Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 12:58 pm GMT

PDB ID	:	7OU6
Title	:	Human O-GlcNAc hydrolase in complex with DNJNAc-thiazolidines
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Deposited on	:	2021-06-11
Resolution	:	2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

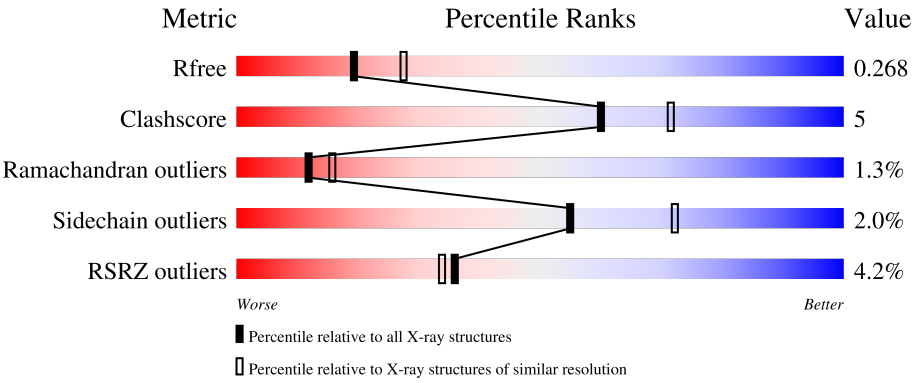
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	AAA	916	2% 40% 7% 53%
1	BBB	916	2% 42% 6% 52%

2 Entry composition

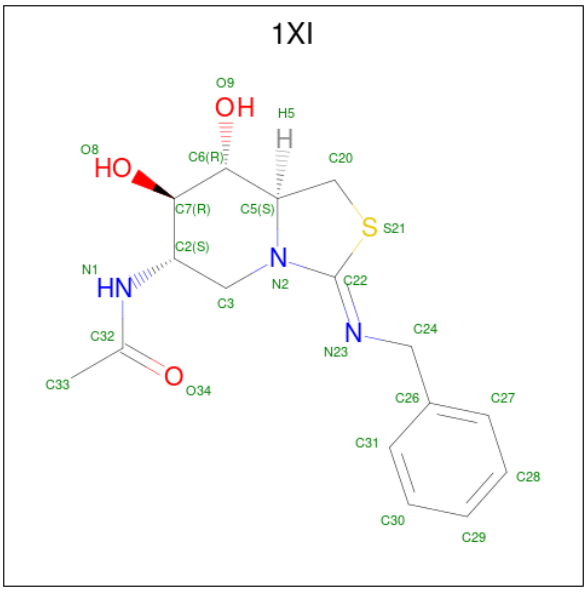
There are 3 unique types of molecules in this entry. The entry contains 13220 atoms, of which 6452 are hydrogens and 0 are deuteriums.

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 O-GlcNAcase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	430	Total	C	H	N	O	S	152	0	0
			6372	2131	3098	531	592	20			
1	BBB	436	Total	C	H	N	O	S	127	0	0
			6742	2236	3312	549	621	24			

- Molecule 2 is {N}-[(3 {Z},6 {S},7 {R},8 {R},8 {a} {S})-7,8-bis(oxidanyl)-3-(phenylmethyl)imino-1,5,6,7,8,8 {a}-hexahydro-[1,3]thiazolo[3,4-a]pyridin-6-yl]ethanamide (three-letter code: 1XI) (formula: $C_{16}H_{21}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	S	2	0
			44	16	21	3	3	1		
2	BBB	1	Total	C	H	N	O	S	2	0
			44	16	21	3	3	1		

- Molecule 3 is water.

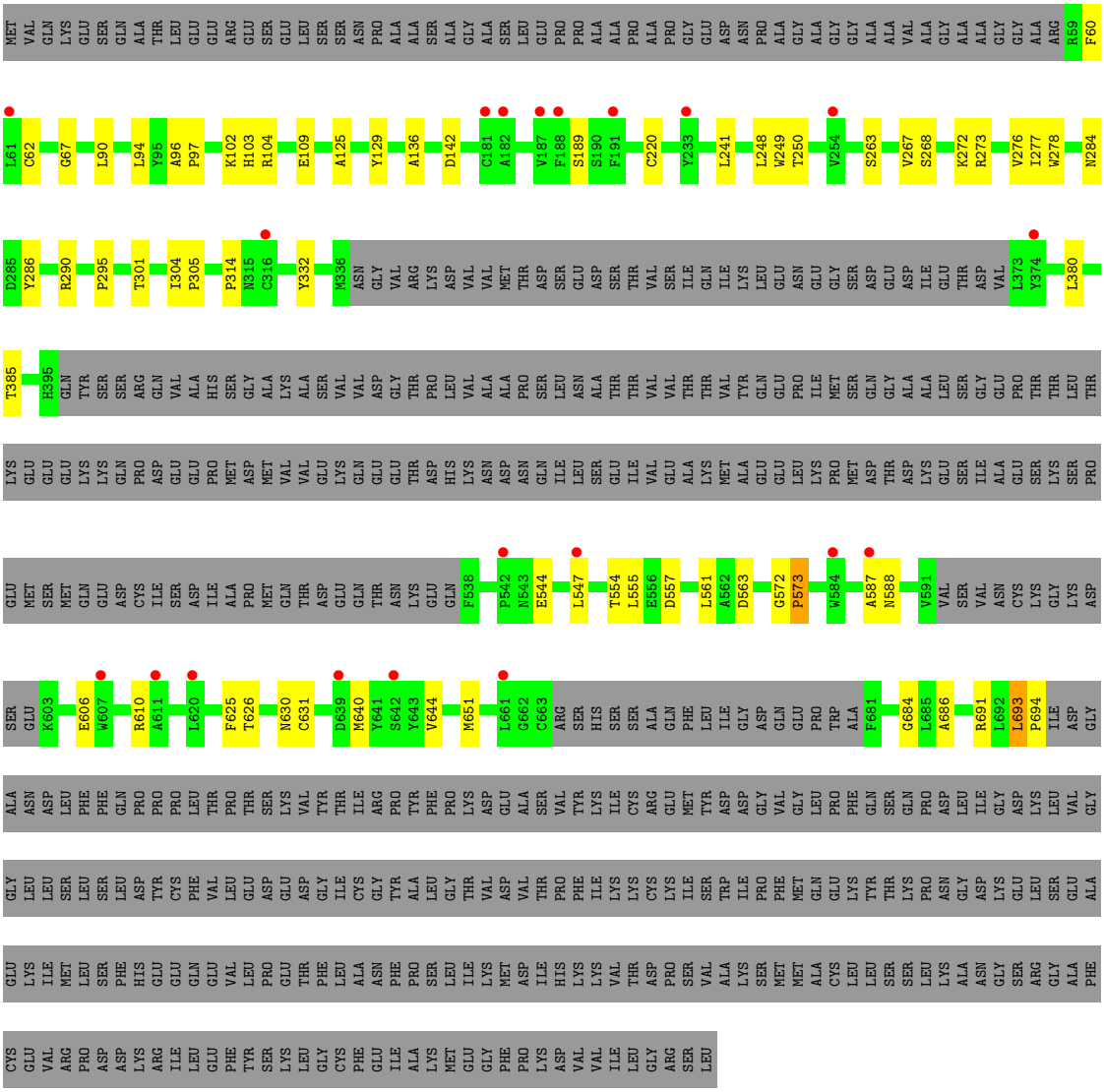
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	8	Total O 8 8	0	0
3	BBB	10	Total O 10 10	0	0

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.

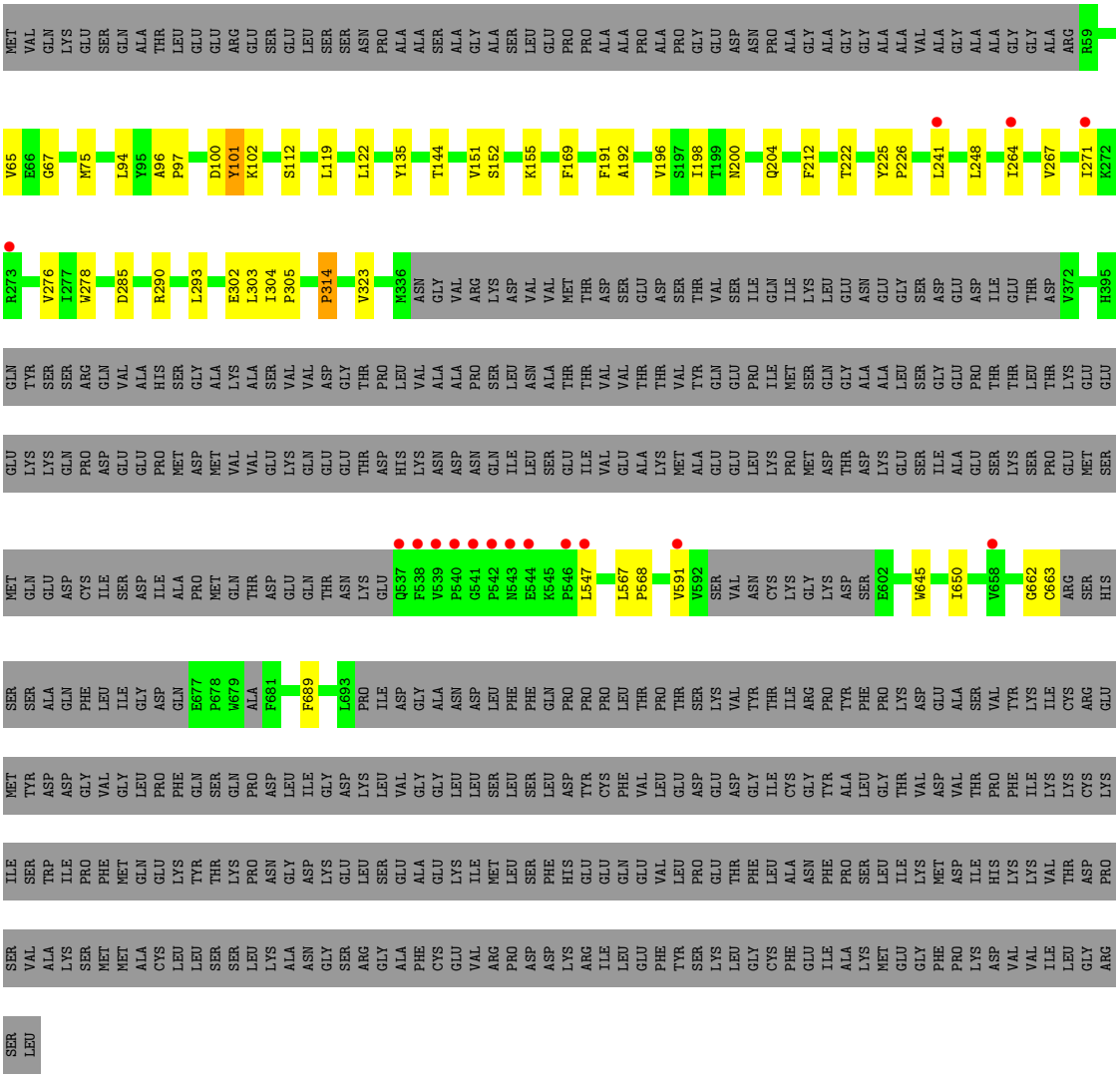
• Molecule 1: Protein O-GlcNAcase

Chain AAA:



• Molecule 1: Protein O-GlcNAcase

Chain BBB:


MET VAL GLN LYS GLU SER GLN ALA THR LEU GLU GLU GLU ARG GLU SER GLU LEU SER SER ASN PRO ALA ALA SER ALA GLY ALA SER LEU GLU PRO PRO ALA ALA PRO ALA PRO GLY GLU ASP ASN PRO ALA GLY ALA GLY GLY ALA ALA VAL ALA GLY ALA ALA ALA GLY GLY ALA ARG R59
V65 E66 G67 M75 L94 Y95 A96 P97 D100 Y101 K102 S112 L119 L122 Y135 T144 V151 S152 K155 F169 F191 A192 V196 S197 I198 T199 N200 Q204 F212 T222 Y225 P226 L241 L248 I264 V267 I271 K272
R273 V276 I277 W278 D285 R290 L293 E302 L303 I304 P305 P314 V323 M336 ASN GLY VAL ARG LYS ASP VAL VAL MET THR THR ASP SER GLU ASP SER THR VAL SER ILE GLN ILE LYS LEU GLU ASN GLU GLY SER GLY ASP GLU ASP ILE GLU THR ASP V372 H395
GLN TYR SER SER ARG GLN VAL ALA HIS SER GLY ALA LYS ALA SER VAL VAL ASP GLY THR PRO LEU VAL ALA ALA PRO SER LEU ASN ALA THR THR THR VAL VAL THR THR VAL TYR GLN GLU PRO ILE MET SER GLN GLY ALA ALA LEU SER GLY GLU PRO THR THR LEU THR LYS GLU GLU
GLU LYS LYS GLN PRO ASP GLU GLU PRO MET ASP MET VAL VAL GLU LYS GLN GLU GLU THR ASP HIS LYS ASN ASP ASN GLN ILE LEU SER GLU ILE VAL GLU ALA LYS MET ALA GLU GLU LEU LYS PRO MET ASP THR ASP LYS GLU GLY SER ILE ALA GLU SER LYS SER PRO GLU MET SER
MET GLN GLU ASP CYS ILE SER ASP ILE ALA PRO MET GLN THR ASP GLU GLN THR ASN LYS GLU Q537 F538 V539 P540 G541 P542 N543 E544 K545 P546 L547 L567 P568 V591 V592 SER VAL ASN CYS LYS GLY LYS ASP SER E602 W645 I650 V658 G662 C663 ARG SER HIS
SER SER ALA GLN PHE LEU ILE GLY ASP GLN E677 P678 W679 ALA F681 F689 L693 PRO ILE ASP GLY ALA ASN ASP LEU PHE PHE GLN PRO PRO PRO LEU THR PRO THR SER LYS VAL TYR THR ILE ARG PRO TYR PHE PRO LYS ASP GLU ALA SER VAL TYR LYS ILE CYS ARG GLU
MET TYR ASP ASP GLY VAL GLY LEU PRO PHE GLN SER GLN PRO ASP LEU ILE GLY ASP LYS LEU VAL GLY GLY LEU LEU SER LEU SER LEU ASP TYR CYS PHE VAL LEU GLU ASP GLU ASP GLY ILE CYS GLY TYR ALA LEU GLY THR VAL ASP VAL THR PRO PHE LYS ILE LYS LYS CYS LYS
ILE SER TRP ILE PRO PHE MET GLN GLU LYS TYR THR LYS PRO ASN GLY ASP LYS GLU LEU SER GLU ALA GLU LYS ILE MET LEU SER PHE HIS GLU GLU GLN GLU VAL LEU PRO GLU THR PHE LEU ALA ASN PHE PRO SER LEU ILE LYS MET ASP ILE HIS LYS LYS VAL THR ASP PRO
SER VAL ALA LYS SER MET MET ALA CYS LEU LEU SER SER LEU LYS ALA ASN GLY SER ARG GLY ALA PHE CYS GLU VAL ARG PRO ASP ASP LYS ARG ILE LEU GLU GLU PHE TYR SER LYS LEU GLY CYS PHE GLU ILE ALA LYS MET GLU GLY PHE PRO LYS ASP VAL VAL ILE LEU GLY ARG
SER LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.29Å 101.29Å 284.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.28 – 2.41 58.21 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.9 (58.28-2.41) 100.0 (58.21-2.41)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.221 , 0.271 0.221 , 0.268	Depositor DCC
R_{free} test set	1735 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å^2)	78.3	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13220	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1XI

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	AAA	0.71	0/3365	0.83	1/4589 (0.0%)
1	BBB	0.70	0/3525	0.84	0/4795
All	All	0.70	0/6890	0.83	1/9384 (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	BBB	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	104	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	100	ASP	Peptide

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	AAA	3274	3098	2955	38	0
1	BBB	3430	3312	3226	30	0
2	AAA	23	21	0	1	0
2	BBB	23	21	0	0	0
3	AAA	8	0	0	0	0
3	BBB	10	0	0	0	0
All	All	6768	6452	6181	59	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 5.

All (59) 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:AAA:693:LEU:HB3	1:AAA:694:PRO:CD	2.20	0.71
1:AAA:693:LEU:HB3	1:AAA:694:PRO:HD3	1.80	0.63
1:AAA:241:LEU:O	1:AAA:273:ARG:NH1	2.32	0.61
1:AAA:626:THR:O	1:AAA:630:ASN:ND2	2.38	0.57
1:AAA:142:ASP:OD1	1:BBB:547:LEU:HA	2.06	0.55
1:AAA:686:ALA:HB1	1:BBB:650:ILE:HD12	1.88	0.54
1:BBB:248:LEU:HA	1:BBB:276:VAL:O	2.08	0.54
1:BBB:293:LEU:O	1:BBB:323:VAL:HG11	2.08	0.54
1:AAA:268:SER:O	1:AAA:272:LYS:N	2.36	0.54
1:AAA:220:CYS:HB3	1:AAA:250:THR:OG1	2.07	0.53
1:AAA:693:LEU:O	1:AAA:694:PRO:C	2.47	0.53
1:AAA:284:ASN:HB2	1:AAA:290:ARG:O	2.08	0.53
1:BBB:196:VAL:HG13	1:BBB:241:LEU:HA	1.90	0.53
1:AAA:67:GLY:HA2	1:AAA:96:ALA:O	2.09	0.52
1:AAA:693:LEU:CB	1:AAA:694:PRO:CD	2.87	0.52
1:BBB:96:ALA:N	1:BBB:97:PRO:HD3	2.24	0.52
1:BBB:101:TYR:CE2	1:BBB:102:LYS:HE3	2.45	0.51
1:AAA:606:GLU:O	1:AAA:610:ARG:HB2	2.12	0.50
1:AAA:60:PHE:CD2	1:AAA:332:TYR:CE1	2.99	0.49
1:AAA:94:LEU:HD11	1:AAA:136:ALA:HB2	1.95	0.49
1:BBB:67:GLY:HA2	1:BBB:96:ALA:O	2.12	0.49
1:BBB:662:GLY:O	1:BBB:663:CYS:SG	2.68	0.49
1:BBB:75:MET:SD	1:BBB:122:LEU:HD22	2.53	0.48
1:BBB:169:PHE:O	1:BBB:212:PHE:HA	2.14	0.47
1:AAA:563:ASP:HA	1:AAA:572:GLY:HA3	1.96	0.47
1:BBB:192:ALA:O	1:BBB:196:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:625:PHE:HD1	1:AAA:644:VAL:HG12	1.79	0.46
1:AAA:263:SER:O	1:AAA:267:VAL:HG12	2.16	0.46
1:AAA:684:GLY:CA	1:BBB:290:ARG:HD3	2.46	0.46
1:AAA:684:GLY:N	1:BBB:290:ARG:HD3	2.30	0.46
1:AAA:62:CYS:SG	1:AAA:90:LEU:CD2	3.04	0.45
1:AAA:125:ALA:O	1:AAA:129:TYR:HD2	1.99	0.45
1:BBB:65:VAL:HG23	1:BBB:94:LEU:HG	1.99	0.45
1:AAA:304:ILE:N	1:AAA:305:PRO:CD	2.80	0.45
1:AAA:385:THR:HG22	1:AAA:555:LEU:HD22	1.97	0.44
1:BBB:302:GLU:O	1:BBB:305:PRO:HD2	2.17	0.44
1:AAA:96:ALA:N	1:AAA:97:PRO:HD3	2.32	0.44
1:AAA:651:MET:HE3	1:BBB:689:PHE:CE2	2.53	0.44
1:AAA:103:HIS:O	1:AAA:103:HIS:CG	2.70	0.44
1:AAA:102:LYS:HE2	1:AAA:109:GLU:HB3	1.99	0.44
1:BBB:304:ILE:HB	1:BBB:305:PRO:HD3	2.00	0.43
1:AAA:554:THR:O	1:AAA:557:ASP:HB2	2.18	0.43
1:AAA:544:GLU:CG	1:BBB:144:THR:HG21	2.49	0.43
1:BBB:135:TYR:O	1:BBB:169:PHE:HA	2.18	0.43
1:AAA:248:LEU:HA	1:AAA:276:VAL:O	2.18	0.43
1:AAA:286:TYR:HA	1:BBB:645:TRP:CZ3	2.53	0.43
1:BBB:267:VAL:O	1:BBB:271:ILE:HG12	2.19	0.42
1:AAA:686:ALA:HB1	1:BBB:650:ILE:CD1	2.49	0.42
1:BBB:567:LEU:HB3	1:BBB:568:PRO:HD2	2.01	0.42
1:BBB:285:ASP:OD1	1:BBB:285:ASP:N	2.52	0.42
1:BBB:264:ILE:HG13	1:BBB:303:LEU:HD22	2.02	0.42
1:BBB:225:TYR:HA	1:BBB:226:PRO:HA	1.89	0.42
1:AAA:250:THR:HA	1:AAA:278:TRP:O	2.19	0.42
1:AAA:295:PRO:HD3	1:AAA:380:LEU:HD22	2.02	0.41
1:AAA:249:TRP:O	1:AAA:277:ILE:HA	2.20	0.41
1:AAA:544:GLU:HG2	1:BBB:144:THR:HG21	2.03	0.41
1:AAA:67:GLY:O	2:AAA:1001:1XI:O8	2.39	0.40
1:BBB:200:ASN:O	1:BBB:204:GLN:HG3	2.21	0.40
1:BBB:151:VAL:HG12	1:BBB:155:LYS:HE3	2.02	0.40

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	AAA	420/916 (46%)	372 (89%)	41 (10%)	7 (2%)	9 11
1	BBB	424/916 (46%)	396 (93%)	24 (6%)	4 (1%)	17 24
All	All	844/1832 (46%)	768 (91%)	65 (8%)	11 (1%)	12 16

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	587	ALA
1	AAA	693	LEU
1	AAA	189	SER
1	AAA	588	ASN
1	BBB	101	TYR
1	BBB	591	VAL
1	BBB	112	SER
1	AAA	691	ARG
1	BBB	314	PRO
1	AAA	573	PRO
1	AAA	314	PRO

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	AAA	306/797 (38%)	300 (98%)	6 (2%)	55 72
1	BBB	348/797 (44%)	341 (98%)	7 (2%)	55 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	654/1594 (41%)	641 (98%)	13 (2%)	55 72

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	301	THR
1	AAA	547	LEU
1	AAA	561	LEU
1	AAA	573	PRO
1	AAA	631	CYS
1	AAA	640	MET
1	BBB	119	LEU
1	BBB	152	SER
1	BBB	191	PHE
1	BBB	198	ILE
1	BBB	222	THR
1	BBB	278	TRP
1	BBB	314	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

2 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	1XI	BBB	1001	-	23,25,25	0.87	1 (4%)	24,35,35	1.05	2 (8%)
2	1XI	AAA	1001	-	23,25,25	0.72	1 (4%)	24,35,35	1.20	3 (12%)

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	1XI	BBB	1001	-	-	3/9/38/38	0/3/3/3
2	1XI	AAA	1001	-	-	1/9/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	1001	1XI	C22-N23	2.15	1.30	1.26
2	AAA	1001	1XI	C3-N2	-2.06	1.44	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	1001	1XI	C2-C3-N2	-3.54	105.11	110.38
2	AAA	1001	1XI	C20-C5-C6	3.08	120.38	115.72
2	BBB	1001	1XI	C7-C6-C5	-2.46	107.21	111.37
2	BBB	1001	1XI	C6-C7-C2	2.41	114.55	111.02
2	AAA	1001	1XI	C6-C7-C2	2.35	114.47	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

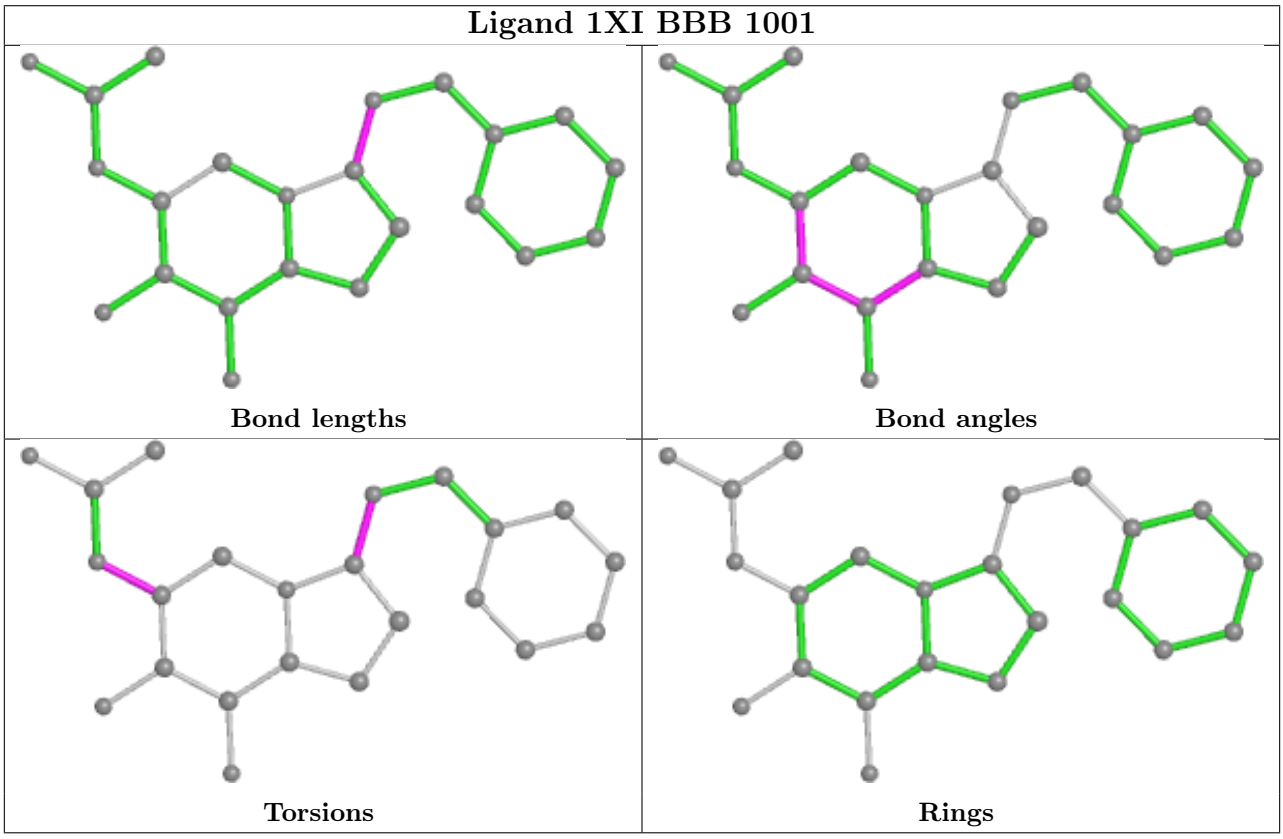
Mol	Chain	Res	Type	Atoms
2	BBB	1001	1XI	N2-C22-N23-C24
2	AAA	1001	1XI	C3-C2-N1-C32
2	BBB	1001	1XI	C3-C2-N1-C32
2	BBB	1001	1XI	C7-C2-N1-C32

There are no ring outliers.

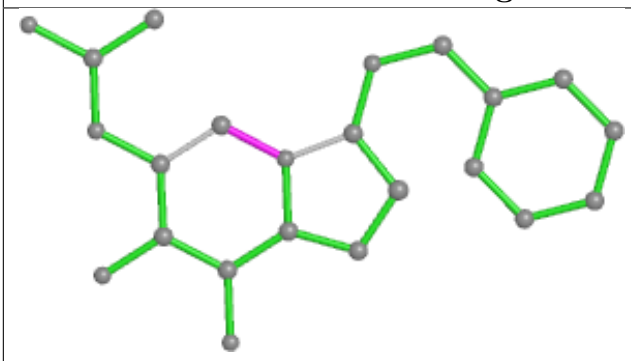
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	1001	1XI	1	0

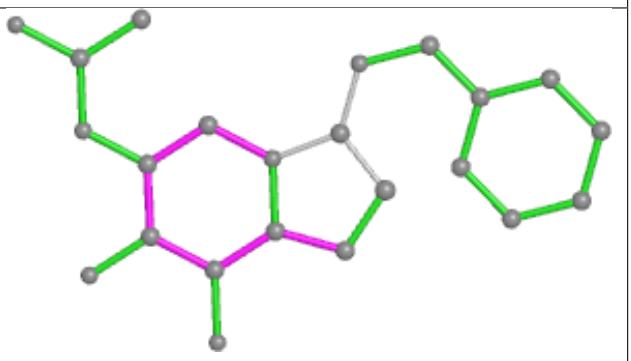
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



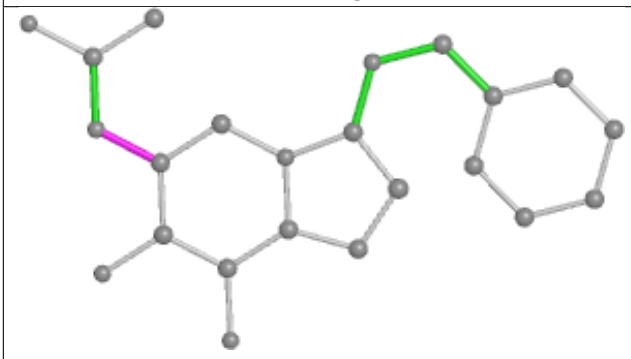
Ligand 1XI AAA 1001



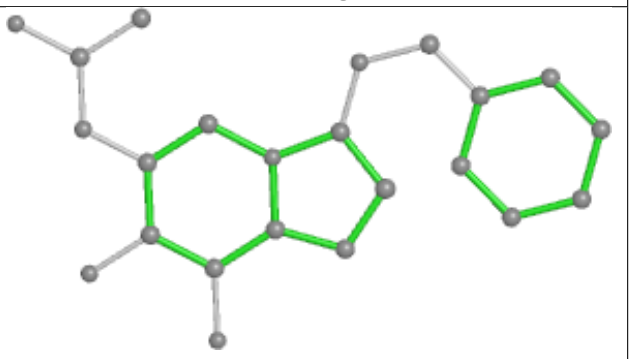
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	AAA	430/916 (46%)	0.27	20 (4%)	31	29	58, 93, 133, 187	0
1	BBB	436/916 (47%)	0.28	16 (3%)	41	40	52, 79, 126, 154	0
All	All	866/1832 (47%)	0.27	36 (4%)	36	34	52, 88, 131, 187	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	661	LEU	4.5
1	BBB	538	PHE	4.1
1	BBB	547	LEU	3.7
1	AAA	542	PRO	3.5
1	AAA	188	PHE	3.4
1	BBB	546	PRO	3.2
1	BBB	540	PRO	3.1
1	BBB	544	GLU	3.0
1	BBB	591	VAL	3.0
1	BBB	658	VAL	2.9
1	AAA	191	PHE	2.8
1	AAA	620	LEU	2.7
1	AAA	547	LEU	2.7
1	AAA	584	TRP	2.6
1	AAA	607	TRP	2.6
1	BBB	264	ILE	2.6
1	AAA	181	CYS	2.5
1	AAA	611	ALA	2.5
1	BBB	537	GLN	2.4
1	BBB	539	VAL	2.4
1	AAA	182	ALA	2.4
1	BBB	542	PRO	2.3
1	BBB	241	LEU	2.3
1	AAA	61	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	271	ILE	2.3
1	AAA	254	VAL	2.2
1	AAA	642	SER	2.1
1	AAA	233	TYR	2.1
1	BBB	541	GLY	2.1
1	AAA	639	ASP	2.1
1	BBB	543	ASN	2.1
1	BBB	273	ARG	2.1
1	AAA	316	CYS	2.0
1	AAA	587	ALA	2.0
1	AAA	187	VAL	2.0
1	AAA	374	TYR	2.0

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)

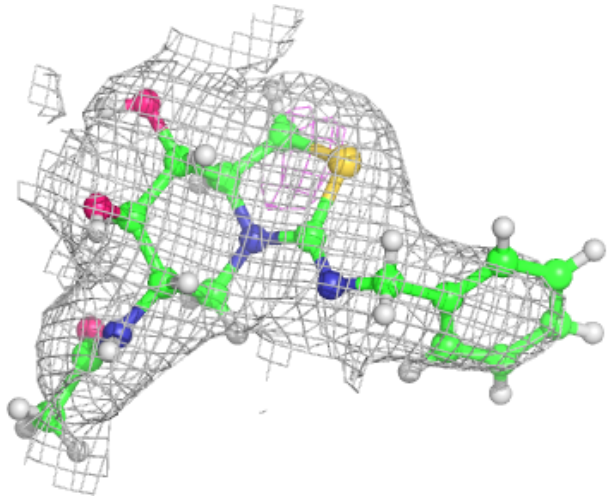
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

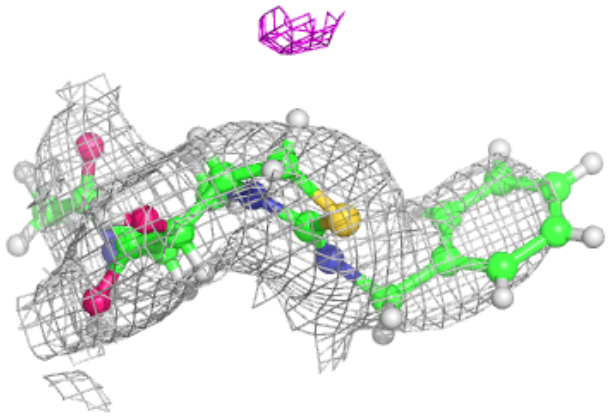
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	1XI	AAA	1001	23/23	0.96	0.17	63,75,124,130	2
2	1XI	BBB	1001	23/23	0.99	0.19	57,65,110,114	2

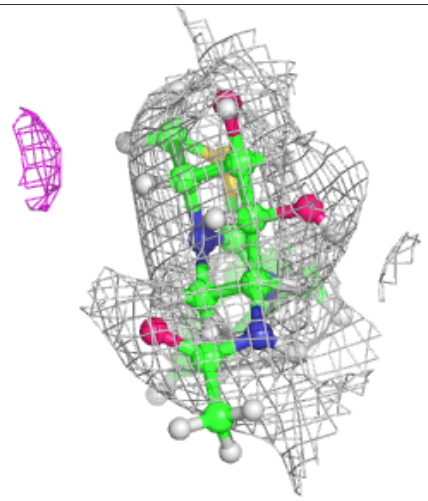
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1XI AAA 1001:

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

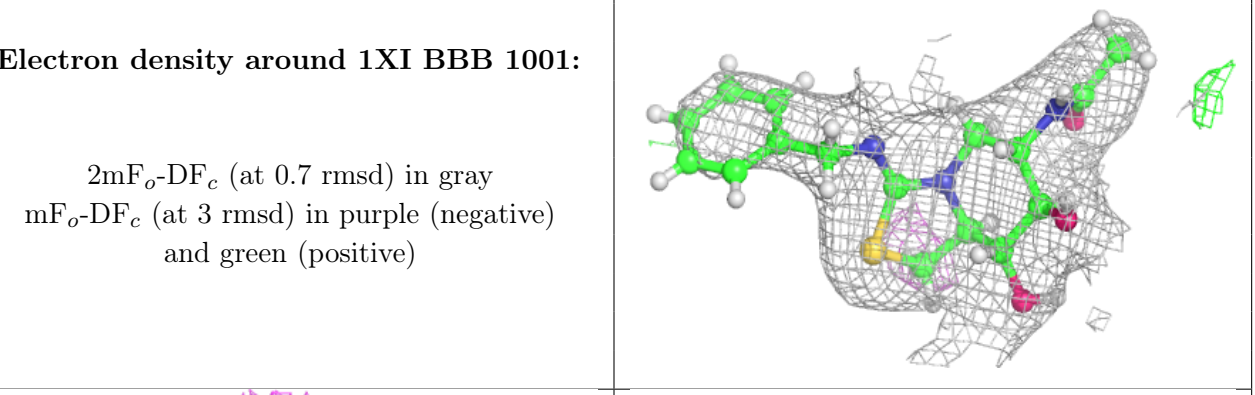


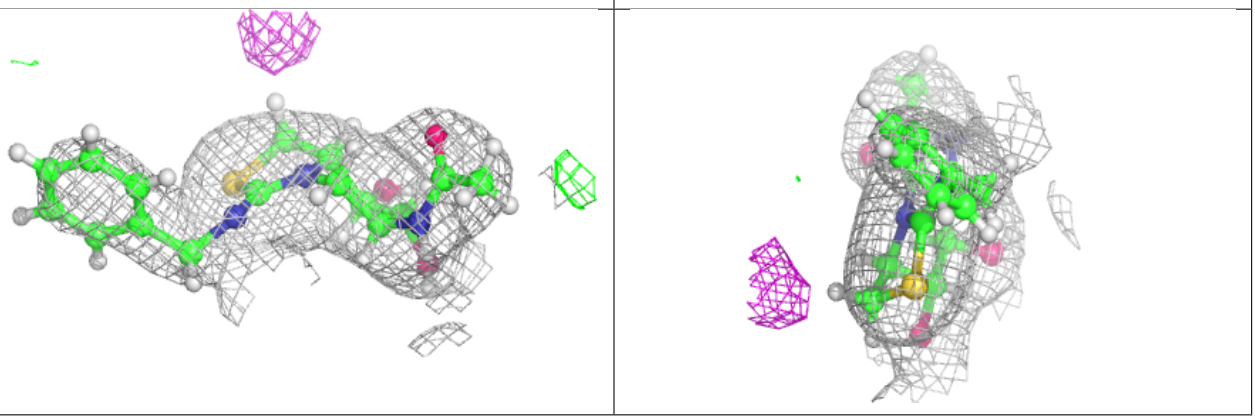




Electron density around 1XI BBB 1001:

$2mF_o$-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.