N,O-dimethyl-L-threonine (three-letter code: OTH) (formula: $C_6H_{13}NO_3$) (labeled as "Ligand of Interest" by depositor).
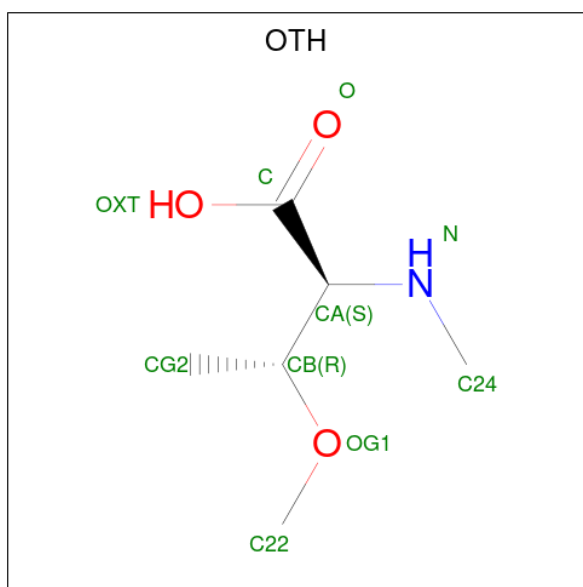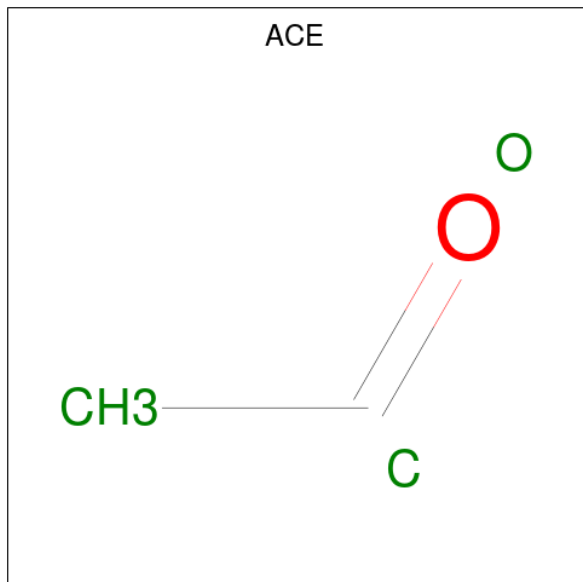
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total 9	C 6	N 1	O 2	0	0

- Molecule 10 is (2S,3R)-2-amino-3-hydroxy-4-methylpentanoic acid (three-letter code: HL2) (formula: $C_6H_{13}NO_3$) (labeled as "Ligand of Interest" by depositor).
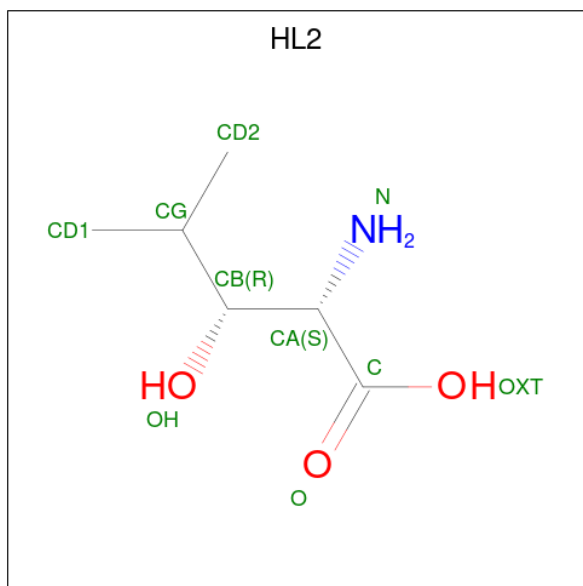
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total 9	C 6	N 1	O 2	0	0
10	A	1	Total 15	C 11	N 1	O 3	0	1

- Molecule 11 is N-methyl-L-alanine (three-letter code: MAA) (formula: $C_4H_9NO_2$) (labeled as "Ligand of Interest" by depositor).
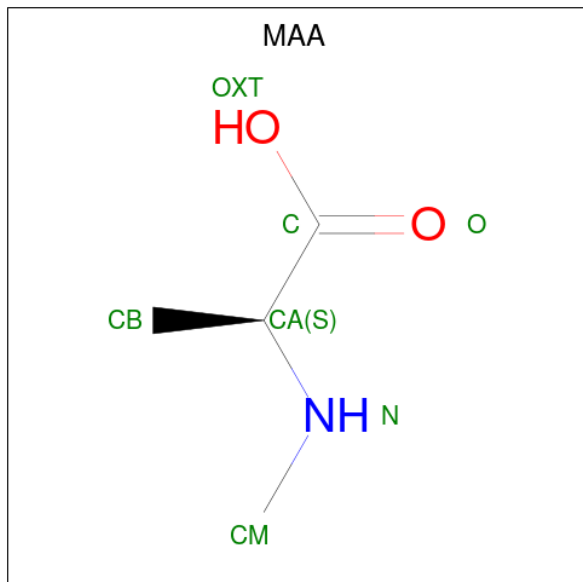
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total 6	C 4	N 1	O 1	0	0

- Molecule 12 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$) (labeled as "Ligand of Interest" by depositor).
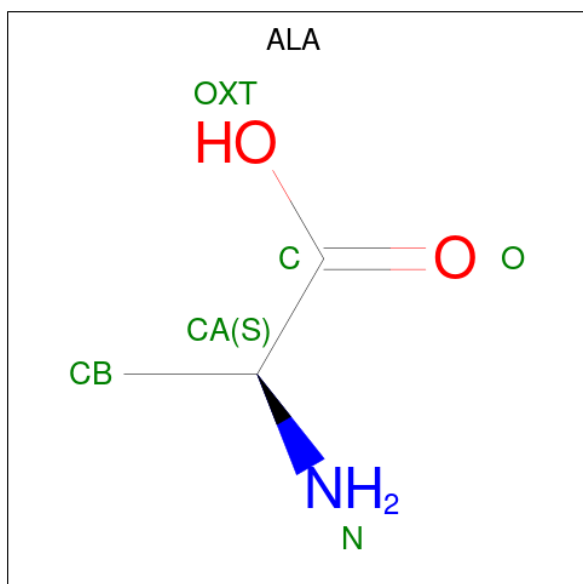
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total 5	C 3	N 1	O 1	0	0

- Molecule 13 is ACETYL GROUP (three-letter code: ACE) (formula: C_2H_4O) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total C O 3 2 1			0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	438	Total O 438 438		0	5
14	B	328	Total O 330 330		0	5
14	G	36	Total O 36 36		0	0

3 Residue-property plots ⓘ

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.
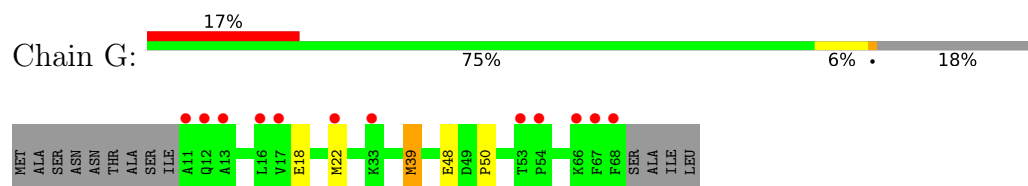
• Molecule 1: Guanine nucleotide-binding protein subunit alpha-11

Chain A:
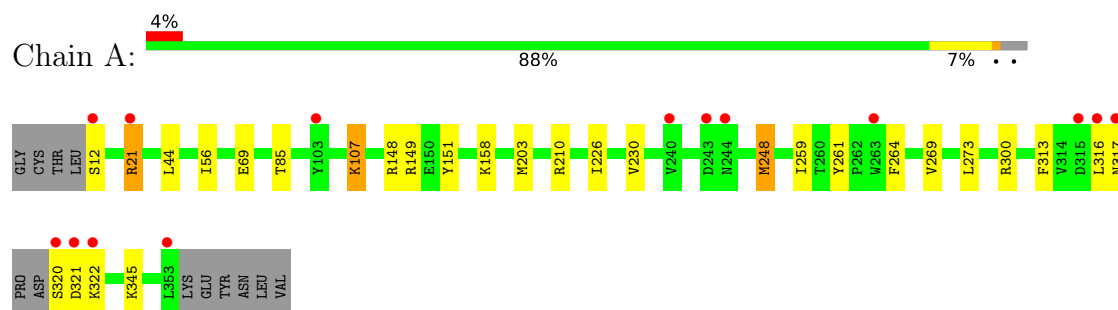
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:
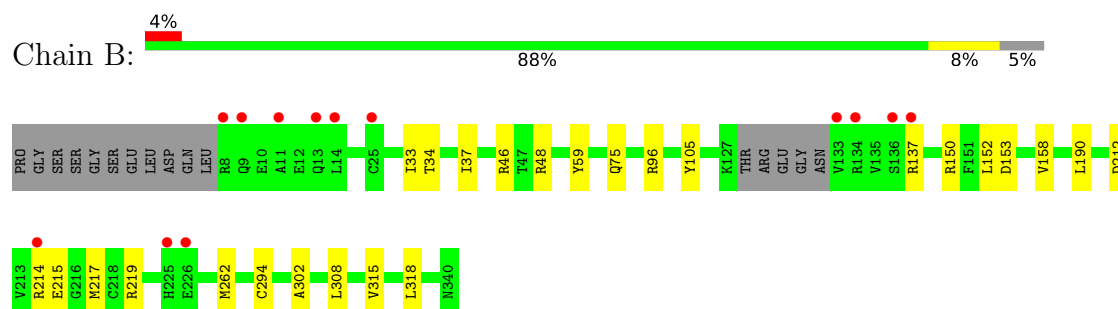
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.60Å　　102.53Å　　154.00Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	59.25　–　1.70 59.25　–　1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.25-1.70) 100.0 (59.25-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.160　,　0.188 0.172　,　0.196	Depositor DCC
R_{free} test set	6216 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6952	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: HF2, GDP, ACE, OTH, HL2, THC, EDO, MAA, DAM

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	0.53	0/3038	0.82	3/4093 (0.1%)
2	B	0.50	0/2639	0.83	0/3579
3	G	0.35	0/450	0.63	0/610
All	All	0.51	0/6127	0.81	3/8282 (0.0%)

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	A	0	1
2	B	0	2
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	149	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	A	248	MET	CG-SD-CE	-6.66	89.54	100.20
1	A	149	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	ARG	Sidechain
2	B	137	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	B	150	ARG	Sidechain

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	A	2979	0	2961	23	0
2	B	2593	0	2468	19	0
3	G	442	0	418	6	0
4	A	28	0	12	0	0
5	A	20	0	30	1	0
5	B	12	0	18	1	0
6	A	6	0	5	1	0
7	A	11	0	8	0	0
8	A	10	0	4	0	0
9	A	9	0	11	0	0
10	A	24	0	29	1	0
11	B	6	0	7	1	0
12	B	5	0	4	1	0
13	B	3	0	3	0	0
14	A	438	0	0	6	0
14	B	330	0	0	3	0
14	G	36	0	0	0	0
All	All	6952	0	5978	47	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 4.

All (47) 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)
2:B:212:ASP:OD2	2:B:219[B]:ARG:NH2	2.17	0.76
2:B:33:ILE:HG22	3:G:39:MET:CE	2.16	0.75
1:A:259:ILE:HD11	1:A:316:LEU:HD13	1.67	0.75
2:B:215:GLU:OE1	2:B:217:MET:CB	2.37	0.72
2:B:46[B]:ARG:HH21	2:B:48:ARG:HH22	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:ILE:HG22	3:G:39:MET:HE1	1.74	0.68
2:B:152:LEU:HD11	2:B:158[A]:VAL:HG23	1.80	0.63
1:A:56:ILE:HG22	6:A:407:DAM:HM3	1.84	0.60
1:A:230[B]:VAL:CG1	1:A:273[B]:LEU:CD2	2.80	0.58
1:A:230[B]:VAL:CG1	1:A:273[B]:LEU:HD23	2.35	0.57
5:B:403:EDO:O1	14:B:501:HOH:O	2.18	0.56
2:B:153:ASP:OD2	14:B:502:HOH:O	2.18	0.55
1:A:21[A]:ARG:HD2	14:A:725:HOH:O	2.08	0.54
1:A:259:ILE:CD1	1:A:316:LEU:HD13	2.38	0.53
2:B:212:ASP:HB3	2:B:215:GLU:HG2	1.92	0.52
2:B:152:LEU:CD1	2:B:158[A]:VAL:HG23	2.41	0.51
1:A:261:TYR:CD1	5:A:405:EDO:H21	2.45	0.50
1:A:85[A]:THR:HG22	14:A:717:HOH:O	2.10	0.50
2:B:318:LEU:C	2:B:318:LEU:HD12	2.32	0.49
2:B:34:THR:HG22	3:G:39:MET:HE2	1.94	0.49
3:G:48:GLU:O	3:G:50:PRO:HD3	2.13	0.48
2:B:294[B]:CYS:HB2	2:B:308:LEU:HB2	1.96	0.47
3:G:18:GLU:O	3:G:22:MET:HG2	2.14	0.47
11:B:404:MAA:C	12:B:405:ALA:O	2.63	0.47
1:A:269:VAL:HG23	1:A:322[A]:LYS:HE3	1.96	0.47
2:B:262[A]:MET:SD	2:B:302:ALA:HB2	2.54	0.46
1:A:300[A]:ARG:NH2	14:A:501[A]:HOH:O	2.33	0.46
1:A:230[A]:VAL:HG21	1:A:313:PHE:CZ	2.51	0.46
2:B:158[A]:VAL:HG12	2:B:190:LEU:HD22	1.98	0.45
1:A:226:ILE:HD11	1:A:264:PHE:CG	2.51	0.45
10:A:412[A]:HL2:HD2A	2:B:96[A]:ARG:NH2	2.32	0.45
2:B:59:TYR:CE1	2:B:75:GLN:HG3	2.53	0.44
1:A:44[B]:LEU:HD21	1:A:203:MET:HE3	1.99	0.44
1:A:107:LYS:HB2	14:A:848:HOH:O	2.17	0.44
1:A:316:LEU:O	1:A:317:ASN:CB	2.66	0.44
1:A:320:SER:C	1:A:322[A]:LYS:H	2.21	0.43
1:A:44[B]:LEU:HD21	1:A:203:MET:CE	2.49	0.43
1:A:320:SER:C	1:A:322[B]:LYS:H	2.22	0.43
2:B:214[B]:ARG:NH1	14:B:509:HOH:O	2.50	0.42
2:B:294[B]:CYS:SG	2:B:315:VAL:HG11	2.59	0.42
1:A:148:ARG:HA	1:A:151:TYR:CE1	2.55	0.42
3:G:39:MET:HE2	3:G:39:MET:HB2	1.92	0.42
1:A:203:MET:HE3	1:A:203:MET:HB3	1.74	0.41
1:A:230[B]:VAL:CG1	1:A:273[B]:LEU:HD22	2.50	0.41
1:A:158[B]:LYS:HE2	14:A:811:HOH:O	2.21	0.41
1:A:69[B]:GLU:HG2	14:A:720:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:THR:O	2:B:37:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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	360/352 (102%)	354 (98%)	5 (1%)	1 (0%)	37	23
2	B	338/344 (98%)	325 (96%)	13 (4%)	0	100	100
3	G	57/71 (80%)	57 (100%)	0	0	100	100
All	All	755/767 (98%)	736 (98%)	18 (2%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	ASP

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	322/317 (102%)	316 (98%)	6 (2%)	52	37
2	B	278/285 (98%)	277 (100%)	1 (0%)	89	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	42/58 (72%)	41 (98%)	1 (2%)	44	27
All	All	642/660 (97%)	634 (99%)	8 (1%)	67	56

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	21[A]	ARG
1	A	21[B]	ARG
1	A	107	LYS
1	A	248	MET
1	A	345	LYS
2	B	105	TYR
3	G	39	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	GLN
1	A	350	GLN
2	B	155	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

19 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	#$|Z| > 2$
8	THC	A	409	9,7	8,9,10	0.48	0	9,11,13	1.03	1 (11%)
5	EDO	B	401	-	3,3,3	0.33	0	2,2,2	0.28	0
6	DAM	A	407	7,12	4,5,6	2.37	2 (50%)	3,5,7	2.24	2 (66%)
5	EDO	B	403	-	3,3,3	0.35	0	2,2,2	0.32	0
5	EDO	A	403	-	3,3,3	0.39	0	2,2,2	0.49	0
12	ALA	B	405	11,6	3,4,5	0.70	0	2,4,6	1.20	0
9	OTH	A	410	8,10	7,8,9	0.83	0	6,9,11	0.81	0
10	HL2	A	412[B]	-	7,8,9	0.80	0	7,10,12	1.02	0
13	ACE	B	406	10	1,2,2	0.17	0	1,1,1	0.46	0
10	HL2	A	412[A]	-	7,8,9	0.81	0	7,10,12	0.79	0
5	EDO	A	404	-	3,3,3	0.27	0	2,2,2	0.16	0
11	MAA	B	404	10,12	4,5,6	0.86	0	1,5,7	0.19	0
5	EDO	B	402	-	3,3,3	0.42	0	2,2,2	0.36	0
10	HL2	A	411	9,10,11	7,8,9	0.49	0	7,10,12	1.04	1 (14%)
5	EDO	A	402	-	3,3,3	0.09	0	2,2,2	0.83	0
5	EDO	A	406	-	3,3,3	0.29	0	2,2,2	0.32	0
7	HF2	A	408	8,6	10,11,12	0.60	0	12,13,15	0.80	1 (8%)
5	EDO	A	405	-	3,3,3	0.09	0	2,2,2	0.31	0
4	GDP	A	401	-	24,30,30	1.02	3 (12%)	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
5	EDO	A	406	-	-	1/1/1/1	-
9	OTH	A	410	8,10	-	4/7/10/12	-
10	HL2	A	411	9,10,11	-	0/9/10/12	-
10	HL2	A	412[B]	-	-	5/9/10/12	-
11	MAA	B	404	10,12	-	1/1/4/6	-
8	THC	A	409	9,7	-	0/8/10/12	-
5	EDO	B	401	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HL2	A	412[A]	-	-	1/9/10/12	-
6	DAM	A	407	7,12	-	0/0/4/6	-
5	EDO	B	403	-	-	0/1/1/1	-
7	HF2	A	408	8,6	-	0/5/6/8	0/1/1/1
5	EDO	A	405	-	-	0/1/1/1	-
4	GDP	A	401	-	-	2/12/32/32	0/3/3/3
5	EDO	A	403	-	-	1/1/1/1	-
5	EDO	B	402	-	-	1/1/1/1	-
5	EDO	A	404	-	-	0/1/1/1	-
5	EDO	A	402	-	-	1/1/1/1	-
12	ALA	B	405	11,6	-	0/0/2/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	407	DAM	O-C	3.35	1.29	1.22
6	A	407	DAM	C-CA	-3.33	1.39	1.45
4	A	401	GDP	C5-C6	-2.37	1.42	1.47
4	A	401	GDP	C6-N1	2.18	1.41	1.37
4	A	401	GDP	C8-N7	-2.17	1.31	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	407	DAM	O-C-CA	2.65	128.62	125.22
10	A	411	HL2	O-C-CA	-2.41	118.47	124.78
4	A	401	GDP	O6-C6-C5	2.33	128.93	124.37
8	A	409	THC	CA-N1-CN	-2.28	120.63	123.12
6	A	407	DAM	CB-CA-N	2.26	131.38	125.91
7	A	408	HF2	CB-CA-C	-2.21	107.26	111.53

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	410	OTH	CB-CA-N-C24
9	A	410	OTH	N-CA-CB-OG1
9	A	410	OTH	C-CA-CB-CG2
10	A	412[B]	HL2	O-C-CA-CB
10	A	412[B]	HL2	OH-CB-CG-CD2
5	A	406	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	401	EDO	O1-C1-C2-O2
9	A	410	OTH	N-CA-CB-CG2
10	A	412[B]	HL2	CA-CB-CG-CD2
4	A	401	GDP	PA-O3A-PB-O1B
5	B	402	EDO	O1-C1-C2-O2
10	A	412[B]	HL2	OH-CB-CG-CD1
4	A	401	GDP	PA-O3A-PB-O3B
10	A	412[B]	HL2	CA-CB-CG-CD1
5	A	403	EDO	O1-C1-C2-O2
11	B	404	MAA	CB-CA-N-CM
5	A	402	EDO	O1-C1-C2-O2
10	A	412[A]	HL2	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	407	DAM	1	0
5	B	403	EDO	1	0
12	B	405	ALA	1	0
10	A	412[A]	HL2	1	0
11	B	404	MAA	1	0
5	A	405	EDO	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 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 THC A 409

Bond lengths

Bond angles

Torsions

Rings

Ligand DAM A 407

Bond lengths

Bond angles

Torsions

Rings

Ligand ALA B 405

Bond lengths

Bond angles

Torsions

Rings

Ligand OTH A 410

Bond lengths

Bond angles

Torsions

Rings

Ligand HL2 A 412 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand ACE B 406

Bond lengths

Bond angles

Torsions

Rings

Ligand HL2 A 412 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand MAA B 404

Bond lengths

Bond angles

Torsions

Rings

Ligand HL2 A 411

Bond lengths

Bond angles

Torsions

Rings

Ligand HF2 A 408

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP A 401

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	340/352 (96%)	0.17	14 (4%)	42	45	12, 31, 54, 86	24 (7%)
2	B	328/344 (95%)	0.02	13 (3%)	43	46	12, 31, 65, 123	14 (4%)
3	G	58/71 (81%)	1.14	12 (20%)	3	2	29, 58, 96, 111	1 (1%)
All	All	726/767 (94%)	0.18	39 (5%)	32	35	12, 32, 68, 123	39 (5%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	LEU	6.9
3	G	11	ALA	6.5
1	A	317	ASN	4.8
2	B	8	ARG	4.7
3	G	68	PHE	4.2
1	A	321	ASP	4.1
1	A	240	VAL	3.9
2	B	214[A]	ARG	3.9
1	A	320	SER	3.7
2	B	136	SER	3.5
2	B	134	ARG	3.4
3	G	53	THR	3.3
2	B	9	GLN	3.3
3	G	67	PHE	3.3
1	A	243	ASP	3.1
3	G	66	LYS	3.1
1	A	316	LEU	3.1
3	G	16	LEU	3.0
1	A	103	TYR	2.9
1	A	263	TRP	2.9
3	G	54	PRO	2.9
3	G	33[A]	LYS	2.9
2	B	11	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
3	G	13	ALA	2.9
3	G	12	GLN	2.8
3	G	22	MET	2.8
1	A	315	ASP	2.6
1	A	244	ASN	2.6
2	B	137	ARG	2.5
1	A	12	SER	2.5
3	G	17	VAL	2.5
1	A	322[A]	LYS	2.4
2	B	14	LEU	2.3
2	B	25	CYS	2.3
2	B	225	HIS	2.3
2	B	133	VAL	2.3
1	A	21[A]	ARG	2.2
2	B	13	GLN	2.2
2	B	226	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
5	EDO	A	406	4/4	0.81	0.23	53,65,71,72	0
5	EDO	A	405	4/4	0.83	0.20	66,66,67,69	0
5	EDO	A	403	4/4	0.83	0.15	33,39,42,51	0
5	EDO	B	402	4/4	0.88	0.15	50,56,57,59	0
5	EDO	B	401	4/4	0.90	0.17	49,52,53,68	0
5	EDO	A	404	4/4	0.91	0.17	55,59,61,64	0
5	EDO	B	403	4/4	0.91	0.14	33,47,51,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	402	4/4	0.97	0.08	27,29,33,34	0
7	HF2	A	408	11/12	0.97	0.05	23,24,27,29	0
6	DAM	A	407	6/7	0.98	0.06	25,25,26,27	0
8	THC	A	409	10/11	0.98	0.05	29,31,34,36	0
9	OTH	A	410	9/10	0.98	0.06	25,30,32,33	0
10	HL2	A	411	9/10	0.98	0.05	24,26,26,28	0
10	HL2	A	412[A]	9/10	0.98	0.05	24,27,28,28	6
10	HL2	A	412[B]	9/10	0.98	0.05	24,27,29,29	6
11	MAA	B	404	6/7	0.98	0.05	28,29,30,30	0
12	ALA	B	405	5/6	0.98	0.05	25,25,27,28	0
13	ACE	B	406	3/3	0.98	0.05	33,33,33,34	0
4	GDP	A	401	28/28	0.99	0.03	20,22,23,25	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 HF2 A 408:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
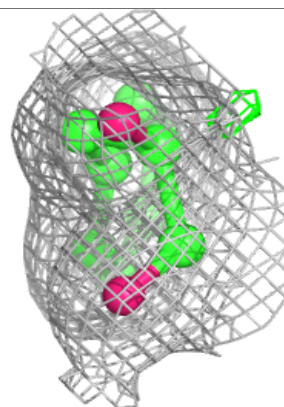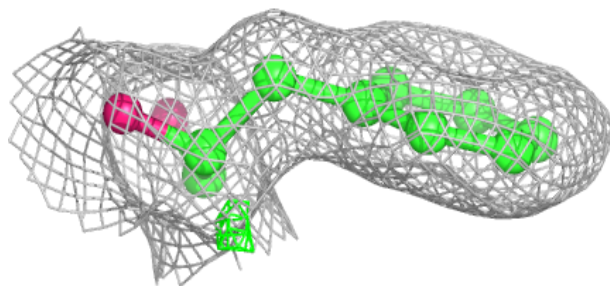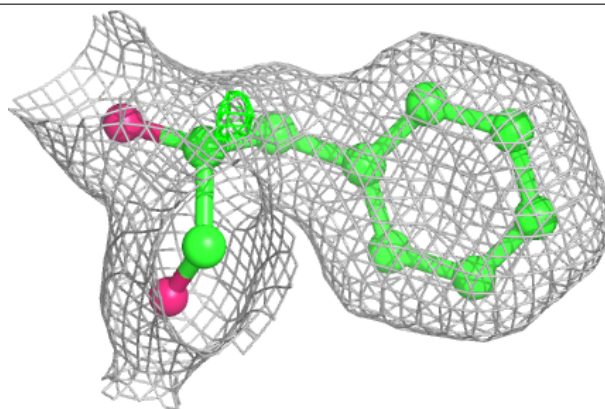
Electron density around DAM A 407:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
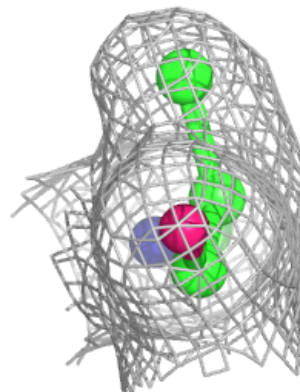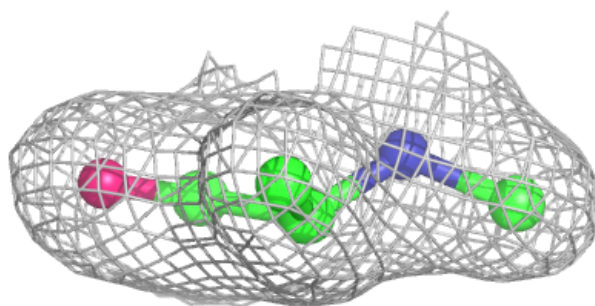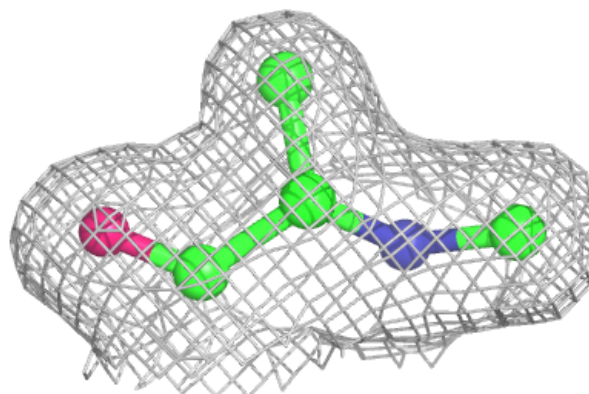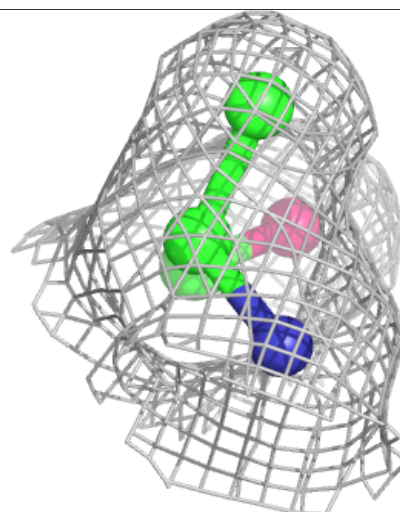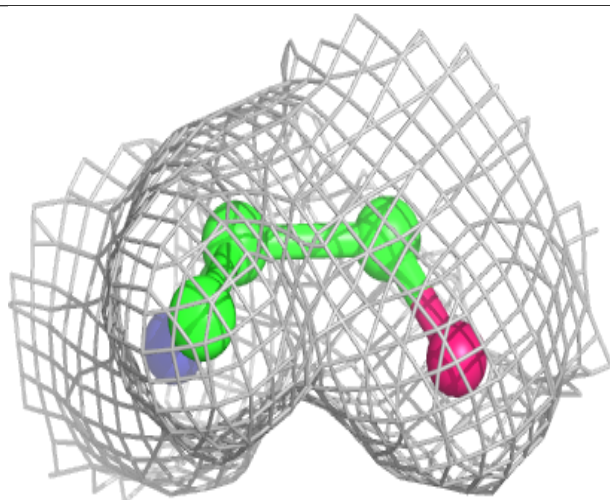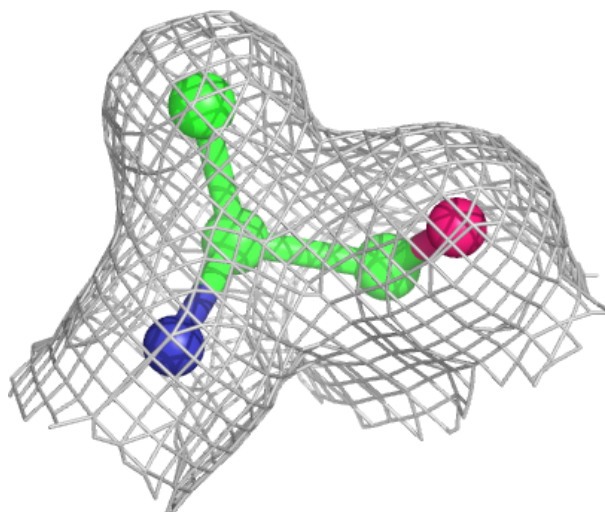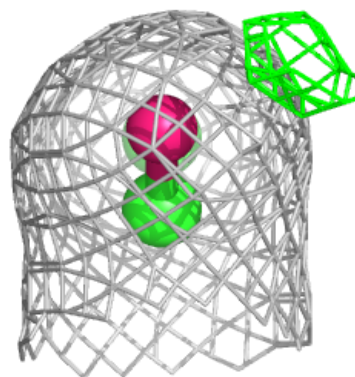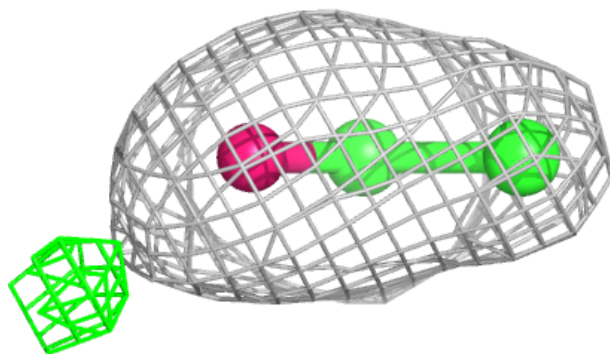mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
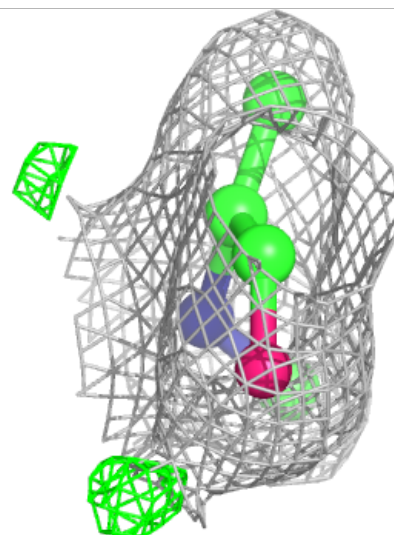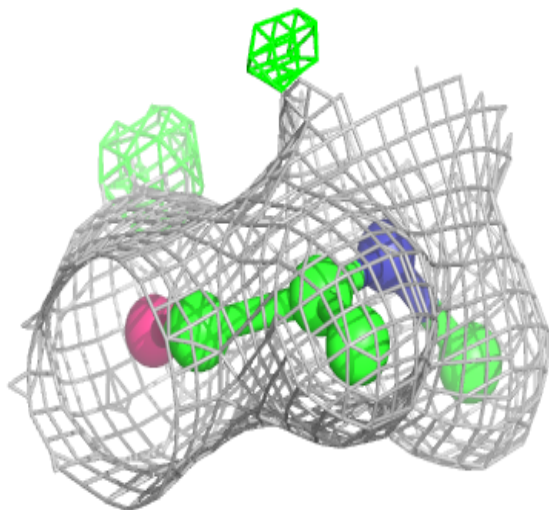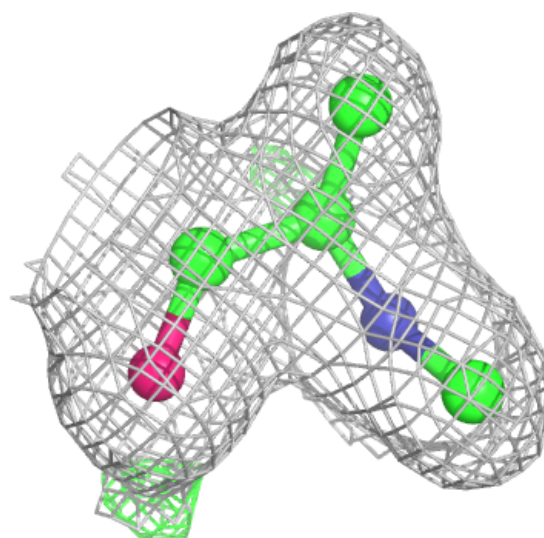
Electron density around THC A 409:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
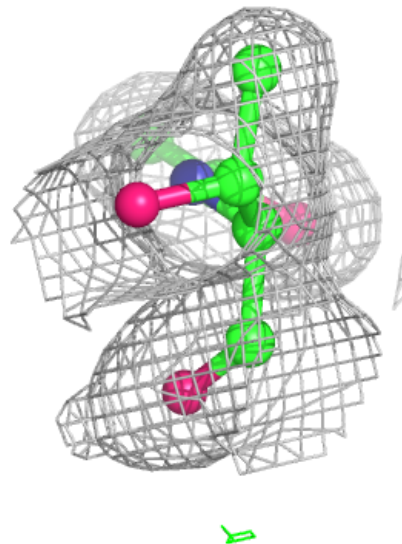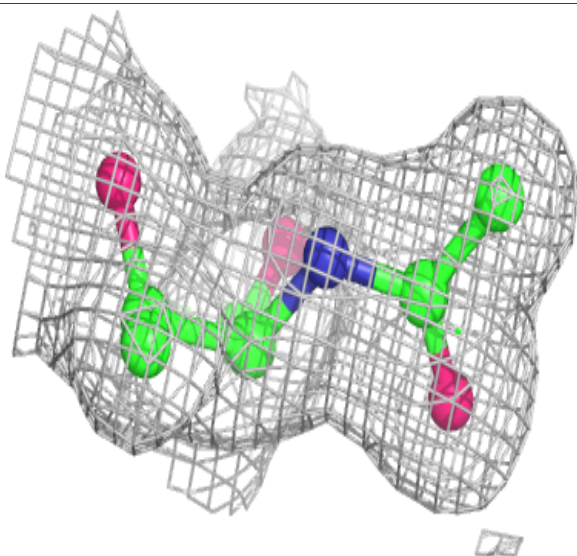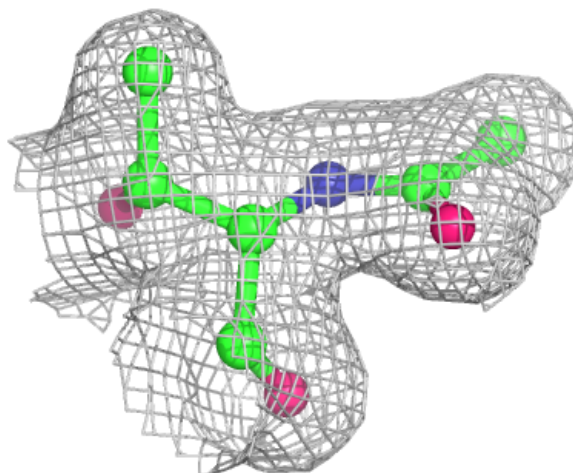
Electron density around OTH A 410:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
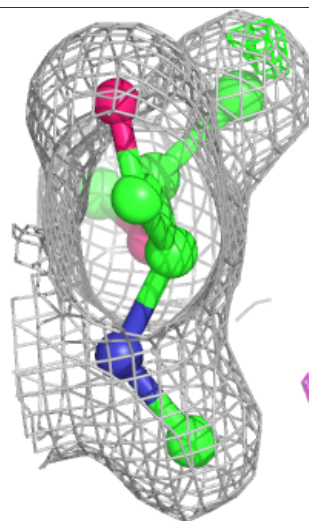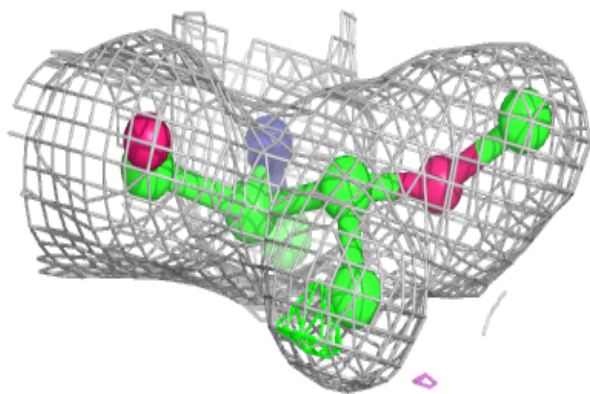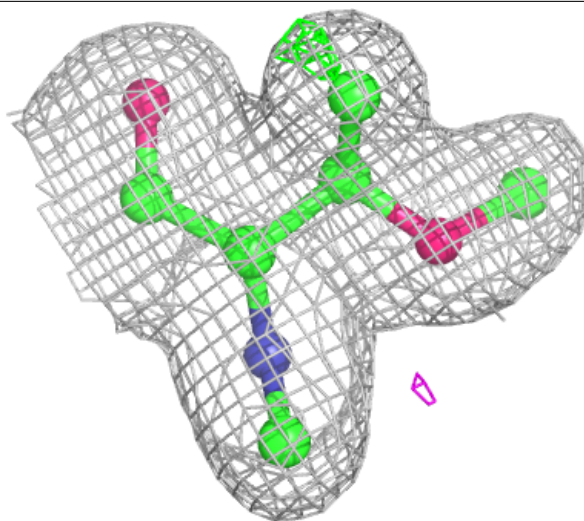
Electron density around HL2 A 411:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
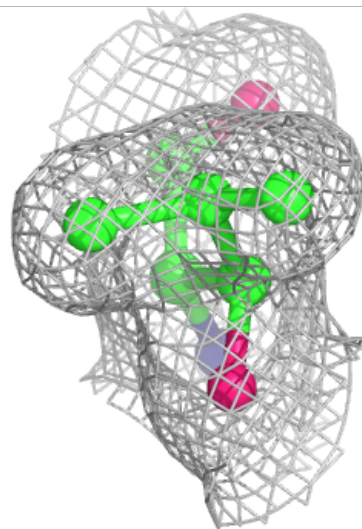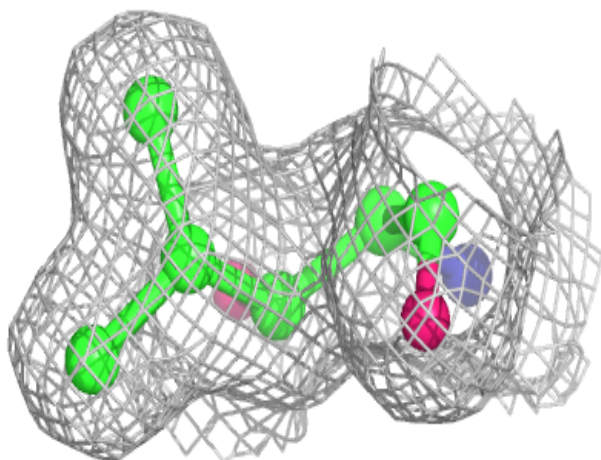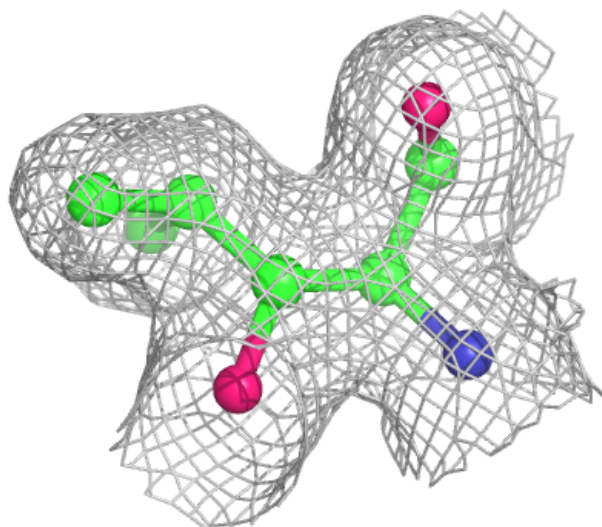
Electron density around HL2 A 412 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
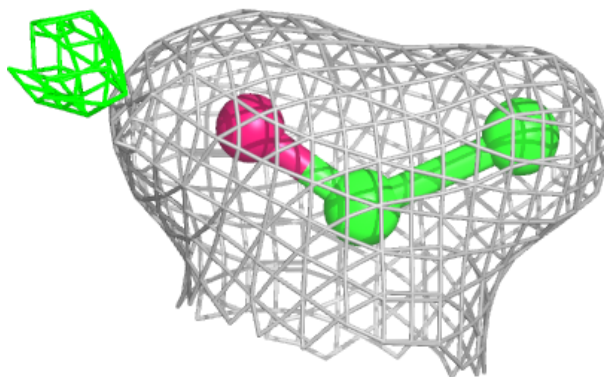mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
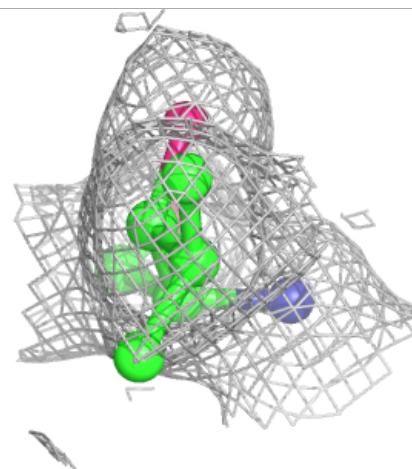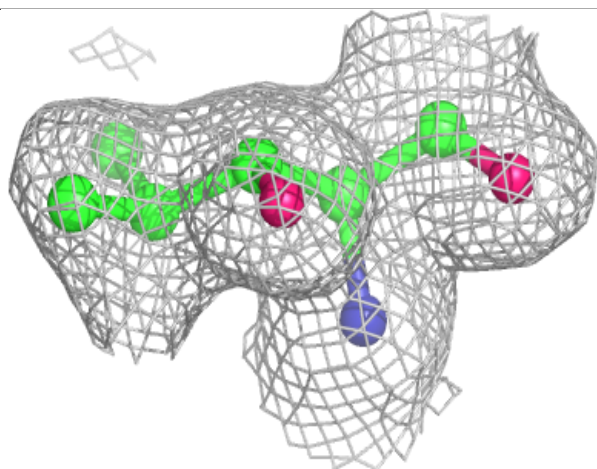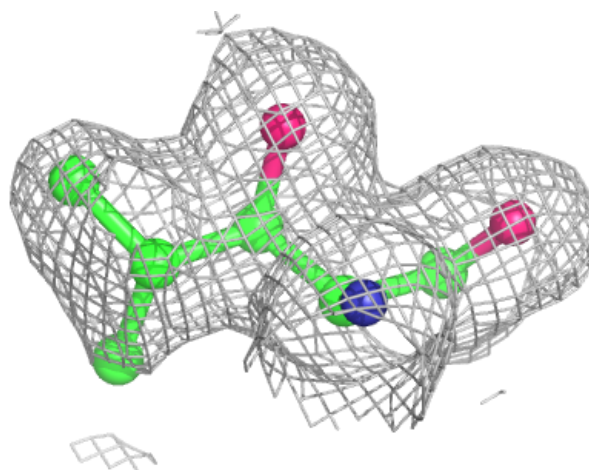
Electron density around HL2 A 412 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
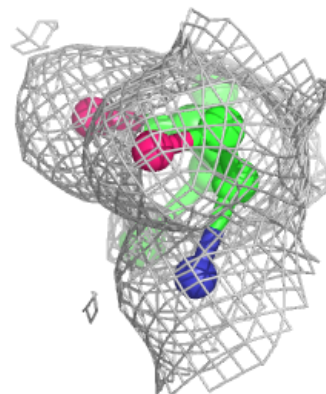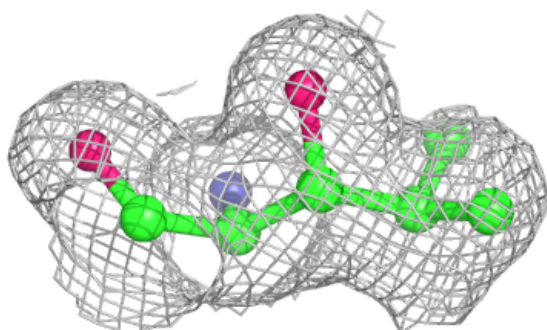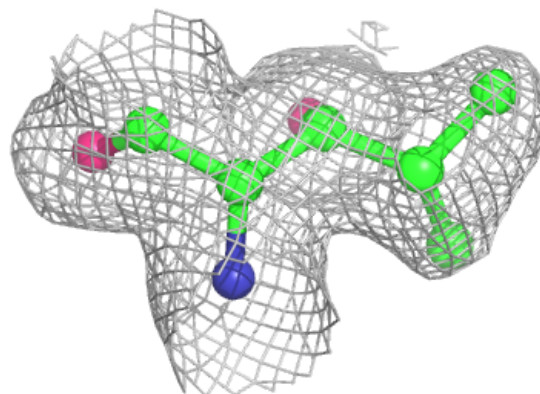
Electron density around MAA B 404:

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

Electron density around ALA B 405:

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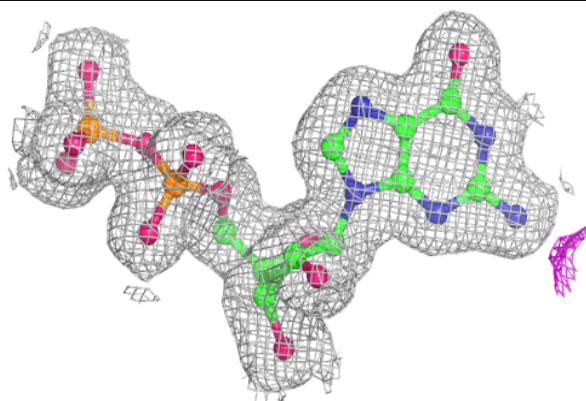and green (positive)

Electron density around ACE B 406:

$2mF_o$-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 401:

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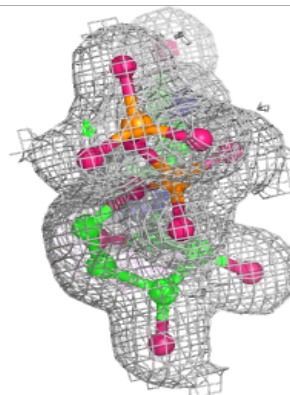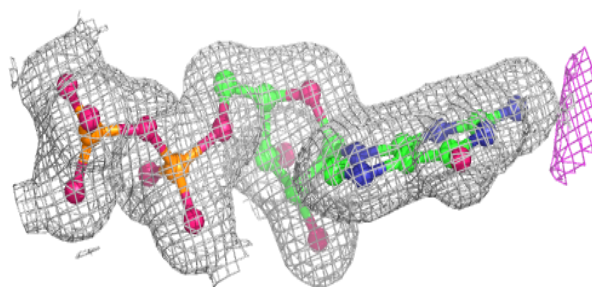
6.5 Other polymers (i)

There are no such residues in this entry.