



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 6, 2022 – 01:14 am BST

PDB ID : 7OU8
Title : Human O-GlcNAc hydrolase in complex with DNJNAc-thiazolidines
Authors : Males, A.; Davies, G.J.; Gonzalez-Cuesta, M.; Mellet, C.O.; Fernandez, J.M.G.; Sidhu, P.; Ashmus, R.; Busmann, J.; Vocadlo, D.J.; Foster, L.
Deposited on : 2021-06-11
Resolution : 1.50 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 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	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

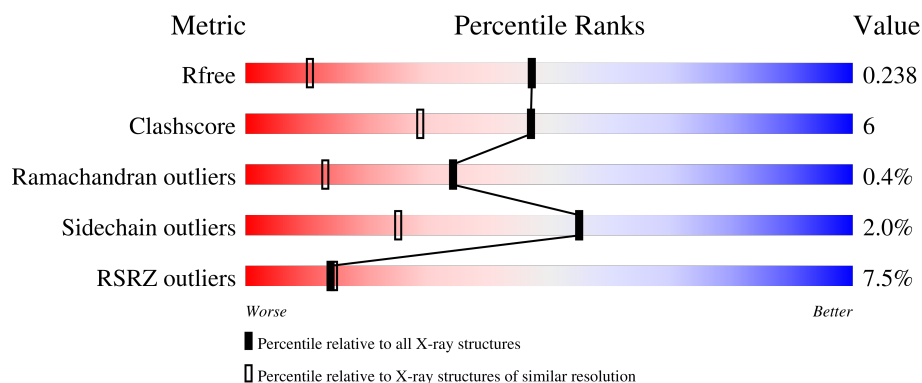
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	AAA	737	<div> <div>4%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	BBB	737	<div> <div>11%</div> <div>86%</div> <div>9%</div> <div>..</div> </div>

2 Entry composition [i](#)

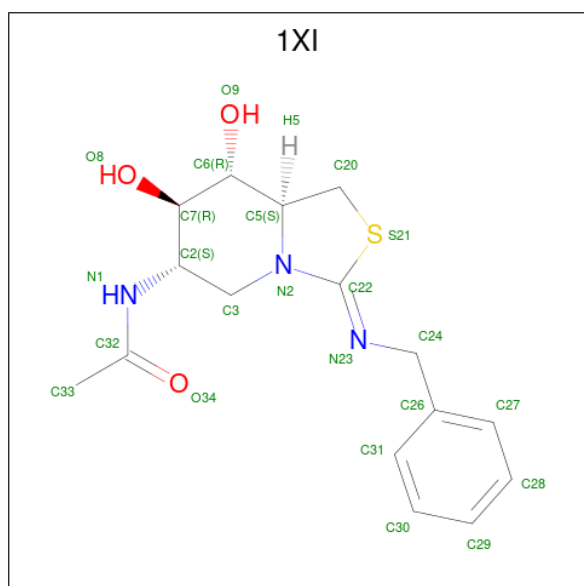
There are 5 unique types of molecules in this entry. The entry contains 23787 atoms, of which 11304 are hydrogens and 0 are deuteriums.

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 BT_4395.

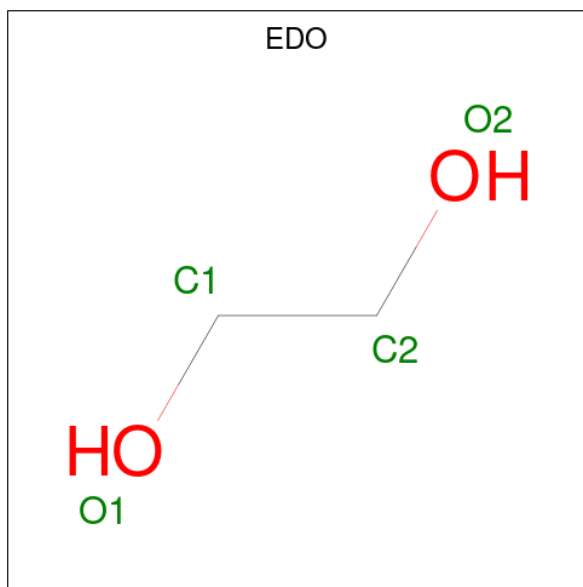
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	714	Total	C	H	N	O	S	165	28	0
			11547	3747	5705	975	1098	22			
1	BBB	708	Total	C	H	N	O	S	174	15	0
			11238	3651	5551	943	1072	21			

- 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: C₁₆H₂₁N₃O₃S) (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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BBB	1	Total	Ca	0	0
			1	1		

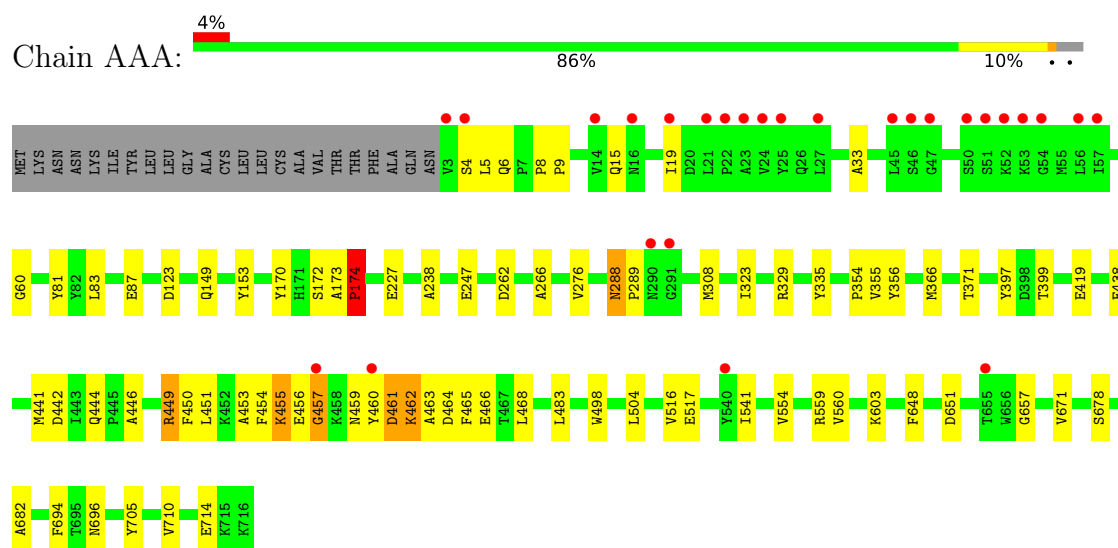
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	458	Total	O	0	5
			463	463		
5	BBB	438	Total	O	0	2
			440	440		

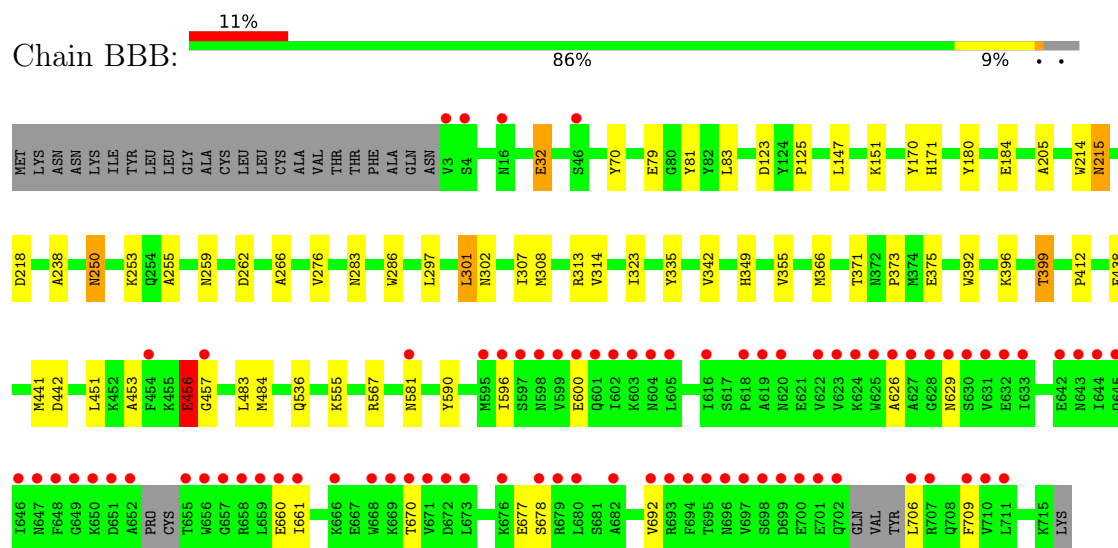
3 Residue-property plots [i](#)

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: O-GlcNAcase BT_4395



• Molecule 1: O-GlcNAcase BT_4395



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	51.53Å 160.62Å 224.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.62 – 1.50 75.62 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (75.62-1.50) 100.0 (75.62-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.232 0.216 , 0.238	Depositor DCC
R_{free} test set	14862 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23787	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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 21.84 % 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 6.4455e-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: CA, EDO, 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	0.78	1/6027 (0.0%)	0.92	3/8188 (0.0%)
1	BBB	0.80	4/5863 (0.1%)	0.92	7/7960 (0.1%)
All	All	0.79	5/11890 (0.0%)	0.92	10/16148 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	375	GLU	CD-OE1	6.12	1.32	1.25
1	BBB	79	GLU	CD-OE2	-5.65	1.19	1.25
1	BBB	32[A]	GLU	CD-OE1	5.53	1.31	1.25
1	BBB	32[B]	GLU	CD-OE1	5.53	1.31	1.25
1	AAA	714	GLU	CD-OE2	-5.47	1.19	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	313	ARG	CG-CD-NE	-7.97	95.06	111.80
1	BBB	442[A]	ASP	CB-CG-OD1	7.10	124.69	118.30
1	BBB	442[B]	ASP	CB-CG-OD1	7.10	124.69	118.30
1	AAA	174[A]	PRO	C-N-CA	6.12	137.00	121.70
1	AAA	174[B]	PRO	C-N-CA	6.12	137.00	121.70
1	BBB	70	TYR	CB-CG-CD1	-5.69	117.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	313	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	BBB	399	THR	CA-CB-CG2	-5.41	104.83	112.40
1	BBB	456	GLU	C-N-CA	5.38	133.59	122.30
1	AAA	329	ARG	NE-CZ-NH2	-5.07	117.76	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	172	SER	Mainchain
1	AAA	456[A]	GLU	Peptide
1	AAA	457[A]	GLY	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	5842	5705	5629	88	1
1	BBB	5687	5551	5464	53	0
2	AAA	23	21	0	0	0
2	BBB	23	21	0	0	0
3	BBB	4	6	6	0	0
4	BBB	1	0	0	0	0
5	AAA	463	0	0	16	0
5	BBB	440	0	0	18	0
All	All	12483	11304	11099	141	1

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.

All (141) 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:174[A]:PRO:HD2	5:AAA:901:HOH:O	1.31	1.29
1:AAA:438[A]:GLU:OE1	1:AAA:441[A]:MET:HE1	1.36	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:438[A]:GLU:OE1	1:AAA:441[A]:MET:CE	1.89	1.19
1:AAA:438[A]:GLU:OE1	1:AAA:441[A]:MET:SD	2.02	1.16
1:AAA:441[B]:MET:SD	1:AAA:559[B]:ARG:NH1	2.18	1.14
1:AAA:174[A]:PRO:CD	5:AAA:901:HOH:O	1.83	1.13
1:AAA:453[B]:ALA:HB3	1:AAA:460:TYR:HB3	1.08	1.07
1:AAA:449[A]:ARG:HG3	1:AAA:449[A]:ARG:HH11	0.93	1.03
1:BBB:441[B]:MET:SD	5:BBB:902:HOH:O	2.17	1.00
1:AAA:453[B]:ALA:CB	1:AAA:460:TYR:HB3	1.94	0.97
1:AAA:449[A]:ARG:HG3	1:AAA:449[A]:ARG:NH1	1.72	0.97
1:AAA:174[A]:PRO:N	5:AAA:901:HOH:O	1.88	0.95
1:BBB:536[A]:GLN:HG2	1:BBB:590:TYR:CD1	2.06	0.90
1:AAA:453[B]:ALA:HB3	1:AAA:460:TYR:CB	2.00	0.90
1:AAA:355:VAL:O	1:AAA:399[A]:THR:HG23	1.73	0.86
1:AAA:438[A]:GLU:CD	1:AAA:441[A]:MET:SD	2.53	0.86
1:AAA:449[A]:ARG:HH11	1:AAA:449[A]:ARG:CG	1.84	0.86
1:BBB:259:ASN:HD21	1:BBB:302:ASN:H	1.26	0.81
1:AAA:462[B]:LYS:O	1:AAA:466[B]:GLU:HG3	1.81	0.81
1:AAA:483:LEU:HD12	5:AAA:1238:HOH:O	1.83	0.78
1:BBB:366[B]:MET:CE	5:BBB:1270:HOH:O	2.33	0.76
1:AAA:288[B]:ASN:ND2	1:AAA:289:PRO:HD2	2.01	0.74
1:BBB:32[A]:GLU:CB	5:BBB:1135:HOH:O	2.35	0.73
1:AAA:483:LEU:CD1	5:AAA:1238:HOH:O	2.36	0.73
1:AAA:461:ASP:O	1:AAA:462[B]:LYS:C	2.27	0.72
1:BBB:32[A]:GLU:HB2	5:BBB:1135:HOH:O	1.89	0.72
1:BBB:451:LEU:HD21	1:BBB:567:ARG:NH1	2.06	0.71
1:AAA:450:PHE:CE1	1:AAA:465[B]:PHE:HD1	2.09	0.69
1:AAA:451[A]:LEU:O	1:AAA:455[A]:LYS:HG3	1.92	0.69
1:AAA:397:TYR:CE2	1:AAA:399[B]:THR:HG22	2.28	0.69
1:AAA:247:GLU:OE1	5:AAA:903:HOH:O	2.11	0.68
1:BBB:314:VAL:HG22	5:BBB:1130:HOH:O	1.94	0.67
1:BBB:355:VAL:O	1:BBB:399:THR:HG23	1.96	0.66
1:AAA:453[A]:ALA:O	1:AAA:457[A]:GLY:N	2.28	0.66
1:AAA:461:ASP:O	1:AAA:463[B]:ALA:N	2.30	0.64
1:AAA:449[A]:ARG:NE	1:AAA:464[A]:ASP:OD2	2.31	0.63
1:BBB:259:ASN:ND2	1:BBB:302:ASN:H	1.96	0.63
1:AAA:461:ASP:C	1:AAA:463[B]:ALA:N	2.53	0.62
1:BBB:483[B]:LEU:HD12	1:BBB:484:MET:HE2	1.81	0.61
1:BBB:171:HIS:HD2	1:BBB:205:ALA:O	1.84	0.59
1:AAA:354:PRO:HB2	1:AAA:399[A]:THR:HG22	1.84	0.59
1:BBB:483[B]:LEU:HD12	1:BBB:484:MET:CE	2.33	0.59
1:BBB:536[A]:GLN:HG2	1:BBB:590:TYR:CG	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:323:ILE:CD1	1:BBB:366[B]:MET:HG2	2.34	0.58
1:BBB:626:ALA:HB3	1:BBB:629:ASN:ND2	2.18	0.58
1:BBB:32[A]:GLU:HB3	5:BBB:1135:HOH:O	1.99	0.58
1:AAA:397:TYR:HE2	1:AAA:399[B]:THR:HG22	1.69	0.58
1:BBB:483[B]:LEU:HD22	5:BBB:1195:HOH:O	2.05	0.57
1:AAA:399[B]:THR:CG2	5:AAA:1156:HOH:O	2.53	0.56
1:AAA:504:LEU:HD12	1:AAA:541:ILE:HD12	1.87	0.56
1:AAA:419[A]:GLU:OE2	5:AAA:904:HOH:O	2.17	0.56
1:AAA:356:TYR:HB3	1:AAA:399[A]:THR:HG21	1.88	0.56
1:BBB:147:LEU:O	1:BBB:151:LYS:HE3	2.06	0.55
1:BBB:184[B]:GLU:OE1	5:BBB:901:HOH:O	2.18	0.55
1:BBB:536[A]:GLN:HG2	1:BBB:590:TYR:CE1	2.41	0.55
1:AAA:15:GLN:NE2	1:AAA:15:GLN:HA	2.22	0.54
1:AAA:462[B]:LYS:O	1:AAA:466[B]:GLU:CG	2.54	0.54
1:AAA:323:ILE:CD1	1:AAA:366[B]:MET:HG2	2.38	0.53
1:AAA:438[B]:GLU:OE1	1:AAA:559[B]:ARG:NH1	2.41	0.53
1:AAA:460:TYR:O	1:AAA:461:ASP:HB2	2.08	0.53
1:AAA:710:VAL:HG21	5:AAA:1292:HOH:O	2.09	0.53
1:BBB:301:LEU:HD23	1:BBB:307:ILE:HD11	1.91	0.52
1:AAA:355:VAL:O	1:AAA:399[B]:THR:HG22	2.10	0.52
1:AAA:651:ASP:OD1	1:AAA:678:SER:HA	2.10	0.52
1:AAA:449[A]:ARG:NH1	1:AAA:449[A]:ARG:CG	2.55	0.51
1:BBB:555[B]:LYS:HE2	5:BBB:1103:HOH:O	2.11	0.51
1:BBB:342:VAL:HG23	5:BBB:1172:HOH:O	2.11	0.50
1:AAA:438[A]:GLU:HB3	1:AAA:441[A]:MET:CE	2.42	0.50
1:AAA:464[B]:ASP:O	1:AAA:468:LEU:HG	2.12	0.50
1:AAA:461:ASP:C	1:AAA:463[B]:ALA:H	2.16	0.49
1:AAA:450:PHE:CE1	1:AAA:465[B]:PHE:CD1	2.97	0.49
1:AAA:399[B]:THR:HG23	5:AAA:1156:HOH:O	2.13	0.48
1:AAA:671:VAL:CG1	1:AAA:682:ALA:HB1	2.43	0.48
1:BBB:215:ASN:ND2	1:BBB:218:ASP:H	2.10	0.48
1:BBB:366[B]:MET:HE2	5:BBB:1270:HOH:O	2.08	0.48
1:AAA:444:GLN:OE1	1:AAA:559[B]:ARG:NH2	2.46	0.48
1:BBB:308:MET:HA	1:BBB:335:TYR:O	2.14	0.48
1:BBB:83:LEU:HD23	1:BBB:83:LEU:C	2.34	0.47
1:AAA:173[A]:ALA:HA	1:AAA:174[A]:PRO:HA	1.55	0.47
1:BBB:238:ALA:HA	1:BBB:276:VAL:O	2.14	0.47
1:AAA:33:ALA:HB2	1:AAA:60:GLY:HA2	1.97	0.47
1:AAA:438[B]:GLU:HA	1:AAA:559[B]:ARG:HH11	1.80	0.47
1:AAA:438[A]:GLU:HB3	1:AAA:441[A]:MET:HE2	1.97	0.47
1:BBB:349:HIS:HE1	5:BBB:1276:HOH:O	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:262:ASP:HA	1:AAA:266:ALA:HB3	1.97	0.47
1:BBB:536[A]:GLN:CG	1:BBB:590:TYR:CD1	2.89	0.46
1:AAA:657:GLY:HA3	1:AAA:694:PHE:CZ	2.50	0.46
1:AAA:450:PHE:HE1	1:AAA:465[B]:PHE:HD1	1.61	0.46
1:AAA:459:ASN:O	1:AAA:460:TYR:CD1	2.69	0.46
1:AAA:397:TYR:CE2	1:AAA:399[B]:THR:CG2	2.99	0.46
1:AAA:454[B]:PHE:CE2	1:AAA:516:VAL:HG22	2.51	0.46
1:AAA:308:MET:HA	1:AAA:335:TYR:O	2.16	0.45
1:AAA:366[B]:MET:HE1	5:AAA:1290:HOH:O	2.16	0.45
1:AAA:81:TYR:CZ	1:AAA:123:ASP:HB3	2.51	0.45
1:AAA:446:ALA:O	1:AAA:464[B]:ASP:HB3	2.16	0.45
1:BBB:171:HIS:HE1	5:BBB:1002:HOH:O	1.99	0.45
1:BBB:214:TRP:CD2	1:BBB:253:LYS:HB3	2.51	0.45
1:BBB:706:LEU:HD11	1:BBB:709:PHE:HB2	1.99	0.45
1:AAA:648:PHE:HA	1:AAA:705:TYR:O	2.17	0.45
1:BBB:151:LYS:HE2	5:BBB:1186:HOH:O	2.16	0.45
1:AAA:446:ALA:HA	1:AAA:449[A]:ARG:HE	1.82	0.45
1:AAA:449[B]:ARG:CG	1:AAA:464[B]:ASP:OD2	2.66	0.44
1:BBB:555[B]:LYS:NZ	5:BBB:921:HOH:O	2.50	0.44
1:AAA:483:LEU:HD11	5:AAA:1238:HOH:O	2.12	0.44
1:AAA:454[B]:PHE:CZ	1:AAA:516:VAL:HG22	2.53	0.44
1:BBB:215:ASN:C	1:BBB:215:ASN:HD22	2.21	0.44
1:BBB:250:ASN:ND2	1:BBB:253:LYS:H	2.16	0.44
1:BBB:396:LYS:CD	5:BBB:1327:HOH:O	2.66	0.44
1:AAA:238:ALA:HA	1:AAA:276:VAL:O	2.18	0.43
1:AAA:323:ILE:HD11	1:AAA:366[B]:MET:HG2	2.00	0.43
1:AAA:8:PRO:HA	1:AAA:9:PRO:HD3	1.88	0.43
1:AAA:149:GLN:HB3	1:AAA:153:TYR:CZ	2.53	0.43
1:AAA:173[A]:ALA:C	5:AAA:901:HOH:O	2.40	0.43
1:BBB:314:VAL:CG2	5:BBB:1130:HOH:O	2.61	0.43
1:AAA:288[B]:ASN:HD22	1:AAA:289:PRO:HD2	1.81	0.43
1:BBB:255:ALA:HA	1:BBB:301:LEU:HD13	2.00	0.42
1:AAA:453[B]:ALA:CB	1:AAA:460:TYR:CB	2.77	0.42
1:AAA:441[B]:MET:SD	1:AAA:559[B]:ARG:CZ	2.99	0.42
1:BBB:262:ASP:HA	1:BBB:266:ALA:HB3	2.02	0.42
1:AAA:81:TYR:CE1	1:AAA:123:ASP:HB3	2.55	0.42
1:BBB:250:ASN:HD22	1:BBB:250:ASN:C	2.23	0.42
1:AAA:227:GLU:OE1	5:AAA:905:HOH:O	2.22	0.41
1:BBB:283:ASN:HD21	1:BBB:286:TRP:HB2	1.85	0.41
1:BBB:451:LEU:HD21	1:BBB:567:ARG:CZ	2.49	0.41
1:BBB:297:LEU:O	1:BBB:301:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:5:LEU:N	5:AAA:922:HOH:O	2.53	0.41
1:BBB:170:TYR:HB2	1:BBB:180:TYR:CE1	2.56	0.41
1:AAA:559[B]:ARG:HD2	1:AAA:560:VAL:HG23	2.02	0.41
1:BBB:125:PRO:HB3	1:BBB:392:TRP:CE3	2.55	0.41
1:BBB:438:GLU:OE2	5:BBB:902:HOH:O	2.21	0.41
1:BBB:483[B]:LEU:CD1	1:BBB:484:MET:CE	2.98	0.41
1:AAA:83:LEU:HD23	1:AAA:83:LEU:C	2.42	0.40
1:AAA:498:TRP:CD1	1:AAA:554:VAL:HG13	2.56	0.40
1:BBB:456:GLU:H	1:BBB:456:GLU:HG3	1.80	0.40
1:BBB:661:ILE:HD11	1:BBB:692:VAL:HG22	2.04	0.40
1:AAA:15:GLN:HA	1:AAA:15:GLN:HE21	1.86	0.40
1:AAA:399[B]:THR:HG23	5:AAA:1012:HOH:O	2.21	0.40
1:AAA:465[A]:PHE:CZ	1:AAA:517:GLU:HG3	2.56	0.40
1:BBB:81:TYR:CZ	1:BBB:123:ASP:HB3	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:170:TYR:HH	1:AAA:442:ASP:OD1[1_455]	1.50	0.10

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	740/737 (100%)	716 (97%)	21 (3%)	3 (0%)	34 13
1	BBB	717/737 (97%)	684 (95%)	29 (4%)	4 (1%)	25 7
All	All	1457/1474 (99%)	1400 (96%)	50 (3%)	7 (0%)	34 9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	461	ASP
1	BBB	457	GLY
1	AAA	462[A]	LYS
1	AAA	462[B]	LYS
1	BBB	581	ASN
1	BBB	453	ALA
1	BBB	677	GLU

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	AAA	611/647 (94%)	596 (98%)	15 (2%)	47	18
1	BBB	593/647 (92%)	581 (98%)	12 (2%)	55	25
All	All	1204/1294 (93%)	1177 (98%)	27 (2%)	55	22

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	4	SER
1	AAA	6	GLN
1	AAA	19	ILE
1	AAA	87	GLU
1	AAA	174[A]	PRO
1	AAA	174[B]	PRO
1	AAA	288[A]	ASN
1	AAA	288[B]	ASN
1	AAA	371	THR
1	AAA	449[A]	ARG
1	AAA	449[B]	ARG
1	AAA	455[A]	LYS
1	AAA	455[B]	LYS
1	AAA	603	LYS
1	AAA	696	ASN
1	BBB	215	ASN
1	BBB	250	ASN

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Mol	Chain	Res	Type
1	BBB	301	LEU
1	BBB	371	THR
1	BBB	373	PRO
1	BBB	412	PRO
1	BBB	456	GLU
1	BBB	596	ILE
1	BBB	600	GLU
1	BBB	660	GLU
1	BBB	670	THR
1	BBB	678	SER

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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
2	1XI	BBB	801	-	23,25,25	1.00	1 (4%)	24,35,35	0.94	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	BBB	802	-	3,3,3	0.11	0	2,2,2	0.29	0
2	1XI	AAA	801	-	23,25,25	0.87	2 (8%)	24,35,35	0.94	2 (8%)

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	801	-	-	2/9/38/38	0/3/3/3
3	EDO	BBB	802	-	-	0/1/1/1	-
2	1XI	AAA	801	-	-	1/9/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	801	1XI	C22-N23	3.88	1.33	1.26
2	AAA	801	1XI	C22-N23	2.34	1.30	1.26
2	AAA	801	1XI	C20-S21	-2.33	1.76	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	801	1XI	C3-N2-C5	-2.20	115.64	119.17
2	AAA	801	1XI	C3-N2-C5	-2.11	115.77	119.17
2	AAA	801	1XI	C20-C5-C6	2.05	118.83	115.72

There are no chirality outliers.

All (3) torsion outliers are listed below:

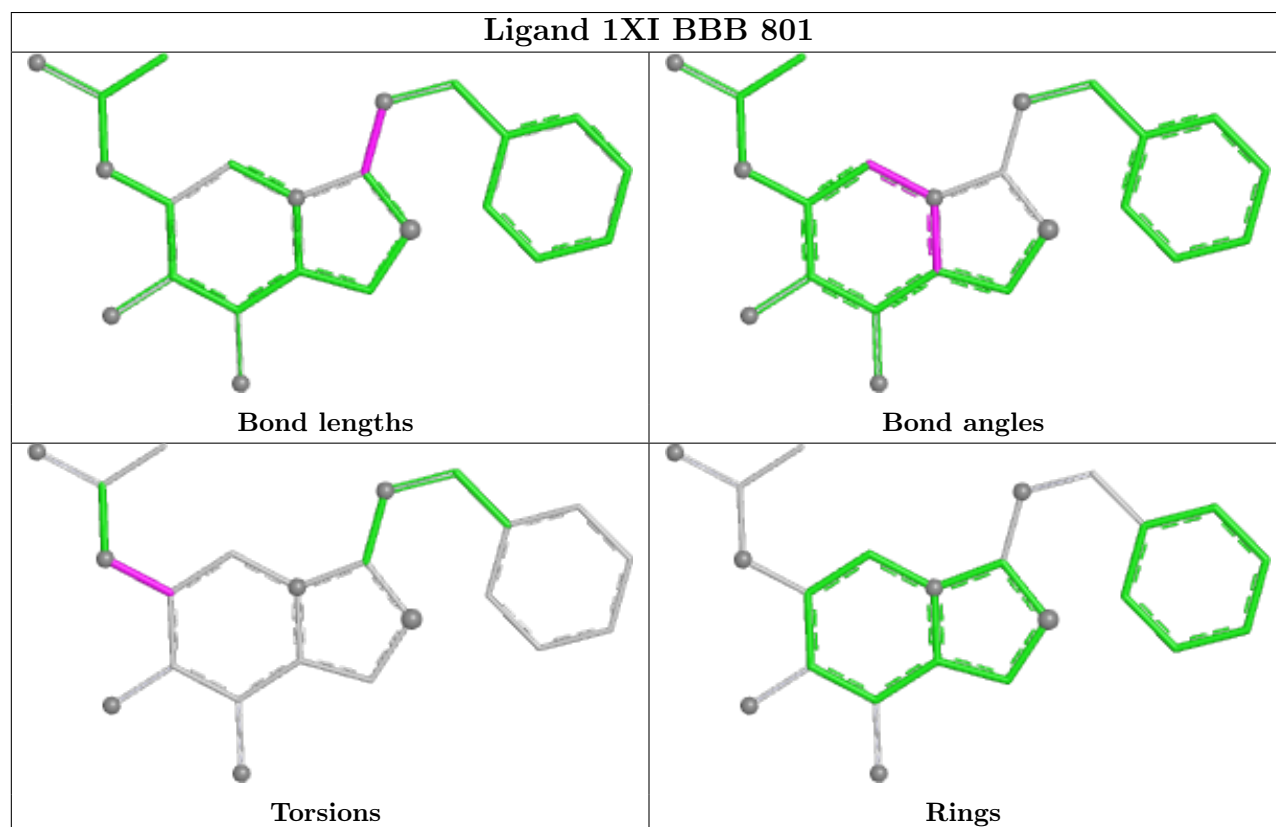
Mol	Chain	Res	Type	Atoms
2	AAA	801	1XI	C3-C2-N1-C32
2	BBB	801	1XI	C3-C2-N1-C32
2	BBB	801	1XI	C7-C2-N1-C32

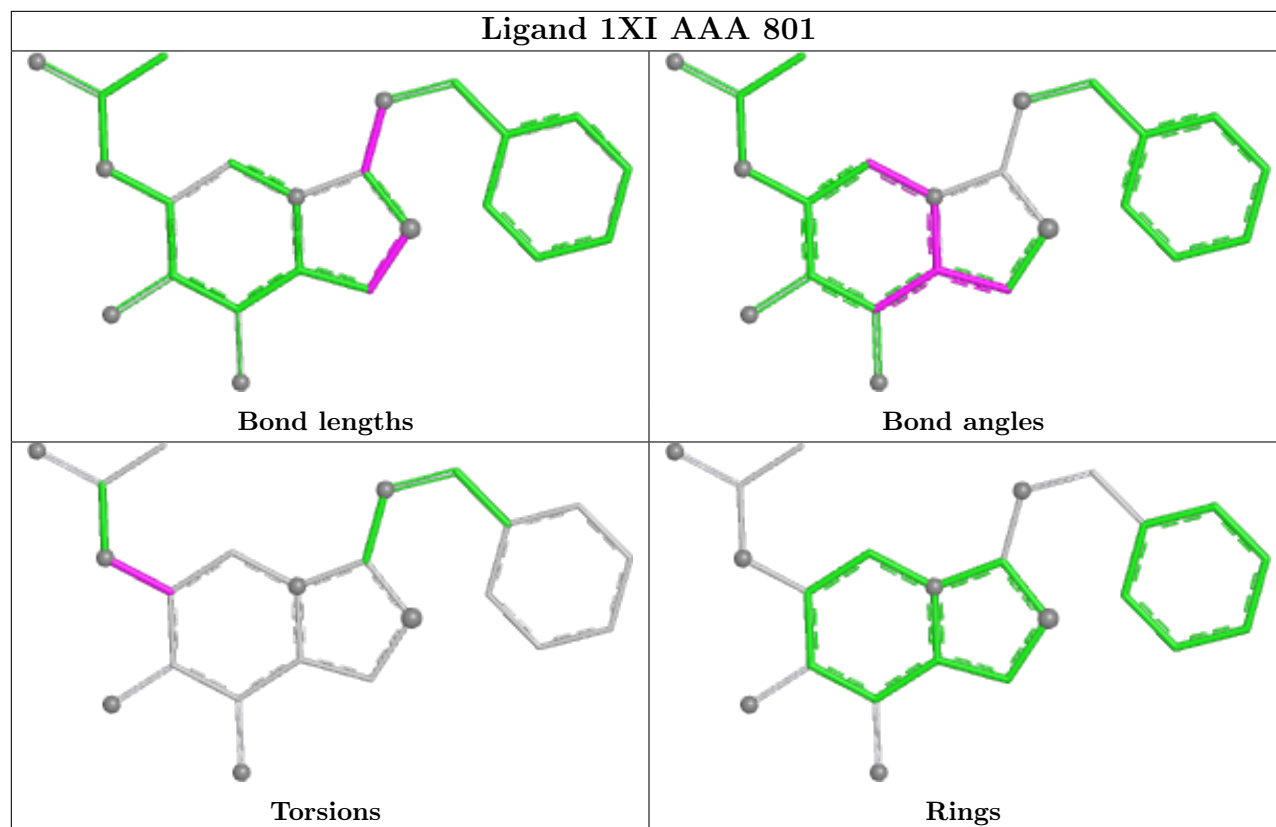
There are no ring outliers.

No monomer is involved in short contacts.

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

also be included. For torsion angles, if less 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

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	AAA	714/737 (96%)	0.10	27 (3%) 40 44	13, 24, 51, 76	0
1	BBB	708/737 (96%)	0.37	80 (11%) 5 5	11, 22, 79, 109	0
All	All	1422/1474 (96%)	0.23	107 (7%) 14 14	11, 23, 67, 109	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	625	TRP	13.8
1	BBB	697	VAL	12.0
1	BBB	656	TRP	11.9
1	BBB	626	ALA	9.3
1	BBB	695	THR	8.7
1	BBB	622	VAL	8.5
1	BBB	659	LEU	8.3
1	BBB	706	LEU	8.1
1	BBB	602	ILE	8.0
1	BBB	627	ALA	7.7
1	BBB	619	ALA	7.5
1	AAA	24	VAL	7.4
1	BBB	657	GLY	7.4
1	BBB	680	LEU	7.3
1	BBB	694	PHE	7.0
1	BBB	698	SER	6.9
1	BBB	598	ASN	6.9
1	BBB	605	LEU	6.8
1	BBB	655	THR	6.6
1	BBB	599	VAL	6.6
1	BBB	673	LEU	6.5
1	AAA	3	VAL	6.5
1	BBB	699	ASP	6.4
1	BBB	629	ASN	6.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	709	PHE	6.3
1	BBB	630	SER	6.2
1	BBB	646	ILE	6.2
1	BBB	628	GLY	6.2
1	BBB	648	PHE	6.0
1	BBB	668	TRP	6.0
1	BBB	671	VAL	5.8
1	BBB	702	GLN	5.6
1	BBB	661	ILE	5.6
1	BBB	652	ALA	5.6
1	BBB	596	ILE	5.5
1	BBB	696	ASN	5.4
1	AAA	47	GLY	5.2
1	BBB	600	GLU	5.0
1	BBB	454	PHE	4.8
1	BBB	644	ILE	4.7
1	BBB	620	ASN	4.7
1	BBB	601	GLN	4.7
1	BBB	670	THR	4.7
1	BBB	678	SER	4.6
1	BBB	597	SER	4.5
1	BBB	693	ARG	4.4
1	BBB	603	LYS	4.3
1	AAA	4	SER	4.2
1	BBB	623	VAL	4.2
1	BBB	692	VAL	4.2
1	BBB	46	SER	4.2
1	BBB	604	ASN	4.1
1	BBB	658	ARG	4.0
1	BBB	650	LYS	3.9
1	AAA	457[A]	GLY	3.9
1	BBB	649	GLY	3.7
1	BBB	679	ARG	3.6
1	BBB	701	GLU	3.5
1	BBB	618	PRO	3.5
1	AAA	56	LEU	3.3
1	BBB	660	GLU	3.3
1	BBB	682	ALA	3.3
1	BBB	669	LYS	3.3
1	AAA	57	ILE	3.3
1	AAA	50	SER	3.3
1	AAA	52	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	595	MET	3.2
1	BBB	624	LYS	3.1
1	BBB	631	VAL	3.1
1	BBB	647	ASN	3.1
1	AAA	54	GLY	3.0
1	AAA	21	LEU	3.0
1	BBB	707	ARG	3.0
1	BBB	616	ILE	3.0
1	AAA	14	VAL	2.9
1	BBB	672	ASP	2.8
1	AAA	46	SER	2.8
1	BBB	457	GLY	2.8
1	AAA	53	LYS	2.7
1	BBB	633	ILE	2.7
1	BBB	16	ASN	2.6
1	AAA	19	ILE	2.6
1	AAA	23	ALA	2.6
1	BBB	645	GLN	2.5
1	AAA	25	TYR	2.5
1	AAA	460	TYR	2.5
1	AAA	540	TYR	2.5
1	BBB	676	LYS	2.4
1	AAA	655	THR	2.4
1	BBB	651	ASP	2.4
1	AAA	16	ASN	2.4
1	AAA	27	LEU	2.4
1	AAA	45	LEU	2.3
1	BBB	642	GLU	2.3
1	AAA	290	ASN	2.3
1	BBB	643	ASN	2.3
1	AAA	291	GLY	2.3
1	AAA	51	SER	2.2
1	BBB	710	VAL	2.2
1	BBB	700	GLU	2.2
1	BBB	4	SER	2.1
1	BBB	632	GLU	2.1
1	BBB	666	LYS	2.1
1	BBB	3	VAL	2.1
1	AAA	22	PRO	2.1
1	BBB	711	LEU	2.1
1	BBB	581	ASN	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](#)

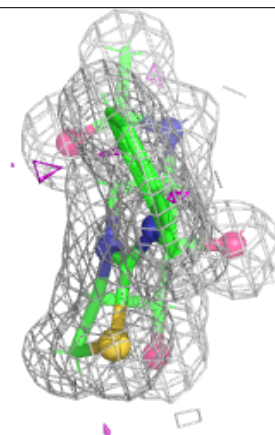
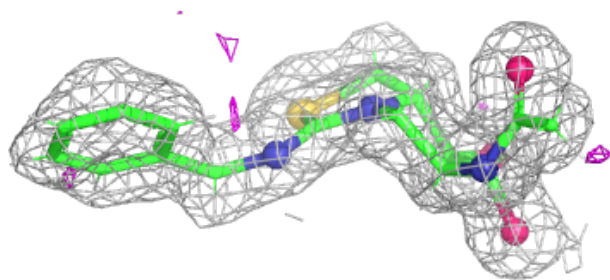
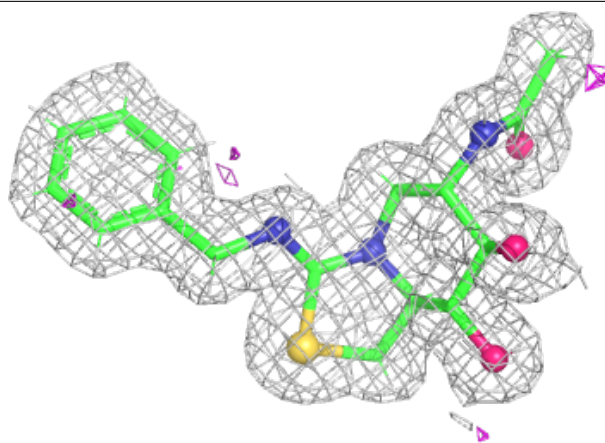
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	BBB	802	4/4	0.93	0.18	37,39,41,41	1
2	1XI	BBB	801	23/23	0.98	0.07	12,13,24,25	2
2	1XI	AAA	801	23/23	0.98	0.08	14,15,32,34	2
4	CA	BBB	803	1/1	0.99	0.04	22,22,22,22	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.

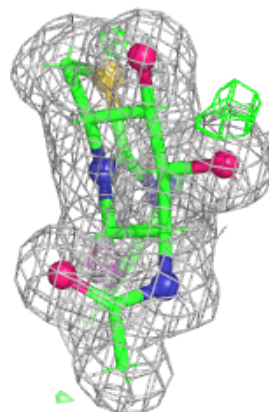
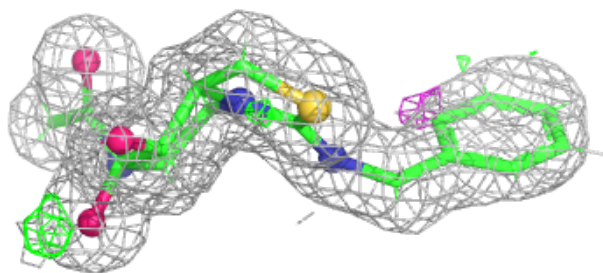
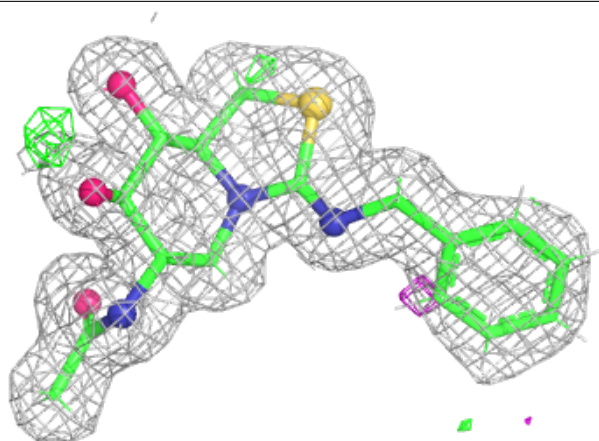
Electron density around 1XI BBB 801:

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



Electron density around 1XI AAA 801:

$2mF_o-DF_c$ (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.