

Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 11:31 am GMT

PDB ID : 6QBG

Title : Crystal structure of human cathepsin D in complex with macrocyclic inhibitor

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Deposited on : 2018-12-21

Resolution : 1.80 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 (i) 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 (1)) 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)

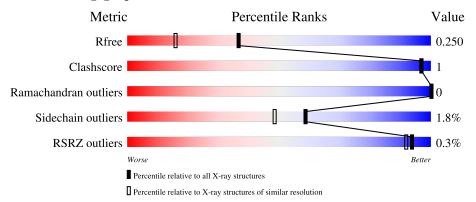
Validation Pipeline (wwPDB-VP) : 2.36

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 1.80 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	A	98	96%	•
2	В	241	95% 5%	•
3	С	2	100%	•



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3002 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 Cathepsin D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total 756	C 483	N 121	O 147	S 5	0	0	0

• Molecule 2 is a protein called Cathepsin D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	241	Total 1861	C 1195	N 305	O 350	S 11	0	3	0

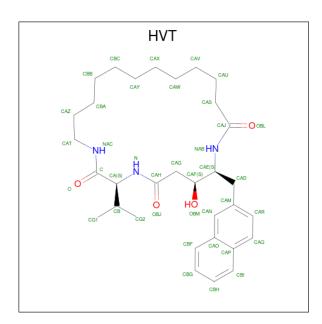
• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	С	2	Total 28	C 16	N 2	O 10	0	0	0

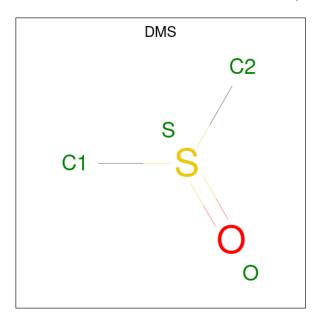
• Molecule 4 is $(3 \{S\}, 7 \{S\}, 8 \{S\})$ -8-(naphthalen-2-ylmethyl)-7-oxidanyl-3-propan-2-yl-1,4,9-triazacyclohenicosane-2,5,10-trione (three-letter code: HVT) (formula: $C_{32}H_{47}N_3O_4$) (labeled as "Ligand of Interest" by depositor).





\mathbf{M}	ol	Chain	Residues	Atoms				ZeroOcc	AltConf
4		A	1	Total 39	C 32			0	0
4		В	1	Total 39	C 32		O 4	0	0

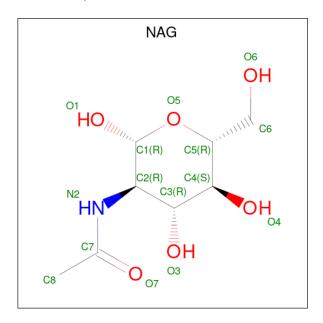
 \bullet Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: $\mathrm{C_2H_6OS}).$



Mo	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0

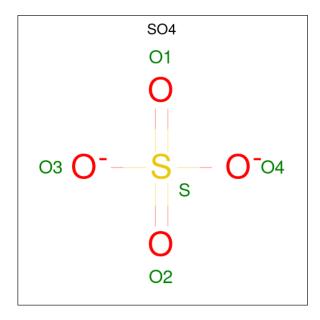


 \bullet Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	В	1	Total 14	C 8	N 1	O 5	0	0

 \bullet Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	В	1	Total 5	O 4	S 1	0	0



• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	73	Total O 73 73	0	0
8	В	177	Total O 179 179	0	2



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: Cathepsin D
Chain A: 96% .
Molecule 2: Cathepsin D
Chain B: 95% 5%
Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
Chain C: 100%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	80.37Å 94.14Å 117.51Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.13 - 1.80	Depositor
rtesolution (A)	43.70 - 1.80	EDS
% Data completeness	98.8 (61.13-1.80)	Depositor
(in resolution range)	98.8 (43.70-1.80)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.10 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
D D.	0.194 , 0.247	Depositor
R, R_{free}	0.202 , 0.250	DCC
R_{free} test set	1246 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 30.7	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3002	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAG, DMS, HVT

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.73	0/779	0.85	0/1063	
2	В	0.76	0/1909	0.89	3/2586 (0.1%)	
All	All	0.75	0/2688	0.88	3/3649 (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
2	В	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	328	ARG	NE-CZ-NH1	7.81	124.20	120.30
2	В	202	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	В	328	ARG	NE-CZ-NH2	-5.72	117.44	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	204	ALA	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	A	756	0	710	1	0
2	В	1861	0	1870	5	0
3	С	28	0	25	0	0
4	A	39	0	0	0	0
4	В	39	0	0	0	0
5	A	8	0	12	0	0
6	В	14	0	13	0	0
7	В	5	0	0	0	0
8	A	73	0	0	0	1
8	В	179	0	0	1	1
All	All	3002	0	2630	5	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 1.

All (5) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:43:SER:HB2	2:B:117:GLU:HB3	1.88	0.56
2:B:164:ILE:HG22	2:B:334:ASP:HA	1.98	0.46
2:B:122:PRO:O	8:B:501:HOH:O	2.21	0.44
2:B:311:ILE:O	2:B:316:GLY:HA3	2.18	0.43
2:B:130:LYS:HA	2:B:130:LYS:HD2	1.95	0.42

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		$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
8:A:257:HOH:O	8:B:637:HOH:O[6_555]	2.19	0.01



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	Perce	\mathbf{ntiles}
1	A	96/98~(98%)	95 (99%)	1 (1%)	0	100	100
2	В	242/241 (100%)	238 (98%)	4 (2%)	0	100	100
All	All	338/339 (100%)	333 (98%)	5 (2%)	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	A	86/87 (99%)	83 (96%)	3 (4%)	36	21	
2	В	202/200 (101%)	200 (99%)	2 (1%)	76	71	
All	All	288/287 (100%)	283 (98%)	5 (2%)	59	51	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	66	THR
1	A	83	LEU
2	В	156	GLN
2	В	307	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:



Mol	Chain	Res	Type
2	В	121	GLN
2	В	337	ASN

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)

2 monosaccharides 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).

Mal True C		Chain Res		Link	Во	ond leng	$ ag{ths}$	В	ond ang	les
Mol	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	С	1	3,1	14,14,15	0.60	0	17,19,21	1.58	5 (29%)
3	NAG	С	2	3	14,14,15	1.00	0	17,19,21	2.51	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	С	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	С	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
3	С	2	NAG	C1-O5-C5	7.83	122.80	112.19
3	С	2	NAG	C1-C2-N2	4.26	117.77	110.49
3	С	1	NAG	O5-C1-C2	-3.37	105.97	111.29
3	С	1	NAG	C2-N2-C7	2.90	127.03	122.90
3	С	1	NAG	C1-O5-C5	2.58	115.69	112.19
3	С	2	NAG	C2-N2-C7	2.16	125.98	122.90
3	С	2	NAG	O5-C1-C2	2.15	114.68	111.29
3	С	1	NAG	O4-C4-C5	2.14	114.61	109.30
3	С	1	NAG	C3-C4-C5	-2.07	106.55	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

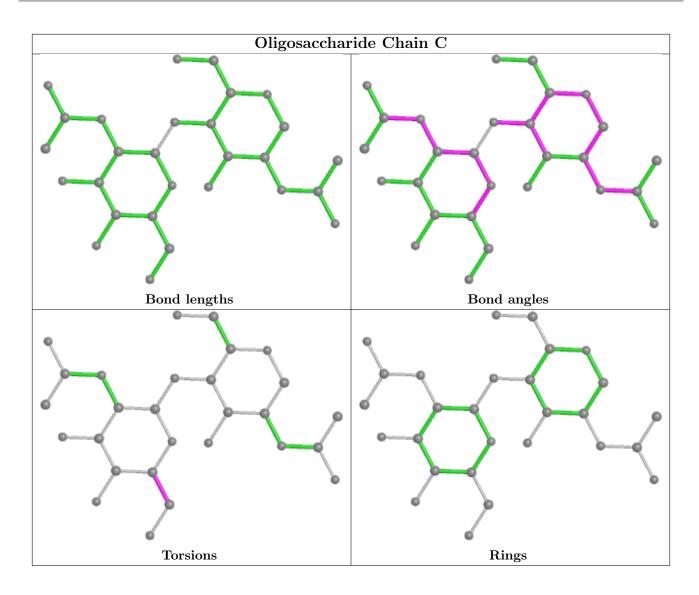
Mol	Chain	Res	Type	Atoms
3	С	2	NAG	O5-C5-C6-O6
3	С	2	NAG	C4-C5-C6-O6

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 oligosaccharide.





5.6 Ligand geometry (i)

6 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	Tuno	Chain	Res	Link	Bond lengths			Bond angles		
IVIOI	Moi Type	Chain	rtes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	HVT	A	103	-	41,41,41	1.65	9 (21%)	51,53,53	1.43	8 (15%)
5	DMS	A	105	-	3,3,3	0.43	0	3,3,3	1.11	0
5	DMS	A	104	-	3,3,3	0.31	0	3,3,3	0.65	0



Mal	Mol Type	Chain	Res	Link	Bo	Bond lengths			Bond angles			
Moi Type	Chain	rtes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2			
6	NAG	В	401	2	14,14,15	0.50	0	17,19,21	2.04	2 (11%)		
7	SO4	В	403	-	4,4,4	0.44	0	6,6,6	0.50	0		
4	HVT	В	402	-	41,41,41	1.82	8 (19%)	51,53,53	1.67	16 (31%)		

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
6	NAG	В	401	2	-	2/6/23/26	0/1/1/1
4	HVT	A	103	-	-	5/43/43/43	0/2/3/3
4	HVT	В	402	-	-	2/43/43/43	0/2/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
4	В	402	HVT	CAS-CAJ	-5.05	1.41	1.51
4	A	103	HVT	CAS-CAJ	-4.93	1.42	1.51
4	В	402	HVT	CAD-CAM	-4.21	1.41	1.51
4	В	402	HVT	CAG-CAH	-4.20	1.42	1.51
4	В	402	HVT	CA-C	-3.96	1.42	1.52
4	В	402	HVT	C-NAC	3.83	1.42	1.33
4	A	103	HVT	CAG-CAH	-3.54	1.43	1.51
4	A	103	HVT	CAH-N	3.43	1.41	1.34
4	A	103	HVT	C-NAC	2.96	1.40	1.33
4	A	103	HVT	CAJ-NAB	2.88	1.40	1.34
4	A	103	HVT	CA-C	-2.84	1.45	1.52
4	В	402	HVT	CAQ-CAP	-2.46	1.36	1.41
4	В	402	HVT	CA-N	2.38	1.50	1.45
4	A	103	HVT	CAD-CAM	-2.35	1.45	1.51
4	A	103	HVT	CAQ-CAP	-2.16	1.36	1.41
4	A	103	HVT	CBF-CAO	-2.14	1.36	1.41
4	В	402	HVT	CAJ-NAB	2.03	1.38	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
6	В	401	NAG	C1-O5-C5	7.14	121.87	112.19
4	В	402	HVT	OBJ-CAH-N	-4.51	115.34	122.95
4	A	103	HVT	OBJ-CAH-N	-4.12	116.00	122.95

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
6	В	401	NAG	C1-C2-N2	-3.58	104.38	110.49
4	A	103	HVT	CBI-CAP-CAO	3.41	125.03	118.92
4	В	402	HVT	CAS-CAJ-NAB	3.28	121.52	115.83
4	A	103	HVT	CAM-CAD-CAE	-3.21	107.76	113.33
4	В	402	HVT	OBL-CAJ-NAB	-3.20	117.55	122.95
4	В	402	HVT	CAD-CAM-CAR	-2.91	115.14	120.91
4	В	402	HVT	CB-CA-N	-2.88	104.31	111.43
4	A	103	HVT	CAG-CAH-N	2.81	120.01	116.33
4	В	402	HVT	CBI-CAP-CAO	2.79	123.92	118.92
4	В	402	HVT	CAG-CAH-N	2.70	119.86	116.33
4	В	402	HVT	CAQ-CAP-CBI	-2.62	117.06	123.19
4	A	103	HVT	CAD-CAM-CAN	2.39	125.83	120.57
4	В	402	HVT	CAT-NAC-C	2.37	126.82	122.59
4	A	103	HVT	CAQ-CAP-CBI	-2.37	117.64	123.19
4	В	402	HVT	CAD-CAM-CAN	2.36	125.76	120.57
4	В	402	HVT	CA-C-NAC	2.25	120.29	116.41
4	A	103	HVT	CAT-NAC-C	2.25	126.61	122.59
4	В	402	HVT	OBJ-CAH-CAG	2.24	124.78	121.50
4	В	402	HVT	CAM-CAN-CAO	-2.06	117.17	121.22
4	В	402	HVT	CB-CA-C	2.05	116.50	111.38
4	В	402	HVT	CAZ-CAT-NAC	-2.04	106.38	112.21
4	В	402	HVT	CAF-CAE-NAB	2.03	113.84	109.92
4	A	103	HVT	CBH-CBI-CAP	-2.01	117.30	120.44

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	103	HVT	CAJ-CAS-CAU-CAV
6	В	401	NAG	C4-C5-C6-O6
4	A	103	HVT	CAV-CAW-CAX-CAY
4	A	103	HVT	CAS-CAU-CAV-CAW
6	В	401	NAG	O5-C5-C6-O6
4	В	402	HVT	CAW-CAX-CAY-CBC
4	A	103	HVT	CAU-CAV-CAW-CAX
4	В	402	HVT	N-CA-CB-CG1
4	A	103	HVT	CBA-CBB-CBC-CAY

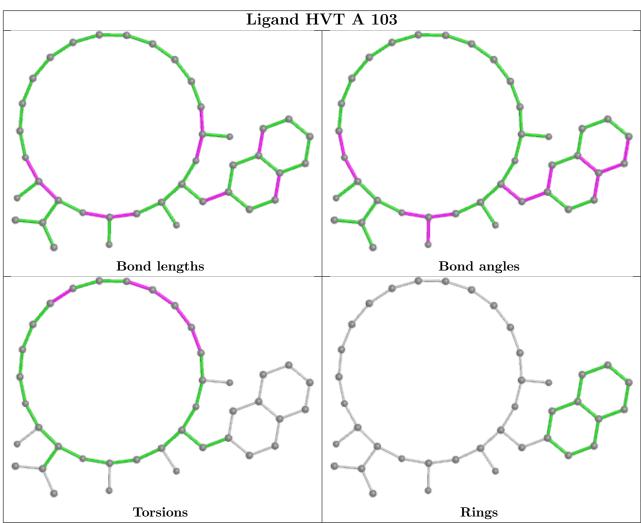
There are no ring outliers.

No monomer is involved in short contacts.

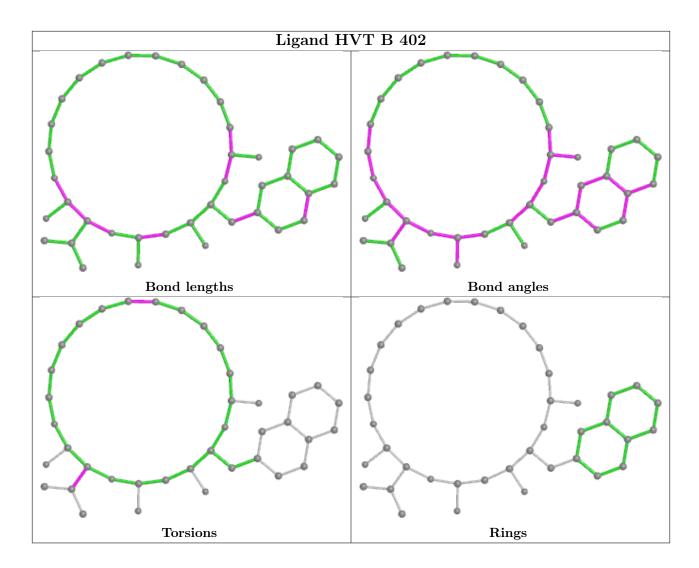
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



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 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.







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 (i)

6.1 Protein, DNA and RNA chains (i)

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		$OWAB(A^2)$	Q<0.9
1	A	98/98 (100%)	-0.38	0 100 100	21, 26, 39, 59	0
2	В	241/241 (100%)	-0.46	1 (0%) 92 90	20, 27, 40, 51	0
All	All	339/339 (100%)	-0.44	1 (0%) 94 92	20, 26, 40, 59	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	161	ASP	2.4

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

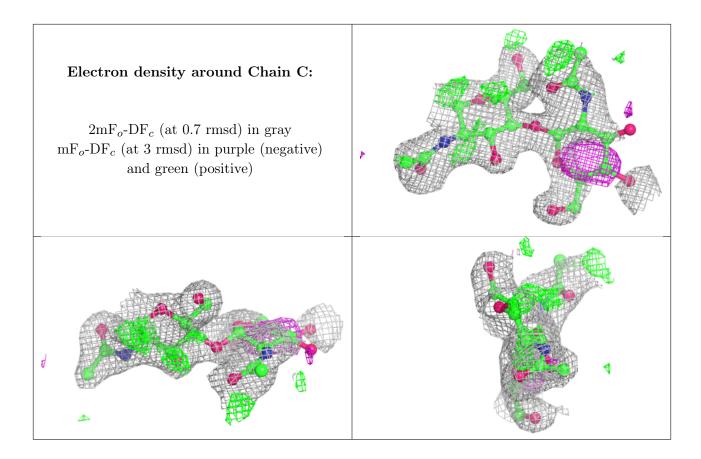
6.3 Carbohydrates (i)

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.

M	Iol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{ ilde{A}}^2)$	Q<0.9
,	3	NAG	С	2	14/15	0.59	0.36	55,60,67,69	0
,	3	NAG	С	1	14/15	0.86	0.13	32,38,43,53	14

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





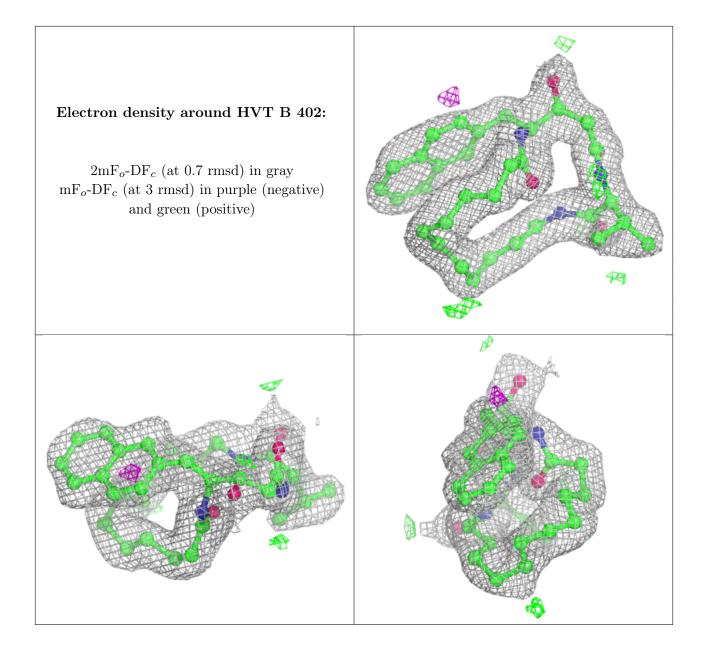
6.4 Ligands (i)

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.

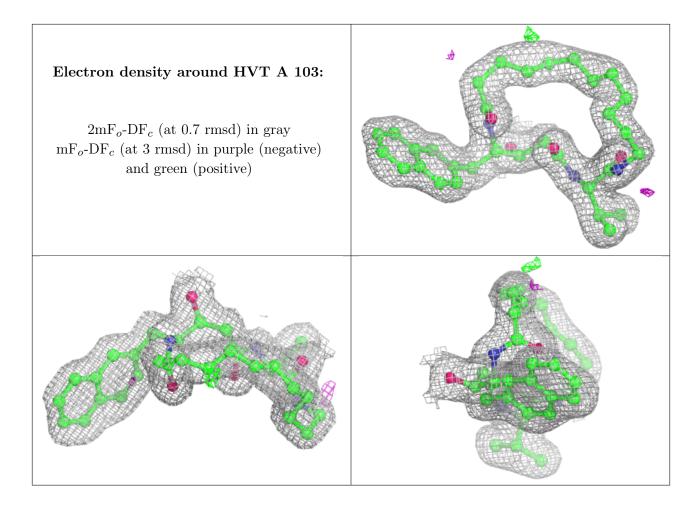
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
6	NAG	В	401	14/15	0.87	0.20	46,53,61,62	0
7	SO4	В	403	5/5	0.89	0.24	65,74,80,82	0
4	HVT	В	402	39/39	0.93	0.11	29,35,44,47	0
5	DMS	A	105	4/4	0.94	0.13	64,66,71,72	0
5	DMS	A	104	4/4	0.96	0.10	25,27,29,30	0
4	HVT	A	103	39/39	0.96	0.10	18,26,37,38	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.









6.5 Other polymers (i)

There are no such residues in this entry.

