



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:35 PM UTC

PDB ID : 8OHX / pdb_00008ohx
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	:	4-5-2 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

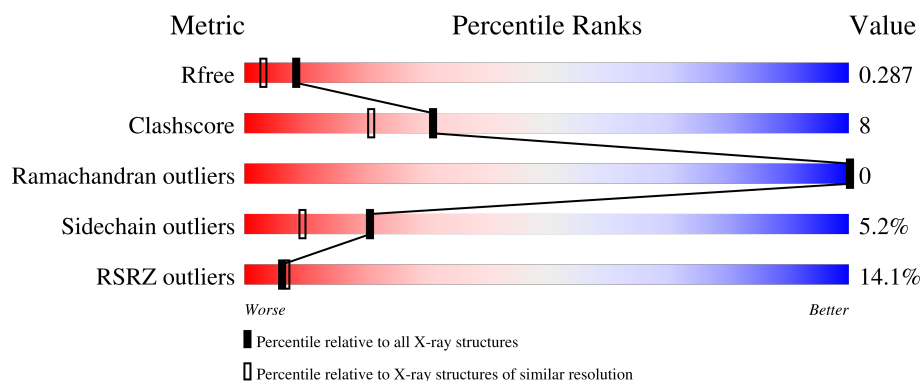
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 $\leq 5\%$. 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	601	6% 83% 16% .
1	BBB	601	22% 73% 24% ..

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.

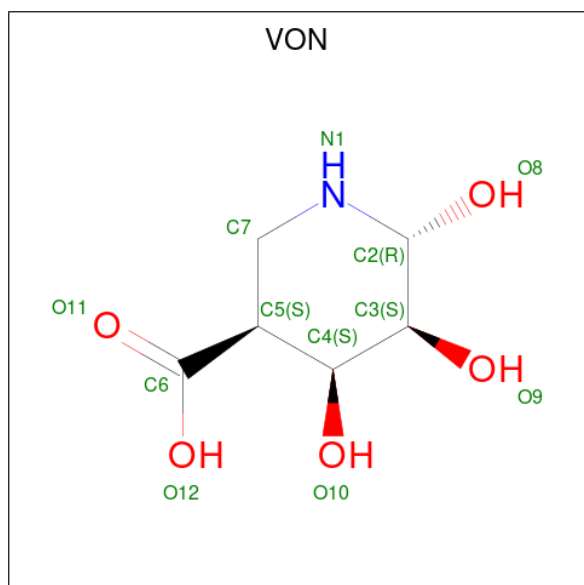
- Molecule 1 is a protein called Beta-D-glucuronidase.

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 (CCD ID: VON) (formula: C₆H₁₁NO₅) (labeled as "Ligand of Interest" by depositor).



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

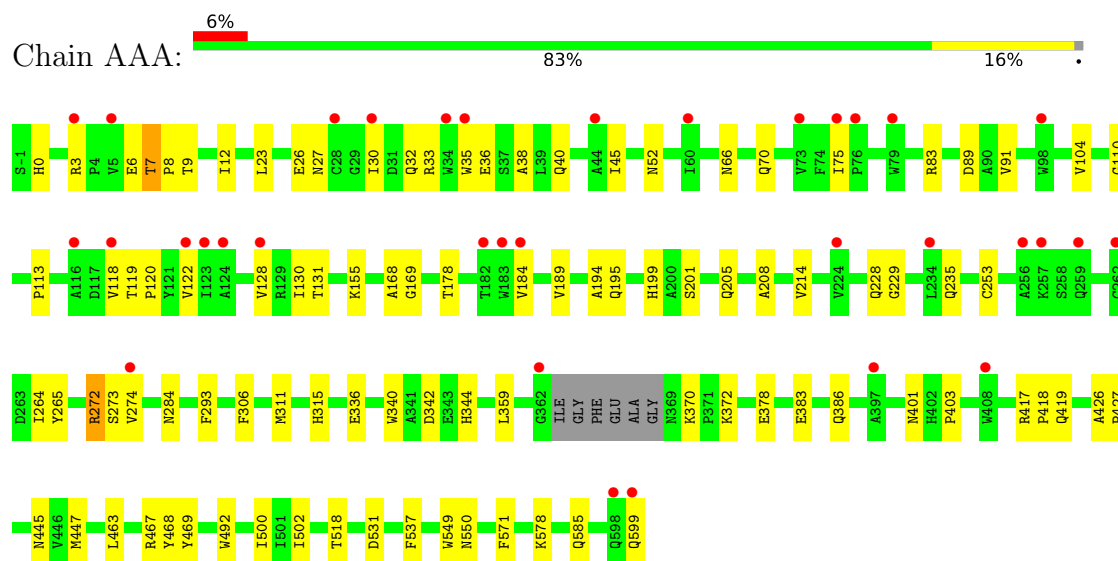
- Molecule 3 is water.

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

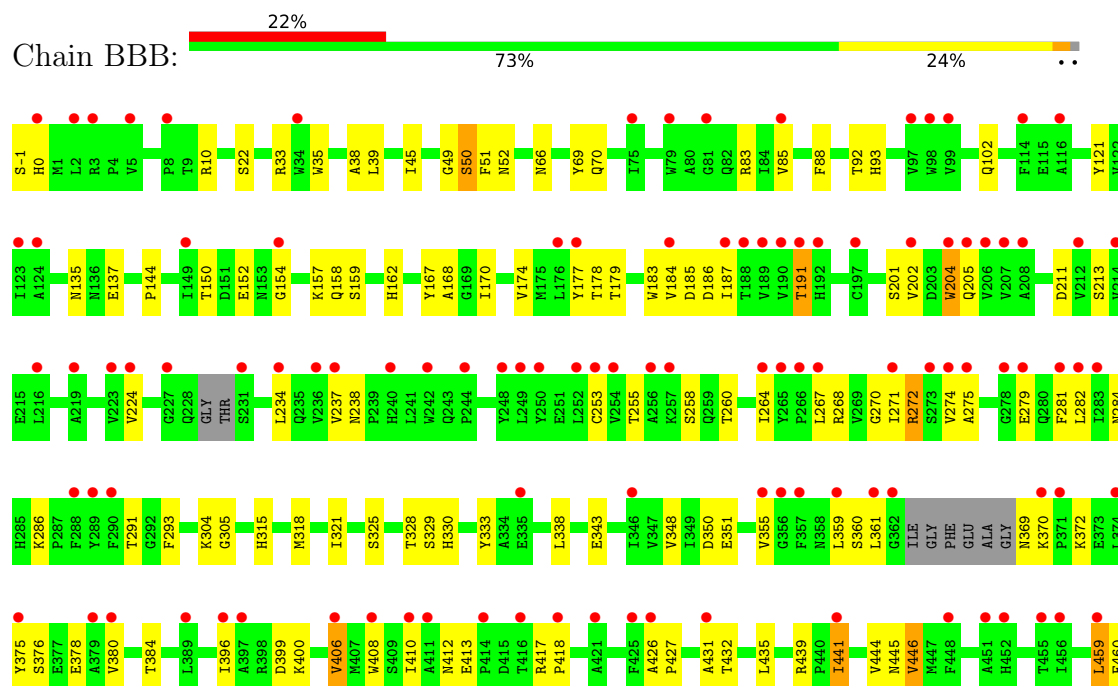
3 Residue-property plots [i](#)

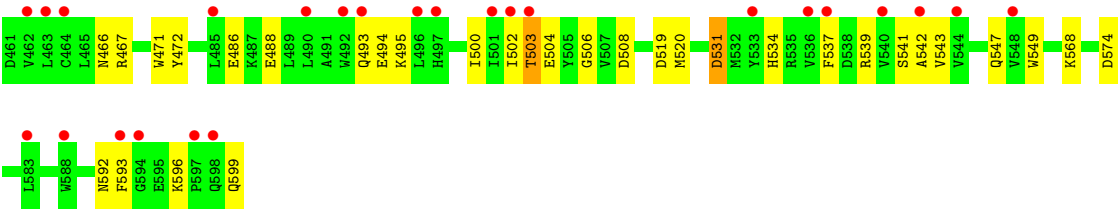
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Beta-D-glucuronidase





4 Data and refinement statistics

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 61.84 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (61.84-1.95) 98.2 (61.84-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.221 , 0.285 0.227 , 0.287	Depositor DCC
R_{free} test set	4644 reflections (4.83%)	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)	0.32 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	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.*

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: 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	1.03	0/4914	1.32	7/6686 (0.1%)
1	BBB	1.05	1/4897 (0.0%)	1.38	8/6663 (0.1%)
All	All	1.04	1/9811 (0.0%)	1.35	15/13349 (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	1
1	BBB	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	224	VAL	N-CA	5.23	1.51	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	574	ASP	CA-CB-CG	5.73	118.33	112.60
1	BBB	446	VAL	CA-C-N	5.68	129.34	120.82
1	BBB	446	VAL	C-N-CA	5.68	129.34	120.82
1	BBB	191	THR	CB-CA-C	5.51	119.94	111.95
1	AAA	169	GLY	CA-C-O	-5.44	117.03	121.76
1	BBB	50	SER	CA-C-O	-5.19	116.05	121.55
1	AAA	578	LYS	CA-C-O	-5.18	115.70	121.81
1	AAA	571	PHE	CA-C-O	-5.17	115.41	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	503	THR	CB-CA-C	5.14	119.60	109.72
1	AAA	229	GLY	CA-C-O	-5.05	117.92	122.57
1	BBB	547	GLN	CB-CA-C	5.04	119.01	110.79
1	AAA	0	HIS	CB-CA-C	5.03	118.25	109.65
1	AAA	194	ALA	CA-C-N	5.03	127.02	120.28
1	AAA	194	ALA	C-N-CA	5.03	127.02	120.28
1	BBB	157	LYS	CB-CA-C	5.01	117.86	110.14

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 [i](#)

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	59	0
1	BBB	4770	0	4546	94	0
2	AAA	12	0	0	0	0
2	BBB	12	0	0	4	0
3	AAA	202	0	0	5	0
3	BBB	110	0	0	5	0
All	All	9892	0	9116	153	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 (153) 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	1.26
1:AAA:130:ILE:O	3:AAA:701:HOH:O	1.53	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:AAA:447:MET:HE2	1:AAA:469:TYR:CE1	2.20	0.77
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:447:MET:HE2	1:AAA:469:TYR:CZ	2.26	0.70
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
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: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:BBB:493:GLN:HG3	1:BBB:542:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:291:THR:O	1:BBB:325:SER:OG	2.26	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:508:ASP:OD1	1:BBB:568:LYS:NZ	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:AAA:33:ARG:HH11	1:AAA:36:GLU:CD	2.23	0.46
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:447:MET:HE1	1:AAA:469:TYR:N	2.31	0.45
1:AAA:447:MET:HE3	1:AAA:467:ARG:HD2	1.97	0.45
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:32:GLN:O	1:AAA:33:ARG:C	2.59	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: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:AAA:447:MET:HE3	1:AAA:467:ARG:HA	1.99	0.44
1:BBB:268:ARG:NH1	1:BBB:343:GLU:HG3	2.32	0.44
1:BBB:592:ASN:O	1:BBB:593:PHE:C	2.61	0.43
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:AAA:359:LEU:HD22	1:AAA:370:LYS:HB3	1.99	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:BBB:486:GLU:CD	1:BBB:539:ARG:HH21	2.25	0.42
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:AAA:342:ASP:CG	1:AAA:403:PRO:HD2	2.45	0.42
1:BBB:33:ARG:HG2	1:BBB:35:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:340:TRP:CD1	1:AAA:344:HIS:CD2	3.08	0.41
1:AAA:447:MET:HE3	1:AAA:467:ARG:CD	2.50	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: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:AAA:447:MET:HE1	1:AAA:469:TYR:H	1.85	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: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:472:TYR:OH	2:BBB:601:VON:O11	2.35	0.40
1:BBB:506:GLY:HA3	1:BBB:549:TRP:O	2.22	0.40
1:BBB:471:TRP:CE3	1:BBB:520:MET:HE3	2.57	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 ⓘ

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%)	26	15
1	BBB	506/511 (99%)	475 (94%)	31 (6%)	17	7
All	All	1014/1022 (99%)	961 (95%)	53 (5%)	21	9

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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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 oligosaccharides 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	1.11	0	11,17,17	2.33	5 (45%)
2	VON	BBB	601	-	11,12,12	1.03	0	11,17,17	1.52	1 (9%)

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	-	-	4/4/21/21	0/1/1/1
2	VON	BBB	601	-	-	0/4/21/21	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	601	VON	C7-N1-C2	4.38	117.27	108.90
2	AAA	601	VON	C4-C3-C2	3.71	115.31	109.86
2	AAA	601	VON	O9-C3-C2	-3.29	103.68	109.42
2	AAA	601	VON	C7-N1-C2	3.20	115.02	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	601	VON	O10-C4-C5	-3.04	104.50	110.59
2	AAA	601	VON	O12-C6-C5	2.65	120.82	113.93

There are no chirality outliers.

All (4) 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
2	AAA	601	VON	C4-C5-C6-O11

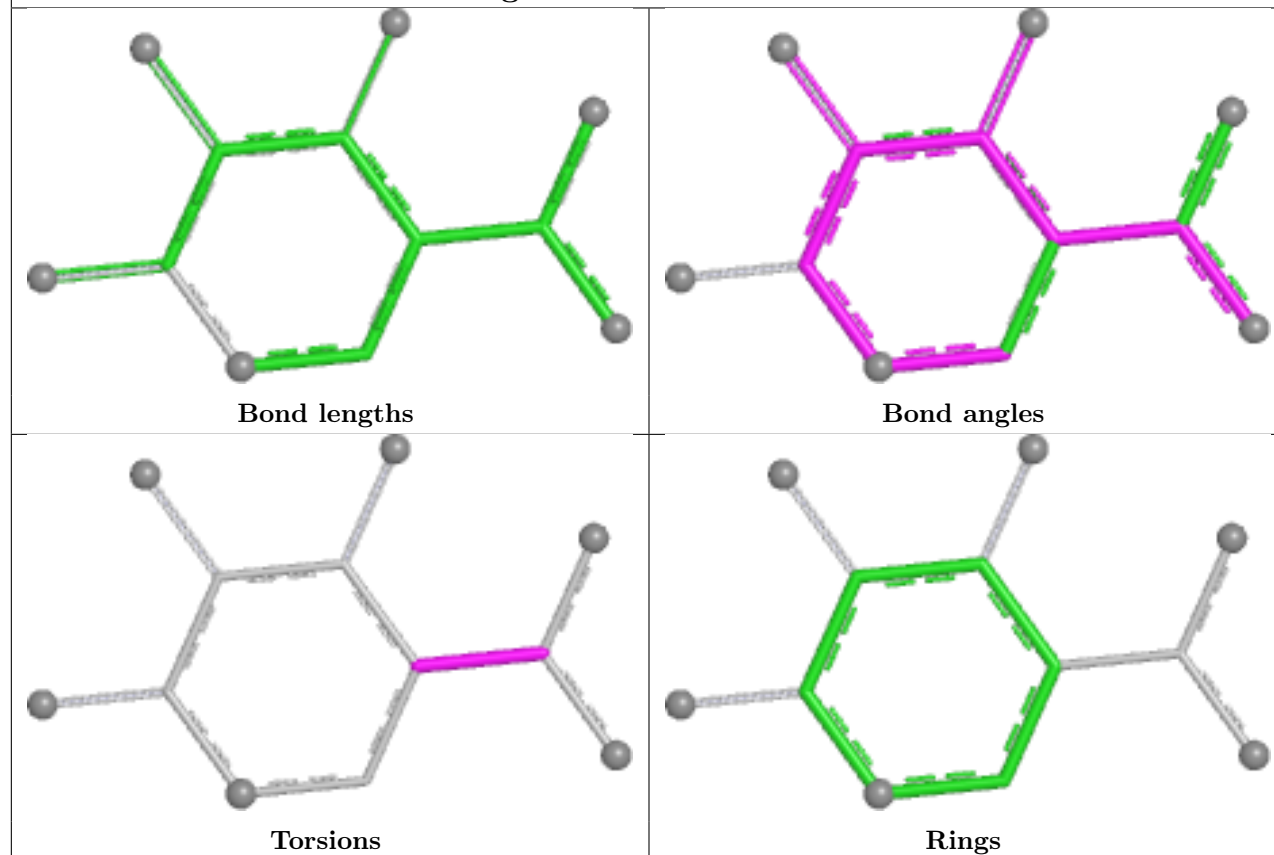
There are no ring outliers.

1 monomer is involved in 4 short contacts:

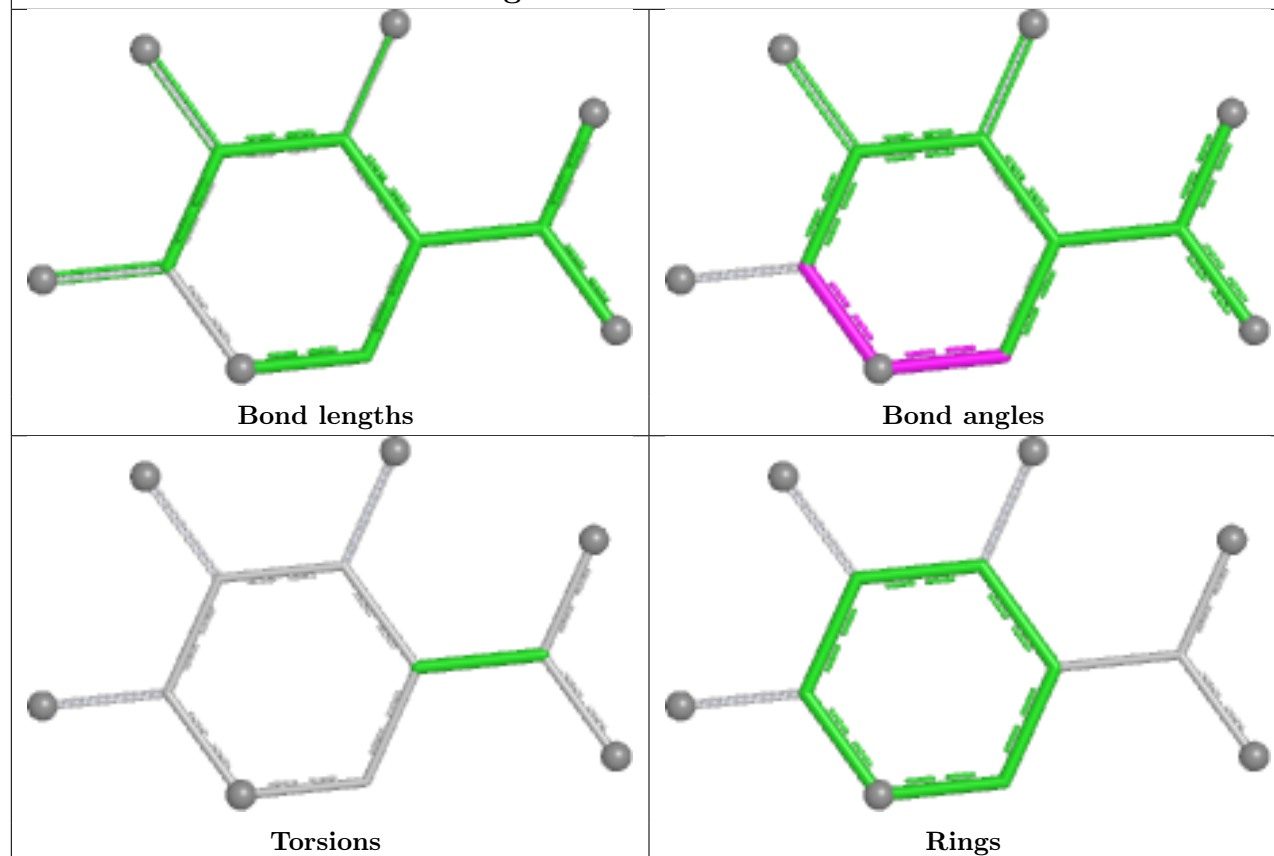
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	601	VON	4	0

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 VON AAA 601



Ligand VON BBB 601



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	595/601 (99%)	0.53	34 (5%)	29 34	22, 43, 71, 97	1 (0%)
1	BBB	593/601 (98%)	1.30	133 (22%)	2 2	33, 61, 97, 115	1 (0%)
All	All	1188/1202 (98%)	0.91	167 (14%)	6 7	22, 51, 87, 115	2 (0%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	361	LEU	6.4
1	BBB	190	VAL	5.7
1	BBB	202	VAL	4.5
1	BBB	206	VAL	4.5
1	BBB	274	VAL	4.1
1	BBB	456	ILE	4.1
1	BBB	357	PHE	4.0
1	BBB	191	THR	3.9
1	BBB	189	VAL	3.8
1	BBB	204	TRP	3.7
1	BBB	362	GLY	3.7
1	BBB	216	LEU	3.7
1	BBB	212	VAL	3.7
1	BBB	463	LEU	3.7
1	BBB	414	PRO	3.7
1	BBB	267	LEU	3.5
1	BBB	252	LEU	3.5
1	BBB	237	VAL	3.4
1	BBB	207	VAL	3.3
1	AAA	123	ILE	3.2
1	BBB	410	ILE	3.2
1	BBB	264	ILE	3.1
1	BBB	418	PRO	3.1
1	BBB	249	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	BBB	256	ALA	3.1
1	BBB	197	CYS	3.1
1	BBB	536	VAL	3.1
1	BBB	288	PHE	3.1
1	BBB	537	PHE	3.1
1	BBB	3	ARG	3.1
1	BBB	275	ALA	3.1
1	BBB	406	VAL	3.0
1	BBB	598	GLN	3.0
1	BBB	588	TRP	3.0
1	BBB	205	GLN	3.0
1	BBB	359	LEU	3.0
1	BBB	5	VAL	3.0
1	BBB	85	VAL	3.0
1	BBB	214	VAL	3.0
1	AAA	182	THR	3.0
1	AAA	183	TRP	3.0
1	BBB	192	HIS	2.9
1	BBB	356	GLY	2.9
1	BBB	455	THR	2.9
1	AAA	30	ILE	2.9
1	BBB	231	SER	2.9
1	BBB	371	PRO	2.9
1	AAA	256	ALA	2.9
1	BBB	411	ALA	2.9
1	AAA	35	TRP	2.9
1	BBB	242	TRP	2.9
1	BBB	346	ILE	2.9
1	BBB	154	GLY	2.9
1	BBB	236	VAL	2.8
1	BBB	187	ILE	2.8
1	BBB	223	VAL	2.8
1	BBB	254	VAL	2.8
1	BBB	250	TYR	2.7
1	BBB	379	ALA	2.7
1	BBB	451	ALA	2.7
1	BBB	282	LEU	2.7
1	BBB	149	ILE	2.7
1	AAA	79	TRP	2.7
1	BBB	114	PHE	2.7
1	BBB	496	LEU	2.7
1	BBB	597	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	BBB	98	TRP	2.6
1	BBB	289	TYR	2.6
1	BBB	389	LEU	2.6
1	BBB	490	LEU	2.6
1	BBB	271	ILE	2.6
1	BBB	425	PHE	2.6
1	AAA	116	ALA	2.6
1	BBB	355	VAL	2.6
1	BBB	188	THR	2.6
1	BBB	583	LEU	2.5
1	BBB	397	ALA	2.5
1	BBB	497	HIS	2.5
1	BBB	548	VAL	2.5
1	BBB	273	SER	2.5
1	BBB	99	VAL	2.5
1	AAA	262	CYS	2.5
1	AAA	362	GLY	2.5
1	BBB	283	ILE	2.5
1	BBB	441	ILE	2.5
1	AAA	124	ALA	2.5
1	BBB	208	ALA	2.5
1	AAA	28	CYS	2.4
1	BBB	416	THR	2.4
1	BBB	224	VAL	2.4
1	BBB	290	PHE	2.4
1	BBB	257	LYS	2.4
1	AAA	5	VAL	2.4
1	BBB	408	TRP	2.4
1	BBB	234	LEU	2.4
1	BBB	375	TYR	2.4
1	BBB	281	PHE	2.4
1	AAA	122	VAL	2.4
1	BBB	540	VAL	2.4
1	BBB	459	LEU	2.3
1	AAA	75	ILE	2.3
1	AAA	397	ALA	2.3
1	BBB	542	ALA	2.3
1	AAA	118	VAL	2.3
1	BBB	462	VAL	2.3
1	BBB	492	TRP	2.3
1	BBB	485	LEU	2.3
1	BBB	265	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	0	HIS	2.3
1	BBB	123	ILE	2.3
1	BBB	244	PRO	2.3
1	BBB	97	VAL	2.3
1	AAA	599	GLN	2.3
1	BBB	248	TYR	2.3
1	BBB	421	ALA	2.3
1	BBB	594	GLY	2.3
1	BBB	184	VAL	2.3
1	BBB	544	VAL	2.3
1	BBB	374	LEU	2.3
1	AAA	3	ARG	2.2
1	AAA	44	ALA	2.2
1	BBB	124	ALA	2.2
1	BBB	227	GLY	2.2
1	BBB	279[A]	GLU	2.2
1	BBB	593	PHE	2.2
1	AAA	598	GLN	2.2
1	BBB	464	CYS	2.2
1	BBB	426	ALA	2.2
1	BBB	34	TRP	2.2
1	BBB	79	TRP	2.2
1	AAA	274	VAL	2.2
1	BBB	253	CYS	2.2
1	AAA	234	LEU	2.2
1	BBB	177	TYR	2.2
1	AAA	98	TRP	2.2
1	BBB	493	GLN	2.2
1	BBB	503	THR	2.2
1	AAA	76	PRO	2.2
1	BBB	370	LYS	2.2
1	BBB	240	HIS	2.1
1	AAA	34	TRP	2.1
1	AAA	184	VAL	2.1
1	BBB	278	GLY	2.1
1	AAA	257	LYS	2.1
1	BBB	448	PHE	2.1
1	AAA	408	TRP	2.1
1	AAA	128	VAL	2.1
1	BBB	81	GLY	2.1
1	BBB	266	PRO	2.1
1	BBB	396	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	BBB	335	GLU	2.1
1	BBB	452	HIS	2.1
1	BBB	380	VAL	2.1
1	BBB	176	LEU	2.1
1	BBB	116	ALA	2.1
1	BBB	219	ALA	2.1
1	AAA	60	ILE	2.0
1	BBB	75	ILE	2.0
1	AAA	259	GLN	2.0
1	AAA	73	VAL	2.0
1	AAA	224	VAL	2.0
1	BBB	2	LEU	2.0
1	BBB	431	ALA	2.0
1	BBB	501	ILE	2.0
1	BBB	502	ILE	2.0
1	BBB	533	TYR	2.0
1	BBB	8	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

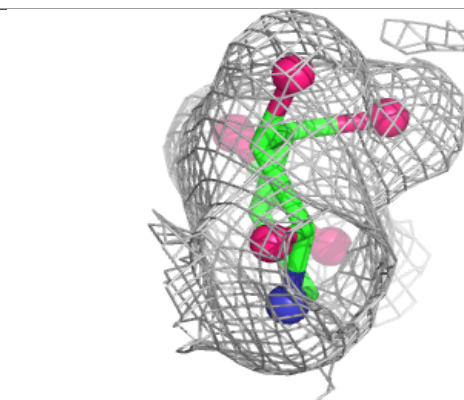
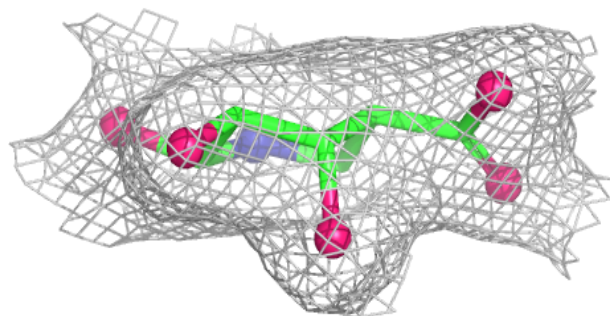
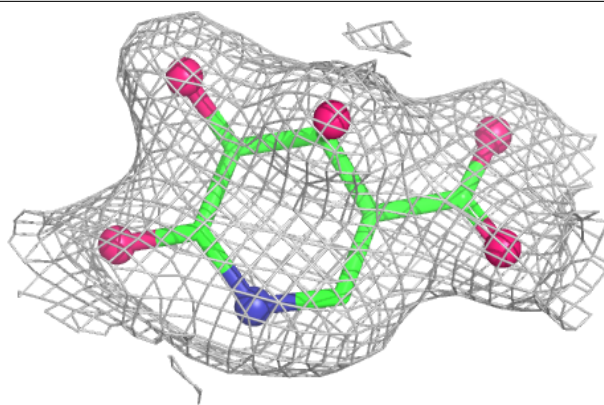
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	VON	BBB	601	12/12	0.93	0.08	42,45,49,52	0
2	VON	AAA	601	12/12	0.94	0.07	30,35,41,44	0

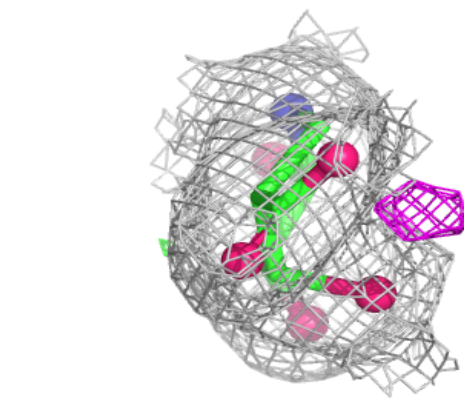
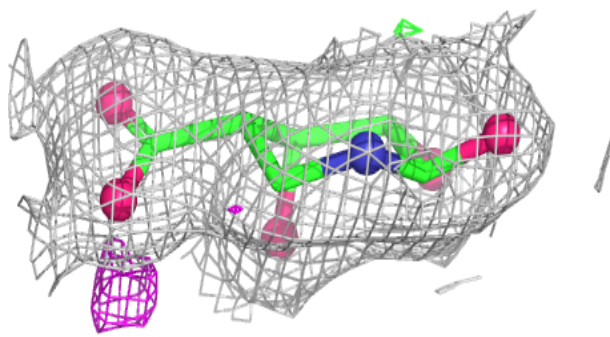
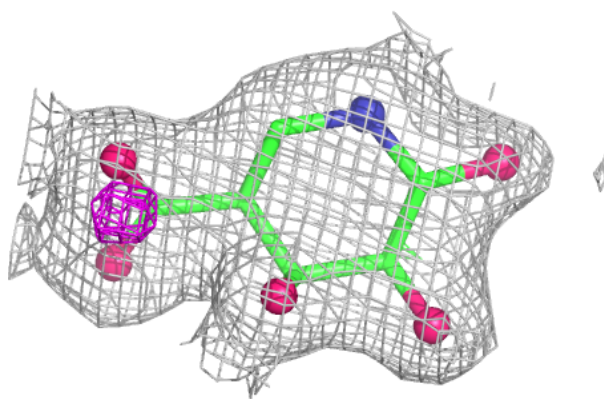
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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