Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 09:16 am GMT

PDB ID	:	8OHX
Title	:	Crystal structure of Beta-glucuronidase from Escherichia coli in complex with siastatin B derived inhibitor
Authors	:	Armstrong, Z.; Yurong, C.; Wu, L.; Overkleeft, H.S.; Davies, G.J.
Deposited on	:	2023-03-21
Resolution	:	1.95 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:

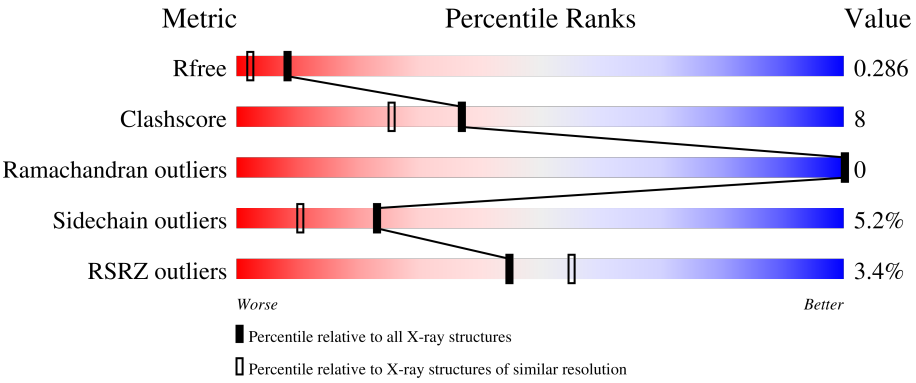
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

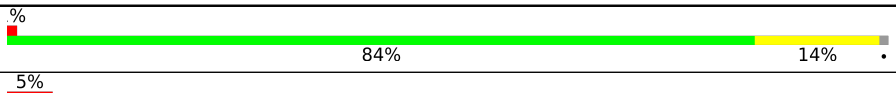
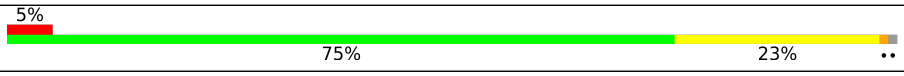
The reported resolution of this entry is 1.95 Å.

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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	601	
1	BBB	601	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9892 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.

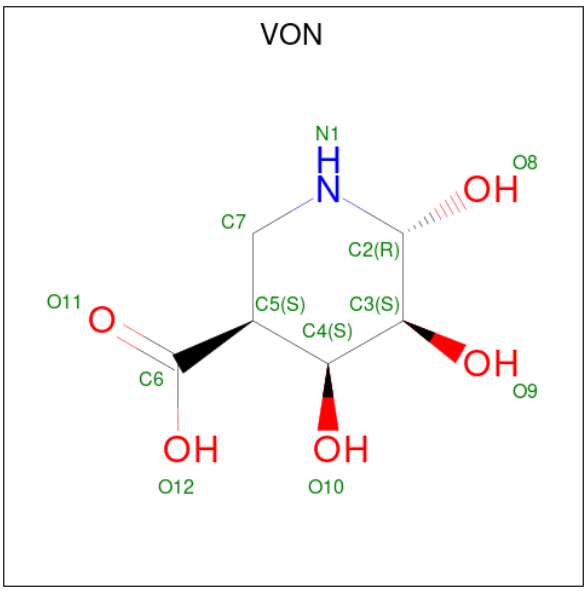
- Molecule 1 is a protein called Beta-D-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	595	Total	C	N	O	S	0	1	0
			4786	3039	826	899	22			
1	BBB	593	Total	C	N	O	S	0	1	0
			4770	3029	823	896	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	SER	-	expression tag	UNP U4Q148
AAA	0	HIS	-	expression tag	UNP U4Q148
BBB	-1	SER	-	expression tag	UNP U4Q148
BBB	0	HIS	-	expression tag	UNP U4Q148

- Molecule 2 is (3 {S},4 {S},5 {S},6 {R})-4,5,6-tris(oxidanyl)piperidine-3-carboxylic acid (three-letter code: VON) (formula: $C_6H_{11}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total 12	C 6	N 1	O 5	0	0
2	BBB	1	Total 12	C 6	N 1	O 5	0	0

- Molecule 3 is water.

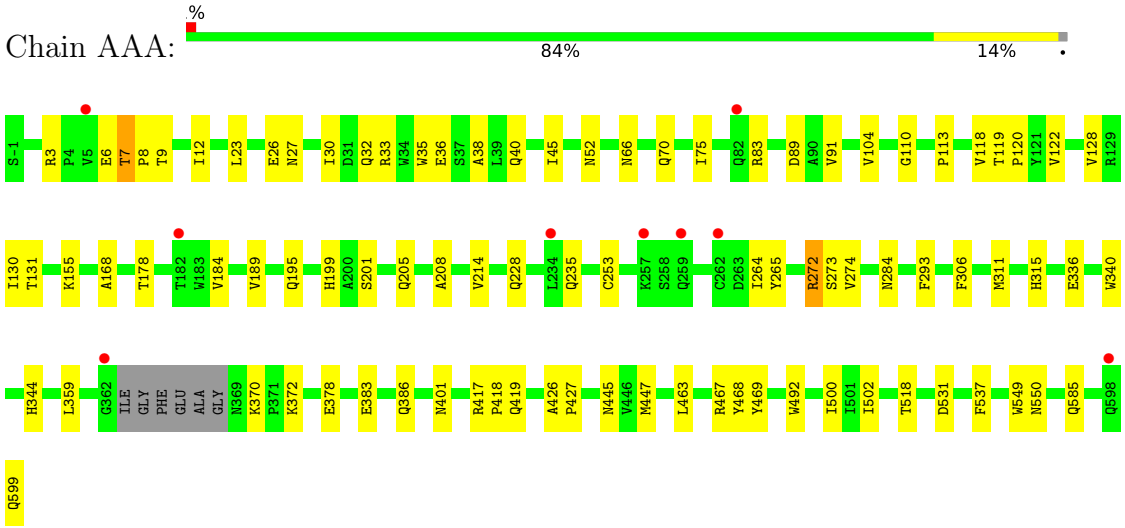
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	202	Total 202	O 202	0	0
3	BBB	110	Total 110	O 110	0	0

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.

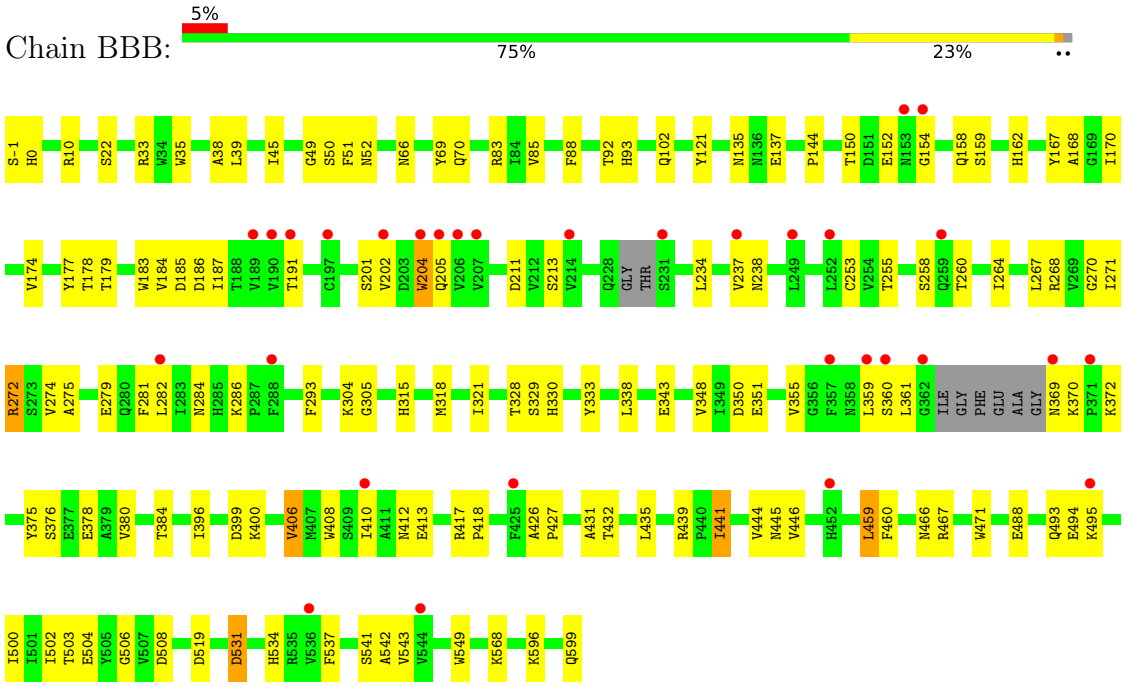
• Molecule 1: Beta-D-glucuronidase

Chain AAA:



• Molecule 1: Beta-D-glucuronidase

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.28Å 76.71Å 141.02Å 90.00° 102.01° 90.00°	Depositor
Resolution (Å)	61.84 – 1.95 67.04 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (61.84-1.95) 98.2 (67.04-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.221 , 0.285 0.227 , 0.286	Depositor DCC
R_{free} test set	4644 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9892	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: VON

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	0.68	0/4914	0.85	0/6686
1	BBB	0.68	0/4897	0.85	0/6663
All	All	0.68	0/9811	0.85	0/13349

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	1
1	BBB	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	293	PHE	Peptide
1	BBB	293	PHE	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	4786	0	4570	57	0
1	BBB	4770	0	4546	89	0
2	AAA	12	0	0	0	0
2	BBB	12	0	0	3	0
3	AAA	202	0	0	5	0
3	BBB	110	0	0	5	0
All	All	9892	0	9116	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (146) 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:130:ILE:C	3:AAA:701:HOH:O	1.71	1.28
1:AAA:130:ILE:O	3:AAA:701:HOH:O	1.53	1.21
1:BBB:543:VAL:O	1:BBB:596:LYS:NZ	2.01	0.92
1:AAA:272:ARG:HA	1:AAA:284:ASN:HD21	1.33	0.91
1:AAA:7:THR:HG21	1:AAA:264:ILE:O	1.71	0.89
1:BBB:191:THR:CG2	1:BBB:271:ILE:HA	2.13	0.78
1:BBB:253:CYS:SG	1:BBB:264:ILE:HG23	2.29	0.72
1:BBB:38:ALA:HA	1:BBB:70:GLN:HE22	1.55	0.71
1:BBB:380:VAL:HG13	1:BBB:384:THR:HG21	1.73	0.71
1:AAA:52:ASN:HD21	1:AAA:168:ALA:H	1.41	0.69
1:AAA:119:THR:HB	1:AAA:120:PRO:HD3	1.75	0.68
1:BBB:445:ASN:ND2	1:BBB:467:ARG:HH12	1.89	0.68
1:BBB:355:VAL:HG23	1:BBB:412:ASN:HD22	1.57	0.68
1:AAA:33:ARG:HA	1:AAA:35:TRP:CZ3	2.28	0.67
1:AAA:33:ARG:HG2	1:AAA:35:TRP:CH2	2.30	0.67
1:BBB:39:LEU:H	1:BBB:70:GLN:NE2	1.92	0.67
1:AAA:70:GLN:HG3	3:AAA:701:HOH:O	1.95	0.66
1:BBB:191:THR:HG21	1:BBB:271:ILE:HA	1.77	0.66
1:AAA:306:PHE:CZ	1:AAA:336:GLU:HG3	2.30	0.66
1:BBB:10:ARG:HB3	3:BBB:795:HOH:O	1.96	0.66
1:BBB:33:ARG:HG2	1:BBB:35:TRP:CH2	2.31	0.65
1:BBB:39:LEU:H	1:BBB:70:GLN:HE22	1.42	0.65
1:AAA:184:VAL:HA	1:AAA:208:ALA:HB2	1.77	0.65
1:AAA:272:ARG:CA	1:AAA:284:ASN:HD21	2.08	0.64
1:AAA:445:ASN:HD21	1:AAA:467:ARG:HH22	1.49	0.61
1:BBB:52:ASN:HD21	1:BBB:168:ALA:H	1.48	0.61
1:BBB:350:ASP:OD2	1:BBB:399:ASP:OD2	2.19	0.61
1:BBB:396:ILE:HG23	1:BBB:408:TRP:CZ2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:500:ILE:O	1:BBB:543:VAL:HA	2.01	0.60
1:BBB:38:ALA:HA	1:BBB:70:GLN:NE2	2.16	0.60
1:AAA:447:MET:HE3	1:AAA:468:TYR:H	1.66	0.60
1:AAA:27:ASN:OD1	1:AAA:66:ASN:ND2	2.35	0.60
1:BBB:400:LYS:O	1:BBB:439:ARG:NH2	2.29	0.59
1:BBB:162:HIS:HD2	3:BBB:706:HOH:O	1.85	0.59
1:BBB:258:SER:OG	1:BBB:260:THR:HG22	2.03	0.59
1:BBB:426:ALA:HB3	1:BBB:427:PRO:HD3	1.83	0.59
1:AAA:122:VAL:HG12	1:AAA:128:VAL:HG11	1.85	0.58
1:BBB:328:THR:HA	1:BBB:333:TYR:CZ	2.39	0.58
1:AAA:38:ALA:HA	1:AAA:70:GLN:HE22	1.69	0.57
1:BBB:187:ILE:HG21	1:BBB:267:LEU:HD23	1.85	0.57
1:BBB:49:GLY:HA2	1:BBB:305:GLY:HA3	1.87	0.57
1:AAA:447:MET:HE2	1:AAA:469:TYR:CZ	2.40	0.56
1:BBB:493:GLN:HG3	1:BBB:542:ALA:HB2	1.88	0.56
1:AAA:104:VAL:HG21	1:AAA:118:VAL:HG12	1.88	0.55
1:AAA:311:MET:O	1:AAA:315:HIS:HD2	1.89	0.55
1:BBB:432:THR:HG22	1:BBB:441:ILE:HG21	1.89	0.55
1:BBB:39:LEU:N	1:BBB:70:GLN:HE22	2.05	0.54
1:AAA:447:MET:HE3	1:AAA:467:ARG:HA	1.88	0.54
1:AAA:445:ASN:ND2	1:AAA:467:ARG:HH22	2.05	0.54
1:AAA:447:MET:CE	1:AAA:468:TYR:H	2.21	0.53
1:BBB:102:GLN:HG2	1:BBB:121:TYR:CD1	2.43	0.53
1:AAA:463:LEU:HD23	1:AAA:500:ILE:HG12	1.91	0.52
1:BBB:279[B]:GLU:O	1:BBB:279[B]:GLU:HG3	2.08	0.52
1:AAA:273:SER:H	1:AAA:284:ASN:ND2	2.07	0.52
1:BBB:268:ARG:HH12	1:BBB:343:GLU:HG3	1.75	0.52
1:BBB:431:ALA:O	1:BBB:435:LEU:HD12	2.09	0.52
1:BBB:66:ASN:OD1	1:BBB:135:ASN:HB2	2.10	0.51
1:BBB:417:ARG:HB2	1:BBB:418:PRO:HD3	1.92	0.51
1:BBB:85:VAL:HB	1:BBB:177:TYR:CE1	2.45	0.51
1:AAA:7:THR:HG23	1:AAA:8:PRO:HD2	1.93	0.51
1:AAA:130:ILE:N	3:AAA:701:HOH:O	2.43	0.51
1:BBB:355:VAL:CG2	1:BBB:412:ASN:HD22	2.24	0.50
1:BBB:467:ARG:NH2	1:BBB:488:GLU:OE2	2.45	0.50
1:AAA:417:ARG:HB2	1:AAA:418:PRO:HD3	1.93	0.49
1:BBB:272:ARG:HA	1:BBB:284:ASN:OD1	2.11	0.49
1:BBB:380:VAL:HG13	1:BBB:384:THR:CG2	2.42	0.49
1:BBB:330:HIS:HE1	2:BBB:601:VON:O9	1.96	0.49
1:BBB:183:TRP:HD1	1:BBB:184:VAL:O	1.96	0.48
1:BBB:413:GLU:HG2	1:BBB:446:VAL:HA	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:189:VAL:H	1:AAA:401:ASN:ND2	2.12	0.48
1:BBB:50:SER:HB3	1:BBB:52:ASN:HD22	1.78	0.48
1:BBB:167:TYR:HB2	1:BBB:304:LYS:HG3	1.95	0.48
1:BBB:502:ILE:HG13	1:BBB:537:PHE:CZ	2.48	0.48
1:AAA:445:ASN:ND2	1:AAA:467:ARG:HH12	2.12	0.47
1:BBB:137:GLU:HA	1:BBB:158:GLN:NE2	2.28	0.47
1:BBB:92:THR:HA	1:BBB:93:HIS:HA	1.66	0.47
1:BBB:167:TYR:CB	1:BBB:304:LYS:HG3	2.44	0.47
1:BBB:361:LEU:HD12	3:BBB:765:HOH:O	2.14	0.47
1:BBB:466:ASN:OD1	1:BBB:503:THR:HG23	2.13	0.47
1:BBB:38:ALA:CA	1:BBB:70:GLN:HE22	2.27	0.47
1:BBB:83:ARG:O	1:BBB:178:THR:HA	2.15	0.47
1:BBB:204:TRP:CZ3	1:BBB:234:LEU:HG	2.49	0.47
1:AAA:315:HIS:HE1	3:AAA:719:HOH:O	1.98	0.47
1:BBB:531:ASP:O	1:BBB:534:HIS:HB2	2.15	0.47
1:AAA:502:ILE:HG13	1:AAA:537:PHE:CE1	2.50	0.47
1:BBB:137:GLU:HA	1:BBB:158:GLN:HE22	1.80	0.47
1:BBB:191:THR:HG23	1:BBB:271:ILE:HA	1.94	0.47
1:BBB:338:LEU:HD21	1:BBB:348:VAL:HG11	1.97	0.46
1:BBB:502:ILE:HG13	1:BBB:537:PHE:CE1	2.50	0.46
1:BBB:0:HIS:ND1	1:BBB:186:ASP:OD2	2.49	0.46
1:BBB:426:ALA:HA	1:BBB:459:LEU:HD22	1.97	0.46
1:BBB:445:ASN:HD22	1:BBB:467:ARG:HH12	1.61	0.46
1:AAA:3:ARG:O	1:AAA:265:TYR:OH	2.28	0.46
1:AAA:426:ALA:HB3	1:AAA:427:PRO:HD3	1.97	0.46
1:AAA:35:TRP:HA	1:AAA:131:THR:HG21	1.99	0.45
1:BBB:282:LEU:HA	1:BBB:286:LYS:O	2.16	0.45
1:BBB:412:ASN:HA	1:BBB:444:VAL:HB	1.98	0.45
1:AAA:91:VAL:O	1:AAA:110:GLY:HA2	2.16	0.45
1:AAA:445:ASN:HD22	1:AAA:467:ARG:HH12	1.65	0.45
1:AAA:75:ILE:HD12	1:AAA:75:ILE:N	2.32	0.44
1:BBB:315:HIS:CE1	3:BBB:707:HOH:O	2.70	0.44
1:AAA:447:MET:HE1	1:AAA:469:TYR:CD1	2.53	0.44
1:AAA:33:ARG:HG2	1:AAA:35:TRP:CZ2	2.52	0.44
1:BBB:281:PHE:CZ	1:BBB:406:VAL:HG13	2.53	0.44
1:BBB:410:ILE:HD11	1:BBB:460:PHE:CE1	2.52	0.44
1:BBB:268:ARG:NH1	1:BBB:343:GLU:HG3	2.32	0.44
1:BBB:33:ARG:HA	1:BBB:35:TRP:CZ3	2.53	0.43
1:BBB:318:MET:O	1:BBB:321:ILE:HG22	2.19	0.43
1:BBB:508:ASP:OD1	1:BBB:568:LYS:NZ	2.38	0.43
1:AAA:359:LEU:HD22	1:AAA:370:LYS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:447:MET:HE2	1:AAA:469:TYR:CE1	2.53	0.43
1:BBB:275:ALA:O	1:BBB:282:LEU:HB2	2.19	0.43
1:BBB:504:GLU:OE1	2:BBB:601:VON:N1	2.52	0.43
1:AAA:83:ARG:O	1:AAA:178:THR:HA	2.18	0.43
1:AAA:199:HIS:CE1	1:AAA:235:GLN:HG3	2.54	0.42
1:BBB:375:TYR:HA	1:BBB:380:VAL:O	2.19	0.42
1:BBB:432:THR:CG2	1:BBB:441:ILE:HG21	2.49	0.42
1:AAA:6:GLU:HG3	1:AAA:12:ILE:HD12	2.02	0.42
1:BBB:33:ARG:HG2	1:BBB:35:TRP:CZ2	2.54	0.42
1:BBB:268:ARG:HH12	1:BBB:343:GLU:CG	2.31	0.42
1:AAA:199:HIS:HE1	1:AAA:235:GLN:HG3	1.83	0.42
1:AAA:463:LEU:CD2	1:AAA:492:TRP:HB3	2.49	0.42
1:AAA:89:ASP:HA	1:AAA:113:PRO:HB3	2.02	0.42
1:BBB:471:TRP:CZ2	1:BBB:508:ASP:HB2	2.55	0.42
1:AAA:33:ARG:HH11	1:AAA:36:GLU:CD	2.23	0.42
1:AAA:340:TRP:CD1	1:AAA:344:HIS:CD2	3.08	0.41
1:AAA:214:VAL:HA	1:AAA:253:CYS:O	2.20	0.41
1:BBB:10:ARG:NH1	1:BBB:179:THR:HG22	2.36	0.41
1:BBB:413:GLU:OE1	2:BBB:601:VON:C2	2.68	0.41
1:AAA:447:MET:HE1	1:AAA:469:TYR:CG	2.55	0.41
1:AAA:549:TRP:HA	1:AAA:550:ASN:HA	1.88	0.41
1:BBB:69:TYR:CD2	1:BBB:170:ILE:HD12	2.55	0.41
1:BBB:330:HIS:HD2	1:BBB:351:GLU:OE2	2.04	0.41
1:BBB:0:HIS:HB3	1:BBB:185:ASP:O	2.21	0.41
1:BBB:191:THR:HG21	1:BBB:270:GLY:O	2.21	0.41
1:BBB:359:LEU:HD22	1:BBB:370:LYS:CE	2.51	0.41
1:BBB:45:ILE:HD11	1:BBB:51:PHE:HA	2.03	0.40
1:BBB:88:PHE:CD2	1:BBB:174:VAL:HG22	2.56	0.40
1:BBB:150:THR:CG2	1:BBB:154:GLY:HA2	2.50	0.40
1:AAA:32:GLN:O	1:AAA:33:ARG:C	2.59	0.40
1:AAA:75:ILE:HD13	1:AAA:128:VAL:HG13	2.03	0.40
1:BBB:85:VAL:HB	1:BBB:177:TYR:CD1	2.56	0.40
1:AAA:7:THR:CG2	1:AAA:9:THR:H	2.35	0.40
1:AAA:52:ASN:HD22	1:AAA:52:ASN:H	1.69	0.40
1:BBB:315:HIS:HE1	3:BBB:707:HOH:O	2.04	0.40
1:BBB:506:GLY:HA3	1:BBB:549:TRP:O	2.22	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	592/601 (98%)	561 (95%)	31 (5%)	0	100 100
1	BBB	588/601 (98%)	532 (90%)	56 (10%)	0	100 100
All	All	1180/1202 (98%)	1093 (93%)	87 (7%)	0	100 100

There are no Ramachandran outliers to report.

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	508/511 (99%)	486 (96%)	22 (4%)	29 16
1	BBB	506/511 (99%)	475 (94%)	31 (6%)	18 7
All	All	1014/1022 (99%)	961 (95%)	53 (5%)	23 10

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	7	THR
1	AAA	23	LEU
1	AAA	26	GLU
1	AAA	30	ILE
1	AAA	40	GLN
1	AAA	45	ILE
1	AAA	155	LYS
1	AAA	195	GLN

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Mol	Chain	Res	Type
1	AAA	201	SER
1	AAA	205	GLN
1	AAA	228	GLN
1	AAA	272	ARG
1	AAA	274	VAL
1	AAA	372	LYS
1	AAA	378	GLU
1	AAA	383	GLU
1	AAA	386	GLN
1	AAA	419	GLN
1	AAA	518	THR
1	AAA	531	ASP
1	AAA	585	GLN
1	AAA	599	GLN
1	BBB	-1	SER
1	BBB	22	SER
1	BBB	144	PRO
1	BBB	152	GLU
1	BBB	159	SER
1	BBB	201	SER
1	BBB	202	VAL
1	BBB	204	TRP
1	BBB	205	GLN
1	BBB	211	ASP
1	BBB	213	SER
1	BBB	237	VAL
1	BBB	238	ASN
1	BBB	255	THR
1	BBB	272	ARG
1	BBB	274	VAL
1	BBB	329	SER
1	BBB	360	SER
1	BBB	369	ASN
1	BBB	372	LYS
1	BBB	376	SER
1	BBB	378	GLU
1	BBB	406	VAL
1	BBB	441	ILE
1	BBB	459	LEU
1	BBB	494	GLU
1	BBB	495	LYS
1	BBB	519	ASP

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Mol	Chain	Res	Type
1	BBB	531	ASP
1	BBB	541	SER
1	BBB	599	GLN

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	VON	AAA	601	-	11,12,12	1.19	0	12,17,17	2.25	5 (41%)
2	VON	BBB	601	-	11,12,12	1.12	1 (9%)	12,17,17	1.47	1 (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	VON	AAA	601	-	-	3/4/21/21	0/1/1/1
2	VON	BBB	601	-	-	0/4/21/21	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	601	VON	C5-C4	-2.22	1.51	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	601	VON	C7-N1-C2	4.30	117.27	108.98
2	AAA	601	VON	C4-C3-C2	3.68	115.31	109.94
2	AAA	601	VON	O10-C4-C5	-3.30	104.50	110.57
2	AAA	601	VON	O9-C3-C2	-3.19	103.68	109.39
2	AAA	601	VON	C7-N1-C2	3.13	115.02	108.98
2	AAA	601	VON	O12-C6-C5	2.47	120.82	114.03

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	601	VON	C7-C5-C6-O12
2	AAA	601	VON	C7-C5-C6-O11
2	AAA	601	VON	C4-C5-C6-O12

There are no ring outliers.

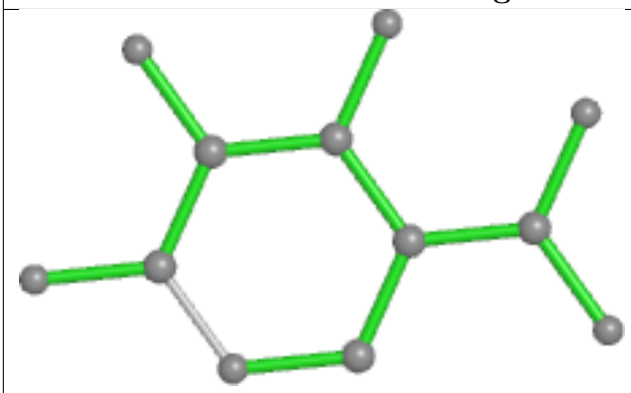
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	601	VON	3	0

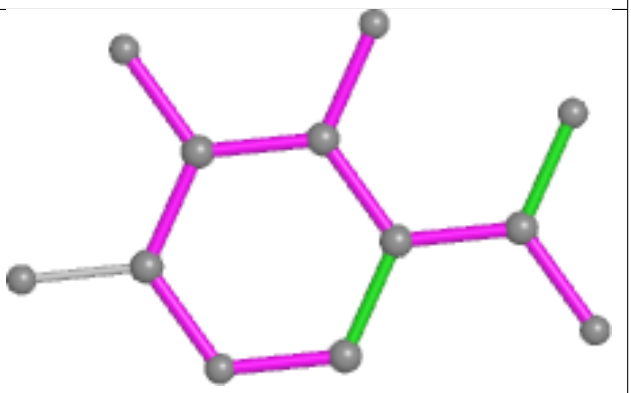
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

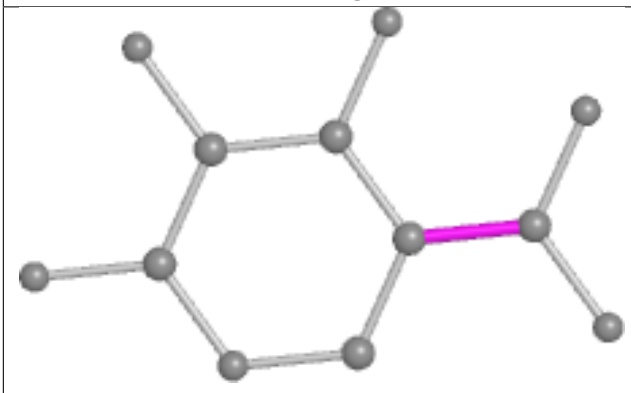
Ligand VON AAA 601



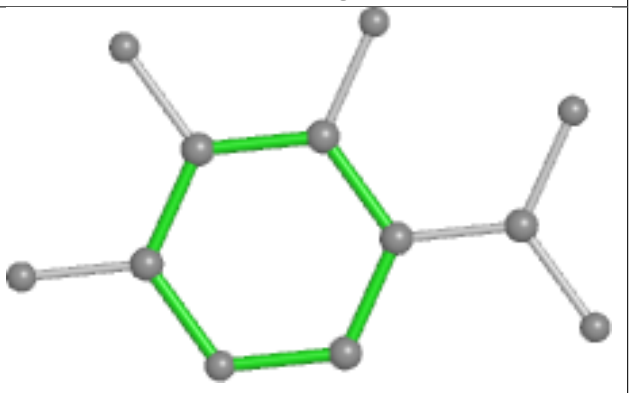
Bond lengths



Bond angles

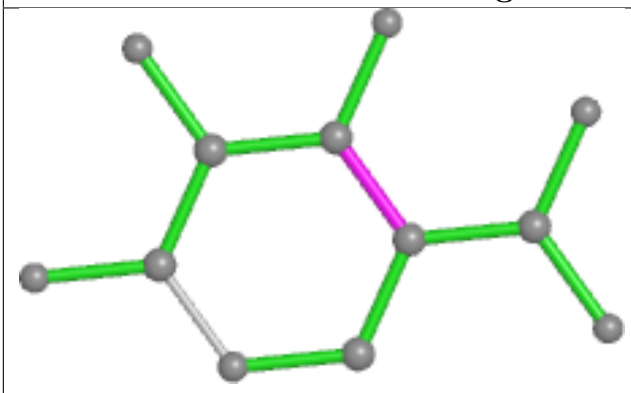


Torsions

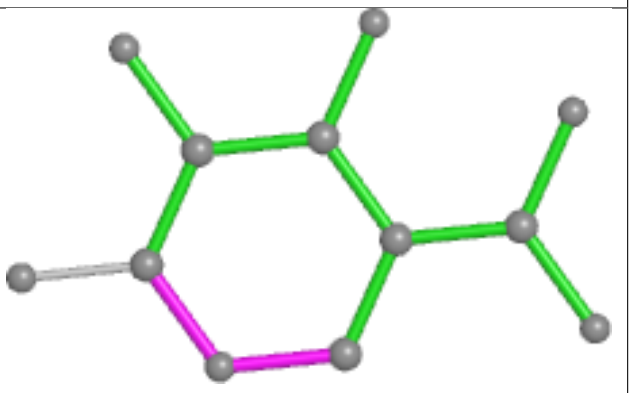


Rings

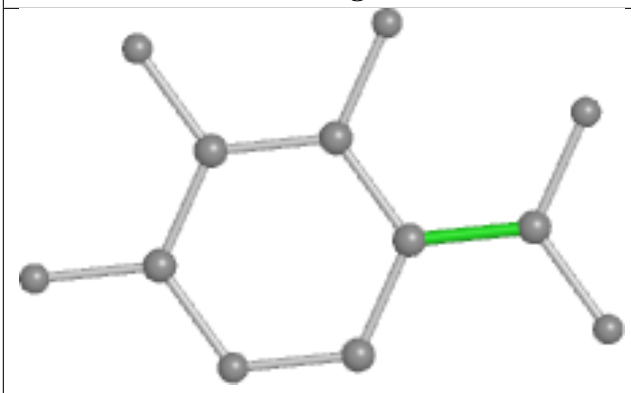
Ligand VON BBB 601



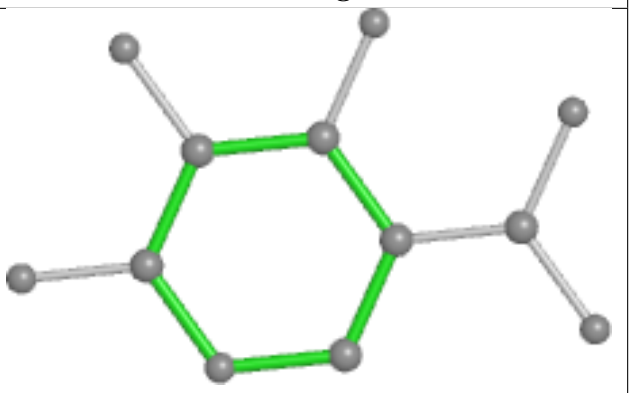
Bond lengths



Bond angles



Torsions



Rings

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, 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	595/601 (99%)	0.12	9 (1%) 73 81	27, 43, 71, 97	0
1	BBB	593/601 (98%)	0.47	31 (5%) 27 37	33, 61, 97, 115	0
All	All	1188/1202 (98%)	0.30	40 (3%) 45 55	27, 51, 87, 115	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	154	GLY	5.6
1	BBB	205	GLN	5.3
1	BBB	357	PHE	3.8
1	BBB	197	CYS	3.7
1	BBB	204	TRP	3.7
1	BBB	153	ASN	3.3
1	AAA	182	THR	3.2
1	BBB	259	GLN	3.2
1	BBB	359	LEU	3.2
1	BBB	362	GLY	3.1
1	BBB	231	SER	2.9
1	AAA	259	GLN	2.9
1	BBB	190	VAL	2.9
1	AAA	598	GLN	2.8
1	BBB	202	VAL	2.8
1	BBB	369	ASN	2.6
1	BBB	371	PRO	2.6
1	BBB	249	LEU	2.5
1	BBB	237	VAL	2.5
1	AAA	362	GLY	2.4
1	BBB	410	ILE	2.4
1	AAA	82	GLN	2.4
1	BBB	206	VAL	2.3
1	BBB	425	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	257	LYS	2.2
1	BBB	360	SER	2.2
1	BBB	288	PHE	2.2
1	BBB	191	THR	2.2
1	BBB	452	HIS	2.2
1	BBB	189	VAL	2.2
1	AAA	262	CYS	2.2
1	BBB	214	VAL	2.2
1	BBB	495	LYS	2.2
1	BBB	207	VAL	2.2
1	BBB	252	LEU	2.1
1	BBB	544	VAL	2.1
1	BBB	282	LEU	2.1
1	BBB	536	VAL	2.1
1	AAA	5	VAL	2.0
1	AAA	234	LEU	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)

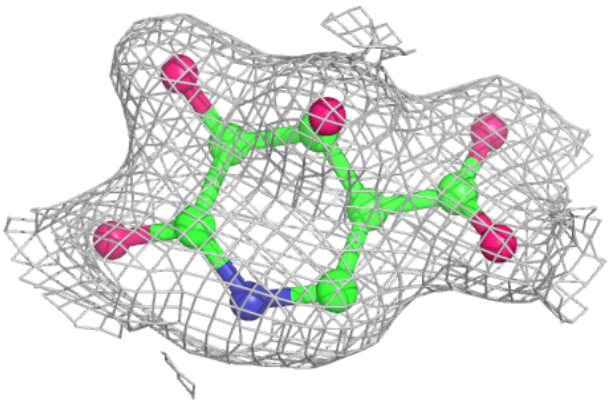
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

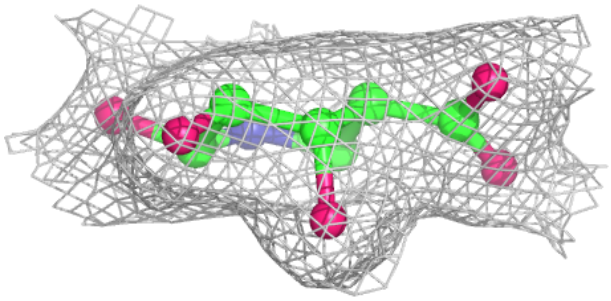
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	VON	BBB	601	12/12	0.91	0.10	42,45,49,52	0
2	VON	AAA	601	12/12	0.96	0.10	30,35,41,44	0

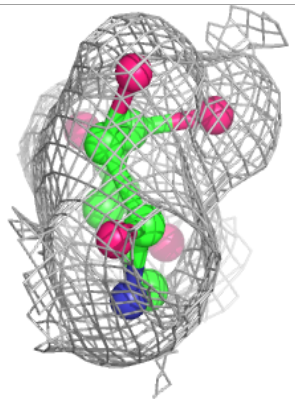
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VON BBB 601:

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

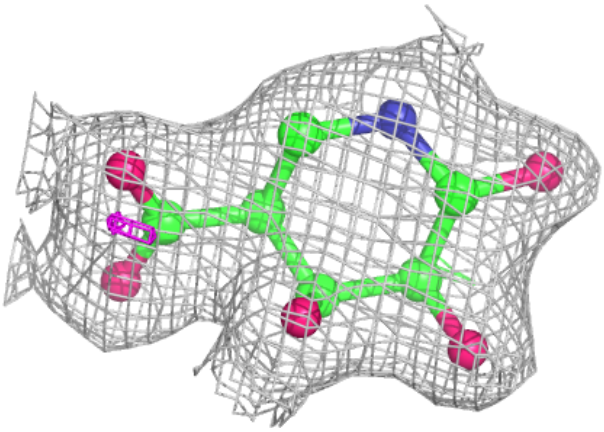


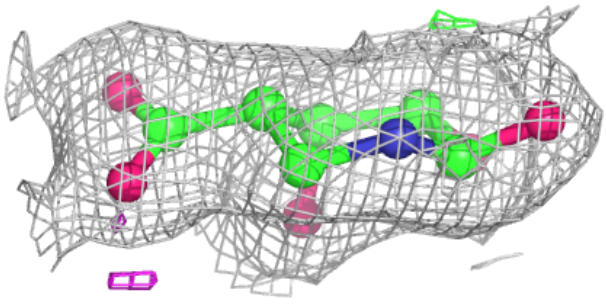


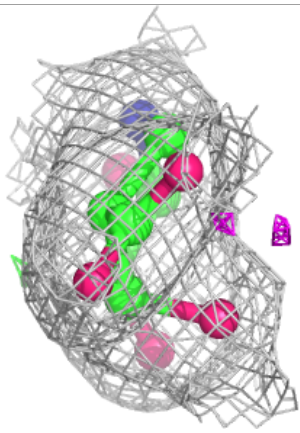


Electron density around VON AAA 601:

$2mF_o$-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.