



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:03 AM UTC

PDB ID : 6PM9 / pdb_00006pm9
Title : Crystal structure of the core catalytic domain of human O-GlcNAcase bound to MK-8719
Authors : Klein, D.J.; Selnick, H.G.; Duffy, J.L.; McEachern, E.J.
Deposited on : 2019-07-01
Resolution : 2.86 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

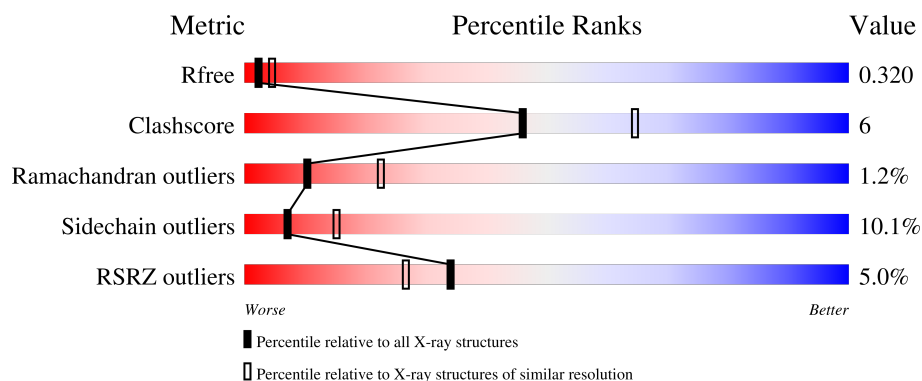
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	A	388	11% 59% 17% 20%
1	B	388	62% 16% 20%
1	C	388	2% 55% 21% 20%
1	D	388	2% 58% 19% 20%
2	E	161	11% 48% 20% 30%

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Mol	Chain	Length	Quality of chain
2	F	161	7%51%12%. .32%
2	G	161	6%53%16%.27%
2	H	161	14%48%19%..30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13916 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 O-GlcNAcase TIM-barrel domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2540	1644	418	464	14			
1	B	309	Total	C	N	O	S	0	0	0
			2536	1641	417	464	14			
1	C	310	Total	C	N	O	S	0	0	0
			2515	1626	416	459	14			
1	D	310	Total	C	N	O	S	0	0	0
			2512	1624	414	460	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP O60502
B	13	GLY	-	expression tag	UNP O60502
C	13	GLY	-	expression tag	UNP O60502
D	13	GLY	-	expression tag	UNP O60502

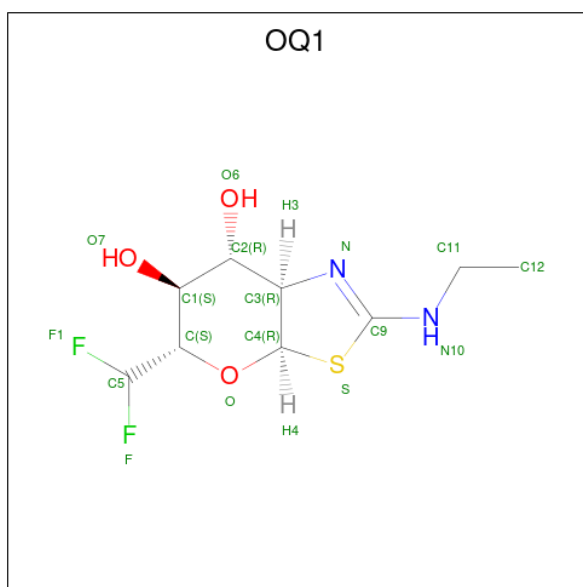
- Molecule 2 is a protein called O-GlcNAcase stalk domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	112	Total	C	N	O	S	0	0	0
			912	588	152	163	9			
2	F	109	Total	C	N	O	S	0	0	0
			896	580	149	158	9			
2	G	117	Total	C	N	O	S	0	0	0
			974	631	163	171	9			
2	H	112	Total	C	N	O	S	0	0	0
			928	600	156	163	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	553	MET	-	initiating methionine	UNP O60502
E	706	HIS	-	expression tag	UNP O60502
E	707	HIS	-	expression tag	UNP O60502
E	708	HIS	-	expression tag	UNP O60502
E	709	HIS	-	expression tag	UNP O60502
E	710	HIS	-	expression tag	UNP O60502
E	711	HIS	-	expression tag	UNP O60502
E	712	HIS	-	expression tag	UNP O60502
E	713	HIS	-	expression tag	UNP O60502
F	553	MET	-	initiating methionine	UNP O60502
F	706	HIS	-	expression tag	UNP O60502
F	707	HIS	-	expression tag	UNP O60502
F	708	HIS	-	expression tag	UNP O60502
F	709	HIS	-	expression tag	UNP O60502
F	710	HIS	-	expression tag	UNP O60502
F	711	HIS	-	expression tag	UNP O60502
F	712	HIS	-	expression tag	UNP O60502
F	713	HIS	-	expression tag	UNP O60502
G	553	MET	-	initiating methionine	UNP O60502
G	706	HIS	-	expression tag	UNP O60502
G	707	HIS	-	expression tag	UNP O60502
G	708	HIS	-	expression tag	UNP O60502
G	709	HIS	-	expression tag	UNP O60502
G	710	HIS	-	expression tag	UNP O60502
G	711	HIS	-	expression tag	UNP O60502
G	712	HIS	-	expression tag	UNP O60502
G	713	HIS	-	expression tag	UNP O60502
H	553	MET	-	initiating methionine	UNP O60502
H	706	HIS	-	expression tag	UNP O60502
H	707	HIS	-	expression tag	UNP O60502
H	708	HIS	-	expression tag	UNP O60502
H	709	HIS	-	expression tag	UNP O60502
H	710	HIS	-	expression tag	UNP O60502
H	711	HIS	-	expression tag	UNP O60502
H	712	HIS	-	expression tag	UNP O60502
H	713	HIS	-	expression tag	UNP O60502

- Molecule 3 is (3aR,5S,6S,7R,7aR)-5-(difluoromethyl)-2-(ethylamino)-5,6,7,7a-tetrahydro-3aH-pyrano[3,2-d][1,3]thiazole-6,7-diol (CCD ID: OQ1) (formula: C₉H₁₄F₂N₂O₃S) (labeled as "Ligand of Interest" by depositor).

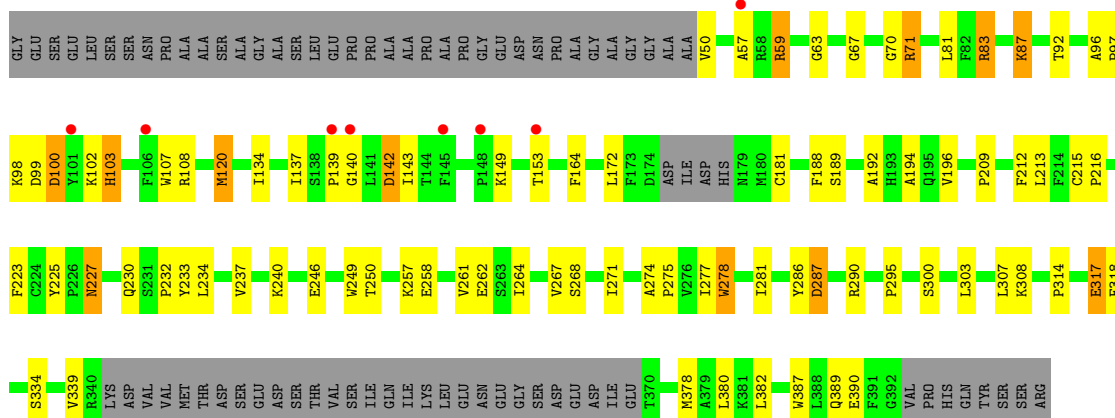


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	
			17	9	2	2	3	1	0
3	B	1	Total	C	F	N	O	S	
			17	9	2	2	3	1	0
3	C	1	Total	C	F	N	O	S	
			17	9	2	2	3	1	0
3	D	1	Total	C	F	N	O	S	
			17	9	2	2	3	1	0

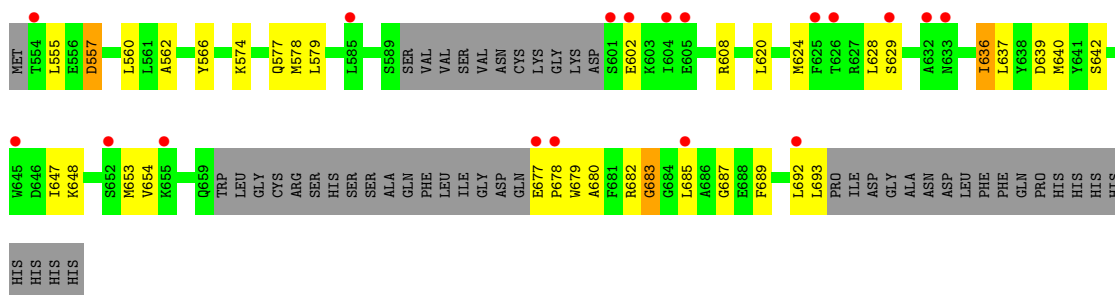
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	9	Total	O	0	0
			9	9		
4	C	8	Total	O	0	0
			8	8		
4	D	3	Total	O	0	0
			3	3		
4	E	2	Total	O	0	0
			2	2		
4	F	3	Total	O	0	0
			3	3		
4	G	1	Total	O	0	0
			1	1		
4	H	3	Total	O	0	0
			3	3		

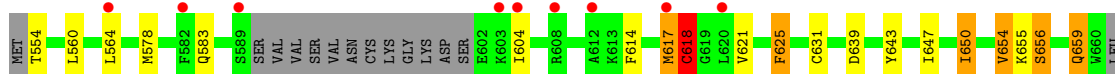
- Molecule 1: O-GlcNAcase TIM-barrel domain

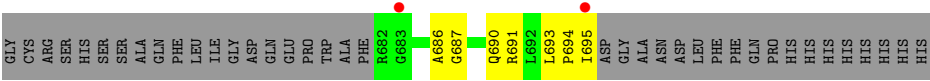


- Molecule 2: O-GlcNAcase stalk domain

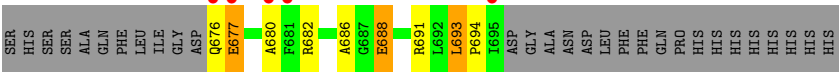


- Molecule 2: O-GlcNAcase stalk domain

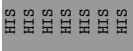
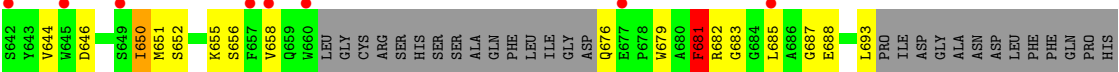




● Molecule 2: O-GlcNAcase stalk domain



● Molecule 2: O-GlcNAcase stalk domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	89.92Å 91.46Å 94.61Å 77.27° 62.61° 62.86°	Depositor
Resolution (Å)	40.69 – 2.86 40.69 – 2.86	Depositor EDS
% Data completeness (in resolution range)	95.1 (40.69-2.86) 95.0 (40.69-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.239 , 0.309 0.251 , 0.320	Depositor DCC
R_{free} test set	2706 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 80.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,l,h-k 0.000 for h,h-l,k 0.000 for h,h-k,h-l 0.000 for -h,-h+k,-l 0.000 for -h,-k,-h+l 0.000 for -h,-l,-k 0.000 for -h,-h+l,-h+k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13916	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7595e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OQ1

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	0.86	0/2610	1.45	30/3539 (0.8%)
1	B	0.88	0/2606	1.48	25/3535 (0.7%)
1	C	0.92	0/2580	1.47	21/3494 (0.6%)
1	D	0.88	0/2577	1.44	17/3491 (0.5%)
2	E	0.84	0/932	1.50	12/1251 (1.0%)
2	F	0.86	0/916	1.57	10/1230 (0.8%)
2	G	0.90	1/998 (0.1%)	1.54	17/1341 (1.3%)
2	H	0.81	0/950	1.48	7/1276 (0.5%)
All	All	0.88	1/14169 (0.0%)	1.48	139/19157 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	677	GLU	CA-C	5.24	1.59	1.52

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	ASP	CA-CB-CG	9.81	122.41	112.60
2	H	605	GLU	N-CA-C	-9.20	102.19	113.41
1	B	140	GLY	N-CA-C	7.86	123.72	113.27
2	F	654	VAL	N-CA-C	-7.71	103.28	110.53
1	A	186	GLU	CA-C-N	7.46	129.96	120.56

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	A	2540	0	2484	32	0
1	B	2536	0	2473	18	0
1	C	2515	0	2474	35	0
1	D	2512	0	2464	39	0
2	E	912	0	887	9	0
2	F	896	0	880	11	0
2	G	974	0	953	12	0
2	H	928	0	905	15	0
3	A	17	0	0	1	0
3	B	17	0	0	0	0
3	C	17	0	0	0	0
3	D	17	0	0	1	0
4	A	6	0	0	0	0
4	B	9	0	0	0	0
4	C	8	0	0	0	0
4	D	3	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
4	G	1	0	0	0	0
4	H	3	0	0	0	0
All	All	13916	0	13520	158	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 6.

The worst 5 of 158 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:264:ILE:HD11	1:D:303:LEU:HG	1.61	0.82
1:D:71:ARG:HE	2:H:641:TYR:HD2	1.24	0.82
1:B:97:PRO:HB2	1:B:100:ASP:HB2	1.62	0.80
1:C:64:VAL:HG23	1:C:85:LEU:HD21	1.64	0.78
1:C:218:GLU:HG2	1:C:223:PHE:O	1.94	0.67

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	305/388 (79%)	287 (94%)	17 (6%)	1 (0%)	36	54
1	B	305/388 (79%)	286 (94%)	16 (5%)	3 (1%)	12	25
1	C	304/388 (78%)	275 (90%)	24 (8%)	5 (2%)	7	17
1	D	304/388 (78%)	279 (92%)	21 (7%)	4 (1%)	9	21
2	E	106/161 (66%)	97 (92%)	6 (6%)	3 (3%)	4	9
2	F	103/161 (64%)	98 (95%)	5 (5%)	0	100	100
2	G	111/161 (69%)	105 (95%)	4 (4%)	2 (2%)	6	15
2	H	106/161 (66%)	99 (93%)	6 (6%)	1 (1%)	14	28
All	All	1644/2196 (75%)	1526 (93%)	99 (6%)	19 (1%)	10	22

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	677	GLU
2	G	680	ALA
1	C	57	ALA
1	D	140	GLY
1	D	181	CYS

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	277/331 (84%)	255 (92%)	22 (8%)	11	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	276/331 (83%)	254 (92%)	22 (8%)	11	24
1	C	270/331 (82%)	243 (90%)	27 (10%)	7	16
1	D	270/331 (82%)	244 (90%)	26 (10%)	8	17
2	E	95/140 (68%)	79 (83%)	16 (17%)	2	3
2	F	94/140 (67%)	84 (89%)	10 (11%)	6	13
2	G	102/140 (73%)	90 (88%)	12 (12%)	5	10
2	H	96/140 (69%)	82 (85%)	14 (15%)	3	5
All	All	1480/1884 (79%)	1331 (90%)	149 (10%)	7	15

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	604	ILE
2	H	644	VAL
2	F	650	ILE
2	G	647	ILE
1	C	114	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	583	GLN
2	H	559	GLN
2	H	630	ASN
2	H	583	GLN
1	C	389	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	OQ1	D	501	-	16,18,18	0.69	0	14,26,26	1.58	3 (21%)
3	OQ1	A	501	-	16,18,18	0.63	0	14,26,26	1.53	3 (21%)
3	OQ1	B	501	-	16,18,18	0.68	0	14,26,26	0.87	0
3	OQ1	C	501	-	16,18,18	0.79	1 (6%)	14,26,26	2.79	7 (50%)

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
3	OQ1	D	501	-	-	4/7/35/35	0/2/2/2
3	OQ1	A	501	-	-	4/7/35/35	0/2/2/2
3	OQ1	B	501	-	-	1/7/35/35	0/2/2/2
3	OQ1	C	501	-	-	3/7/35/35	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	OQ1	C2-C3	-2.02	1.50	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	OQ1	C4-O-C	6.40	122.56	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	OQ1	O-C-C1	4.87	114.82	107.94
3	D	501	OQ1	C4-O-C	3.92	119.32	114.17
3	A	501	OQ1	F1-C5-F	3.83	112.92	105.53
3	C	501	OQ1	C2-C3-N	-3.28	105.97	110.56

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	OQ1	C1-C-C5-F
3	A	501	OQ1	O-C-C5-F
3	A	501	OQ1	C1-C-C5-F1
3	A	501	OQ1	O-C-C5-F1
3	B	501	OQ1	O-C-C5-F1

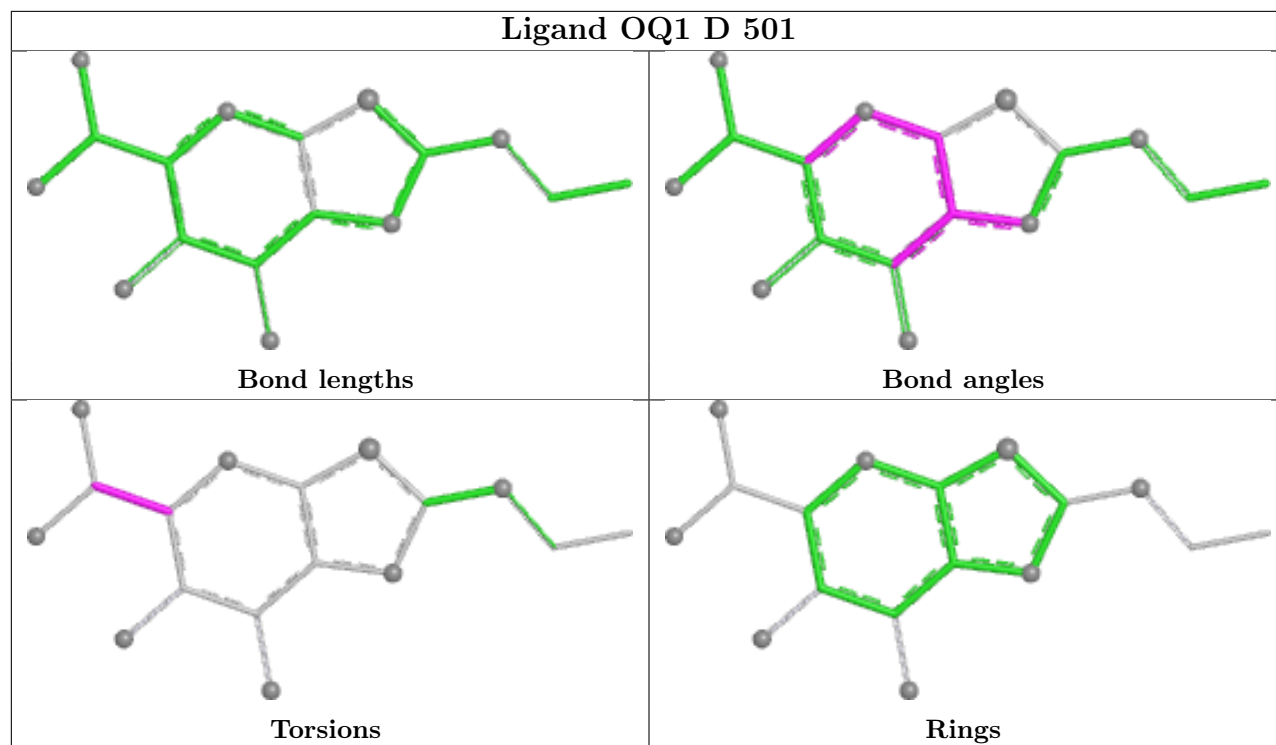
There are no ring outliers.

2 monomers are involved in 2 short contacts:

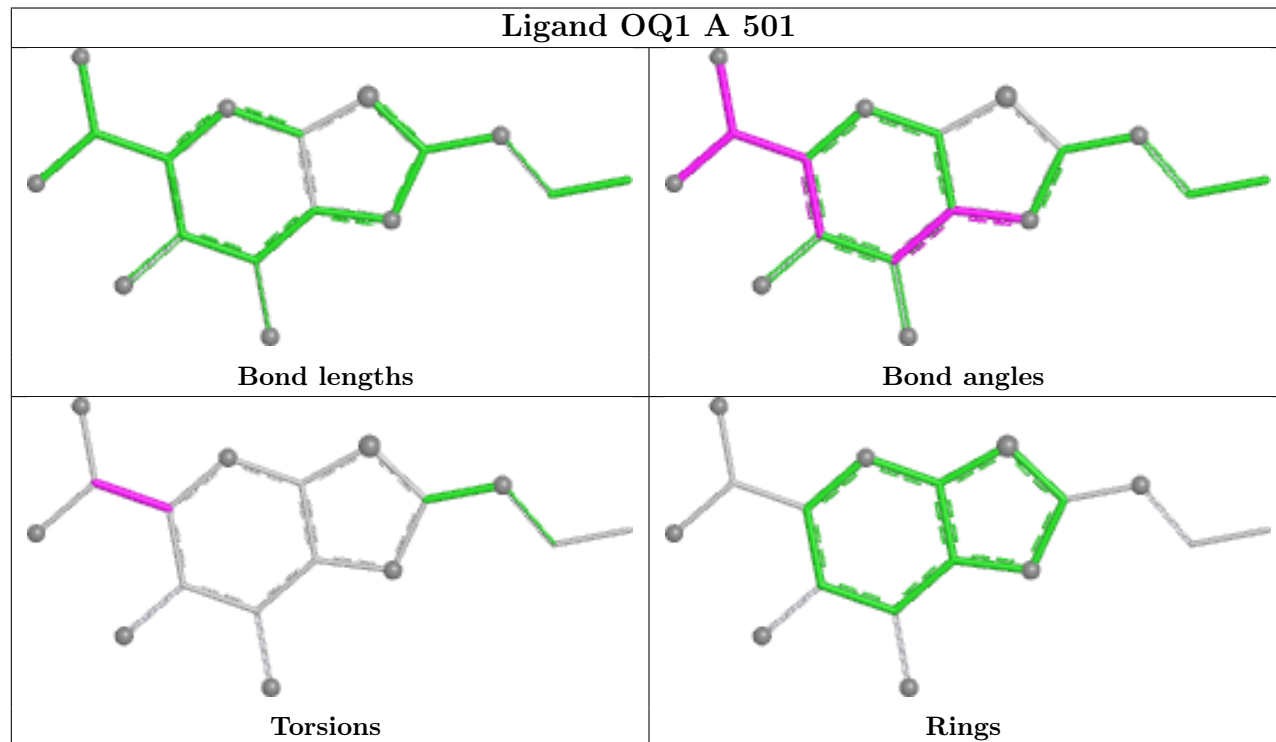
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	OQ1	1	0
3	A	501	OQ1	1	0

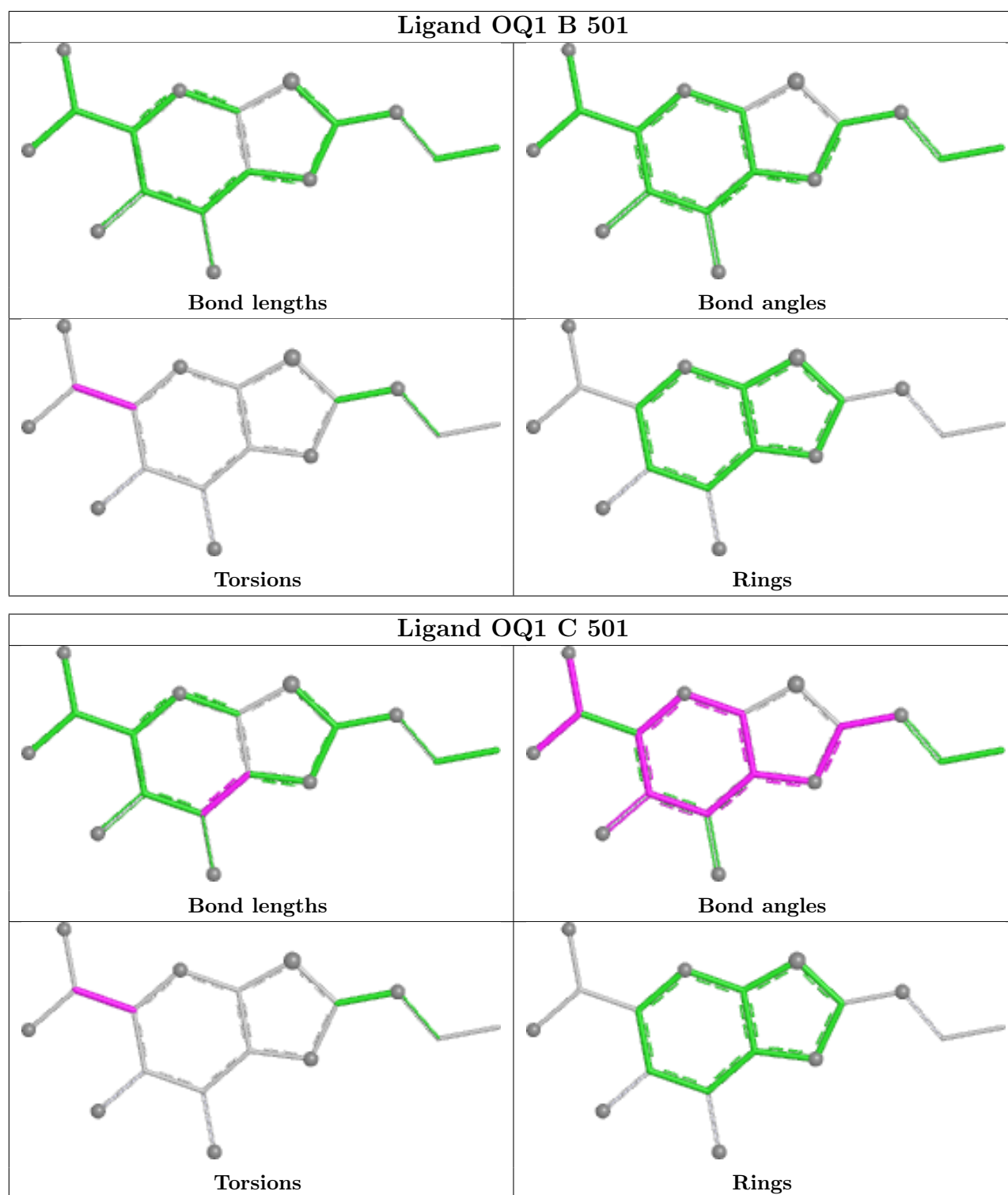
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand OQ1 D 501



Ligand OQ1 A 501





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	309/388 (79%)	0.17	4 (1%) 75 68	35, 51, 70, 88	0
1	B	309/388 (79%)	-0.05	3 (0%) 79 74	33, 47, 63, 76	0
1	C	310/388 (79%)	0.28	9 (2%) 53 45	35, 53, 75, 99	0
1	D	310/388 (79%)	0.57	8 (2%) 57 48	37, 67, 96, 116	0
2	E	112/161 (69%)	1.10	18 (16%) 4 4	55, 84, 117, 129	0
2	F	109/161 (67%)	0.72	11 (10%) 12 10	41, 60, 82, 96	0
2	G	117/161 (72%)	0.70	9 (7%) 19 14	34, 59, 88, 106	0
2	H	112/161 (69%)	1.23	22 (19%) 3 3	47, 78, 113, 134	0
All	All	1688/2196 (76%)	0.43	84 (4%) 34 27	33, 56, 95, 134	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	601	SER	5.3
2	G	680	ALA	4.3
2	E	645	TRP	4.0
2	E	677	GLU	3.8
2	H	641	TYR	3.7

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 ⓘ

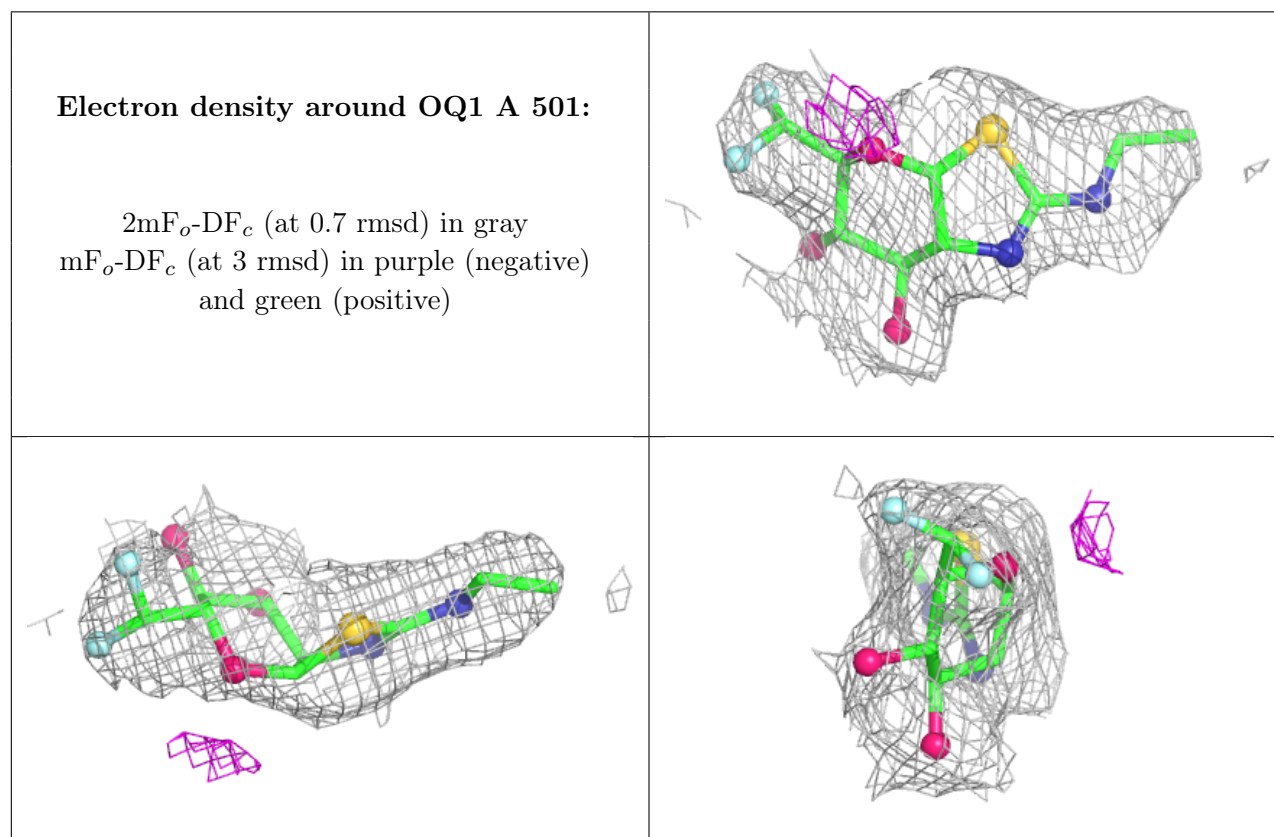
There are no oligosaccharides in this entry.

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.

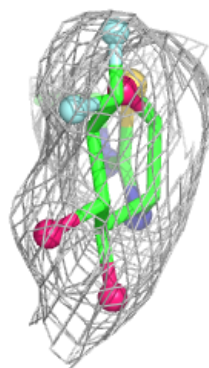
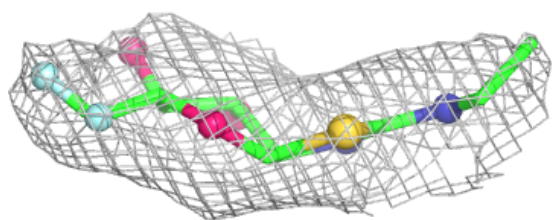
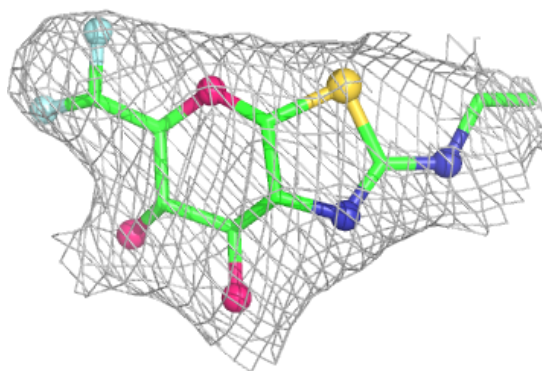
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OQ1	A	501	17/17	0.91	0.11	29,54,59,59	0
3	OQ1	C	501	17/17	0.93	0.10	44,52,57,57	0
3	OQ1	D	501	17/17	0.94	0.12	49,52,58,58	0
3	OQ1	B	501	17/17	0.95	0.10	25,45,55,57	0

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.

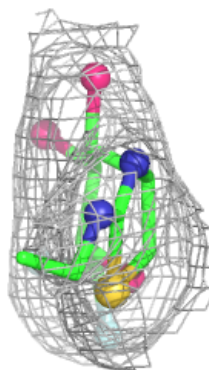
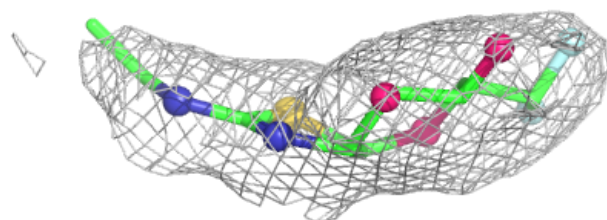
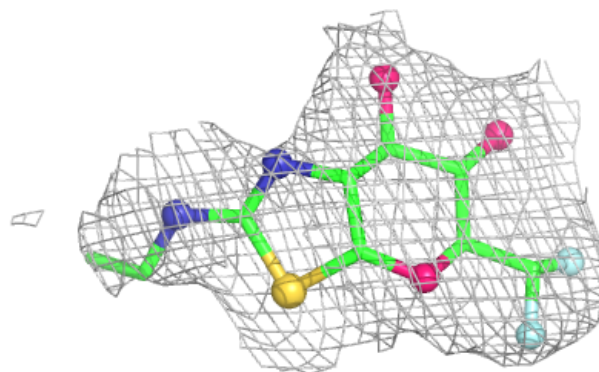


Electron density around OQ1 C 501:

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

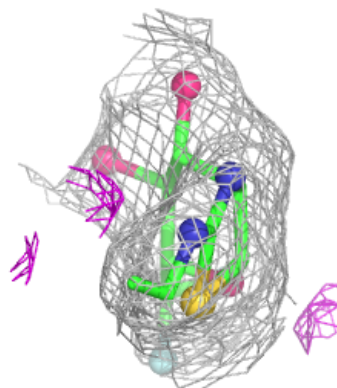
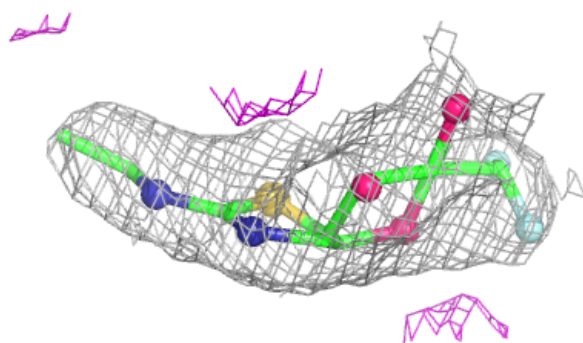
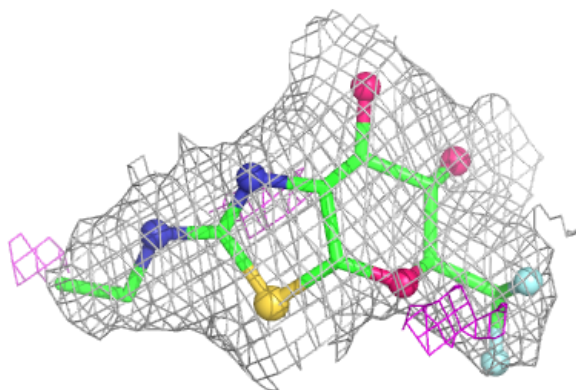
**Electron density around OQ1 D 501:**

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



Electron density around OQ1 B 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.