



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 06:05 AM UTC

PDB ID : 6YYQ / pdb_00006yyq
Title : Structure of Cathepsin S in complex with Compound 3
Authors : Wagener, M.; Schade, M.; Merla, B.; Hars, U.; Kueckelhaus, S.Q.
Deposited on : 2020-05-05
Resolution : 2.51 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

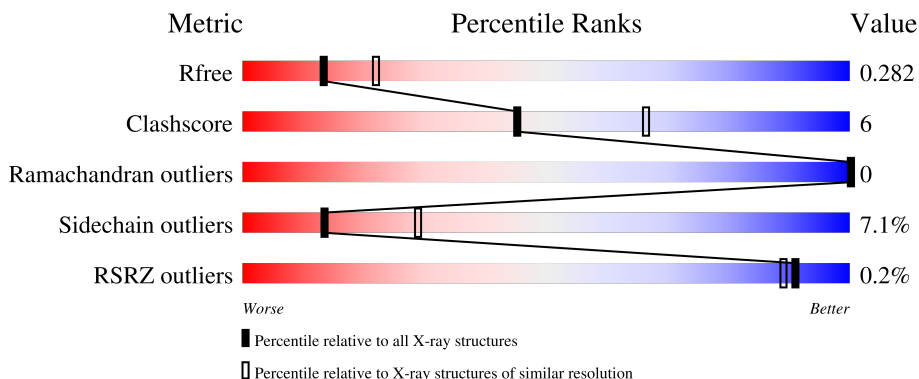
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	225	84% 12% ..
1	BBB	225	84% 13% ..
1	CCC	225	82% 16% ..
1	DDD	225	% 78% 18% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7158 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 S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	220	Total	C	N	O	S	0	0	0
			1713	1082	293	326	12			
1	BBB	220	Total	C	N	O	S	0	1	0
			1720	1087	295	326	12			
1	CCC	222	Total	C	N	O	S	0	0	0
			1733	1094	299	328	12			
1	DDD	222	Total	C	N	O	S	0	1	0
			1740	1099	301	328	12			

There are 24 discrepancies between the modelled and reference sequences:

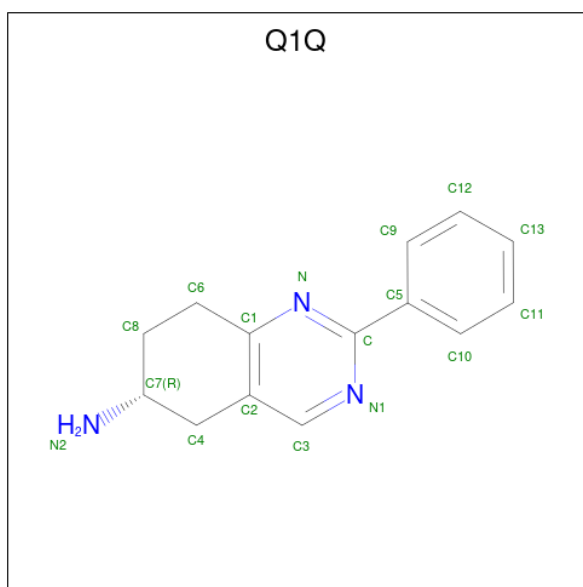
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	218	HIS	-	expression tag	UNP P25774
AAA	219	HIS	-	expression tag	UNP P25774
AAA	220	HIS	-	expression tag	UNP P25774
AAA	221	HIS	-	expression tag	UNP P25774
AAA	222	HIS	-	expression tag	UNP P25774
AAA	223	HIS	-	expression tag	UNP P25774
BBB	218	HIS	-	expression tag	UNP P25774
BBB	219	HIS	-	expression tag	UNP P25774
BBB	220	HIS	-	expression tag	UNP P25774
BBB	221	HIS	-	expression tag	UNP P25774
BBB	222	HIS	-	expression tag	UNP P25774
BBB	223	HIS	-	expression tag	UNP P25774
CCC	218	HIS	-	expression tag	UNP P25774
CCC	219	HIS	-	expression tag	UNP P25774
CCC	220	HIS	-	expression tag	UNP P25774
CCC	221	HIS	-	expression tag	UNP P25774
CCC	222	HIS	-	expression tag	UNP P25774
CCC	223	HIS	-	expression tag	UNP P25774
DDD	218	HIS	-	expression tag	UNP P25774
DDD	219	HIS	-	expression tag	UNP P25774
DDD	220	HIS	-	expression tag	UNP P25774

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	221	HIS	-	expression tag	UNP P25774
DDD	222	HIS	-	expression tag	UNP P25774
DDD	223	HIS	-	expression tag	UNP P25774

- Molecule 2 is (6 {R})-2-phenyl-5,6,7,8-tetrahydroquinazolin-6-amine (CCD ID: Q1Q) (formula: C₁₄H₁₅N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	N	0	0
			17	14	3		
2	BBB	1	Total	C	N	0	0
			17	14	3		
2	CCC	1	Total	C	N	0	0
			17	14	3		

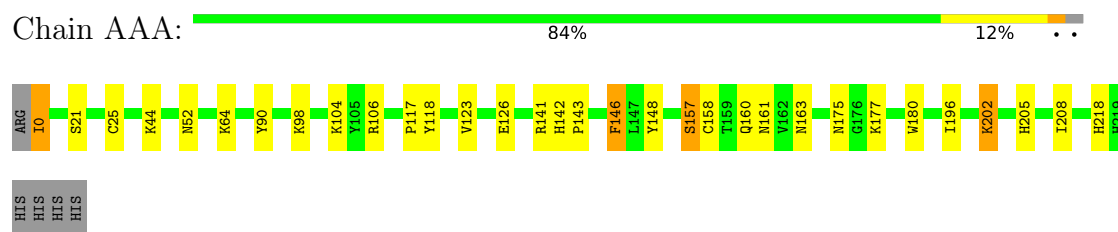
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	53	Total	O	0	0
			53	53		
3	BBB	51	Total	O	0	0
			51	51		
3	CCC	59	Total	O	0	0
			59	59		
3	DDD	38	Total	O	0	0
			38	38		

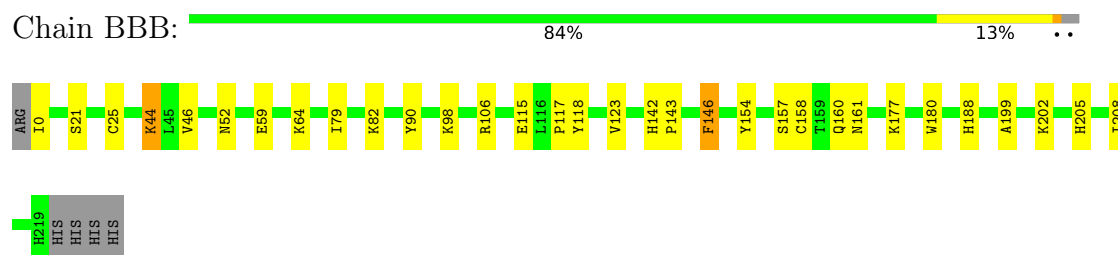
3 Residue-property plots [i](#)

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.

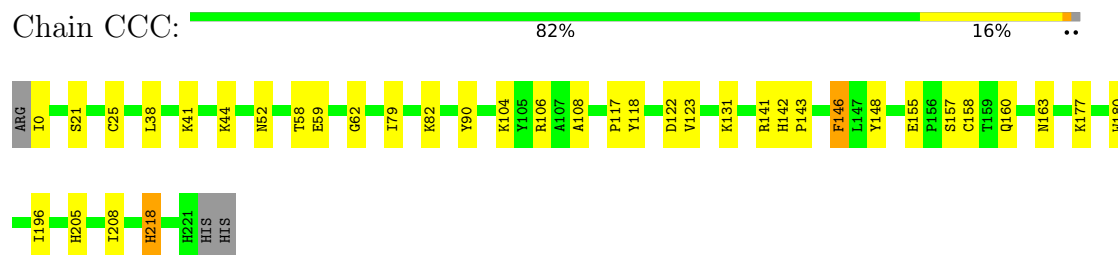
- Molecule 1: Cathepsin S



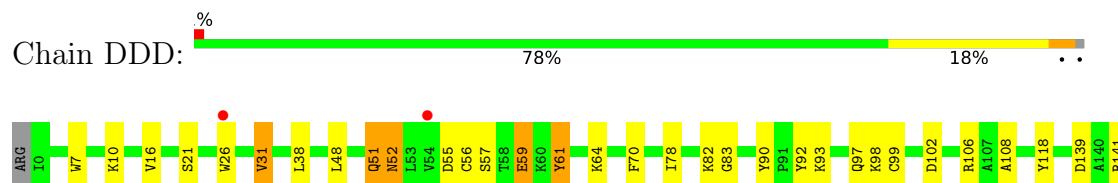
- Molecule 1: Cathepsin S



- Molecule 1: Cathepsin S



- Molecule 1: Cathepsin S



F146	L147	Y148	R149	S157	C158	T159	Q160	N161	K177	W180	H188	I196	I208	F211	H218	H221	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.77 Å 92.77 Å 182.89 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.82 – 2.51 28.82 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.82-2.51) 99.7 (28.82-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.210 , 0.280 0.213 , 0.282	Depositor DCC
R_{free} test set	1599 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.766	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7158	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: Q1Q

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	1.07	2/1757 (0.1%)	1.42	4/2376 (0.2%)
1	BBB	1.02	0/1768	1.41	2/2391 (0.1%)
1	CCC	1.02	0/1779	1.40	3/2406 (0.1%)
1	DDD	1.04	0/1790	1.46	5/2421 (0.2%)
All	All	1.04	2/7094 (0.0%)	1.42	14/9594 (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	DDD	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	205	HIS	CE1-NE2	5.98	1.38	1.32
1	AAA	202	LYS	C-O	5.60	1.29	1.23

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	218	HIS	CA-CB-CG	10.16	123.96	113.80
1	DDD	51	GLN	CB-CG-CD	-8.61	97.96	112.60
1	AAA	146	PHE	CB-CA-C	-6.86	97.94	110.63
1	CCC	218	HIS	CB-CA-C	6.80	122.20	110.72
1	DDD	211	PHE	CA-CB-CG	6.71	120.52	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DDD	61	TYR	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	1713	0	1632	12	0
1	BBB	1720	0	1639	19	0
1	CCC	1733	0	1646	16	0
1	DDD	1740	0	1655	38	0
2	AAA	17	0	0	0	0
2	BBB	17	0	0	0	0
2	CCC	17	0	0	0	0
3	AAA	53	0	0	1	0
3	BBB	51	0	0	2	0
3	CCC	59	0	0	4	0
3	DDD	38	0	0	14	0
All	All	7158	0	6572	79	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 6.

The worst 5 of 79 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:DDD:51:GLN:NE2	1:DDD:92:TYR:HA	1.13	1.42
1:DDD:51:GLN:NE2	1:DDD:92:TYR:CA	2.09	1.14
1:DDD:51:GLN:HE22	1:DDD:92:TYR:CA	1.62	1.09
1:DDD:159:THR:HG23	3:DDD:302:HOH:O	1.51	1.09
1:DDD:78:ILE:HA	3:DDD:301:HOH:O	1.53	1.08

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	218/225 (97%)	212 (97%)	6 (3%)	0	100	100
1	BBB	219/225 (97%)	214 (98%)	5 (2%)	0	100	100
1	CCC	220/225 (98%)	211 (96%)	9 (4%)	0	100	100
1	DDD	221/225 (98%)	214 (97%)	7 (3%)	0	100	100
All	All	878/900 (98%)	851 (97%)	27 (3%)	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	181/186 (97%)	165 (91%)	16 (9%)	9	20
1	BBB	182/186 (98%)	172 (94%)	10 (6%)	19	40
1	CCC	183/186 (98%)	171 (93%)	12 (7%)	15	32
1	DDD	184/186 (99%)	170 (92%)	14 (8%)	12	26
All	All	730/744 (98%)	678 (93%)	52 (7%)	13	29

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	44	LYS
1	CCC	158	CYS
1	DDD	161	ASN

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Mol	Chain	Res	Type
1	CCC	52	ASN
1	CCC	106	ARG

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	Q1Q	BBB	2001	-	19,19,19	1.52	4 (21%)	25,26,26	1.86	9 (36%)
2	Q1Q	AAA	2001	-	19,19,19	1.69	5 (26%)	25,26,26	2.16	6 (24%)
2	Q1Q	CCC	2001	-	19,19,19	1.29	4 (21%)	25,26,26	2.02	6 (24%)

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	Q1Q	BBB	2001	-	-	0/4/13/13	0/3/3/3
2	Q1Q	AAA	2001	-	-	1/4/13/13	0/3/3/3
2	Q1Q	CCC	2001	-	-	4/4/13/13	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	2001	Q1Q	C1-N	4.09	1.41	1.34
2	BBB	2001	Q1Q	C-N1	3.86	1.40	1.34
2	CCC	2001	Q1Q	C-N1	3.49	1.40	1.34
2	AAA	2001	Q1Q	C-N1	3.08	1.39	1.34
2	AAA	2001	Q1Q	C3-N1	2.86	1.40	1.34

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	2001	Q1Q	N1-C-N	-7.17	118.20	125.23
2	CCC	2001	Q1Q	N1-C-N	-6.05	119.30	125.23
2	BBB	2001	Q1Q	N1-C-N	-4.51	120.81	125.23
2	BBB	2001	Q1Q	C5-C-N1	3.94	121.56	117.34
2	CCC	2001	Q1Q	C3-N1-C	3.88	121.73	116.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

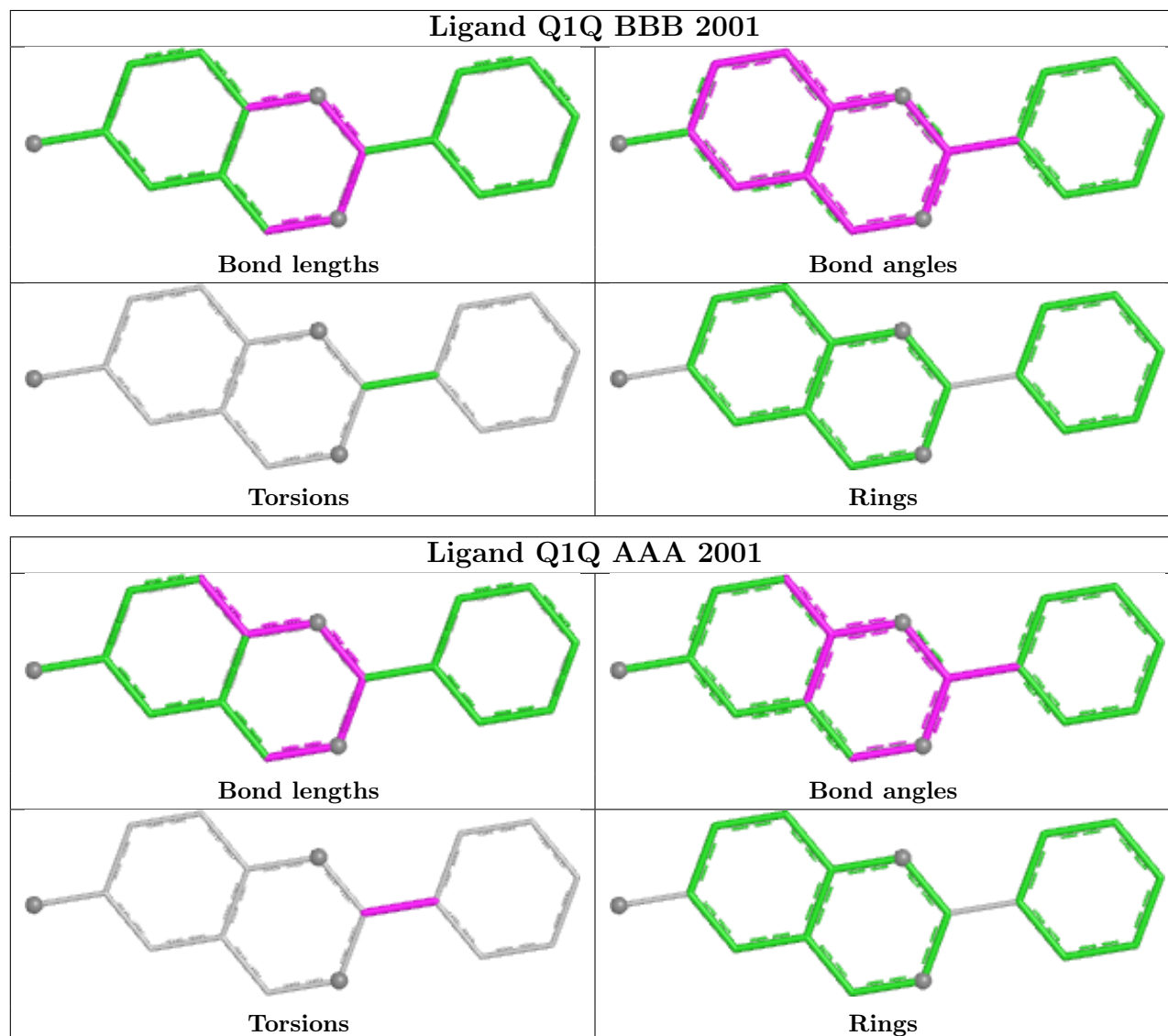
Mol	Chain	Res	Type	Atoms
2	CCC	2001	Q1Q	N-C-C5-C9
2	CCC	2001	Q1Q	N-C-C5-C10
2	CCC	2001	Q1Q	N1-C-C5-C9
2	CCC	2001	Q1Q	N1-C-C5-C10
2	AAA	2001	Q1Q	N-C-C5-C10

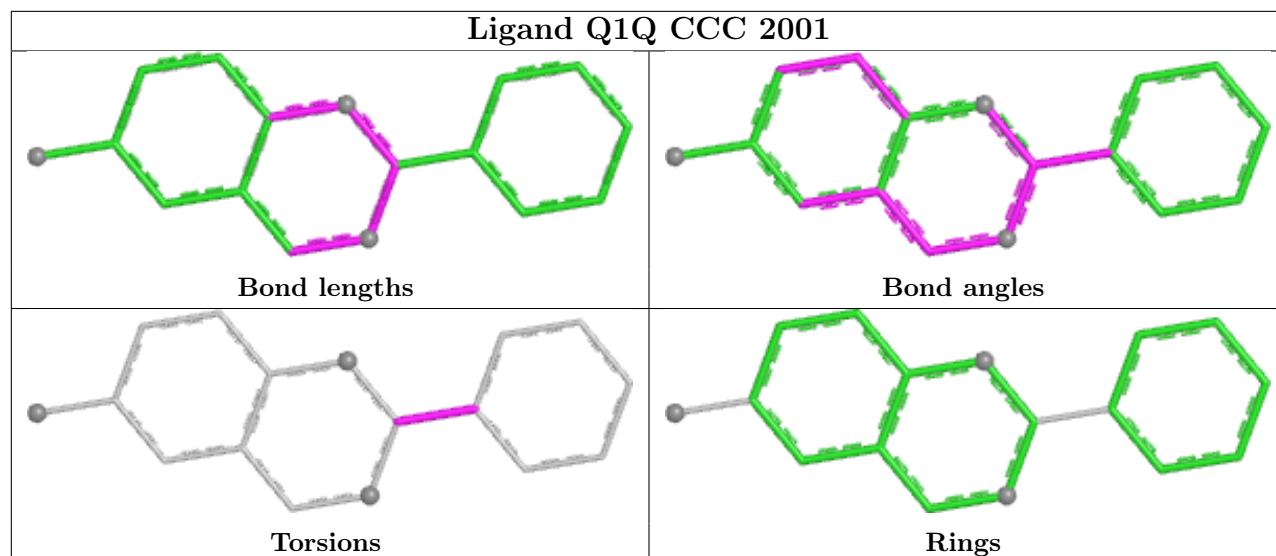
There are no ring outliers.

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 [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, 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	220/225 (97%)	-0.30	0	100 100	54, 72, 95, 132	0
1	BBB	220/225 (97%)	-0.28	0	100 100	43, 75, 109, 137	1 (0%)
1	CCC	222/225 (98%)	-0.23	0	100 100	44, 76, 106, 137	0
1	DDD	222/225 (98%)	0.16	2 (0%)	81 78	43, 91, 128, 148	1 (0%)
All	All	884/900 (98%)	-0.16	2 (0%)	91 89	43, 77, 117, 148	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	54	VAL	2.4
1	DDD	26	TRP	2.2

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](#)

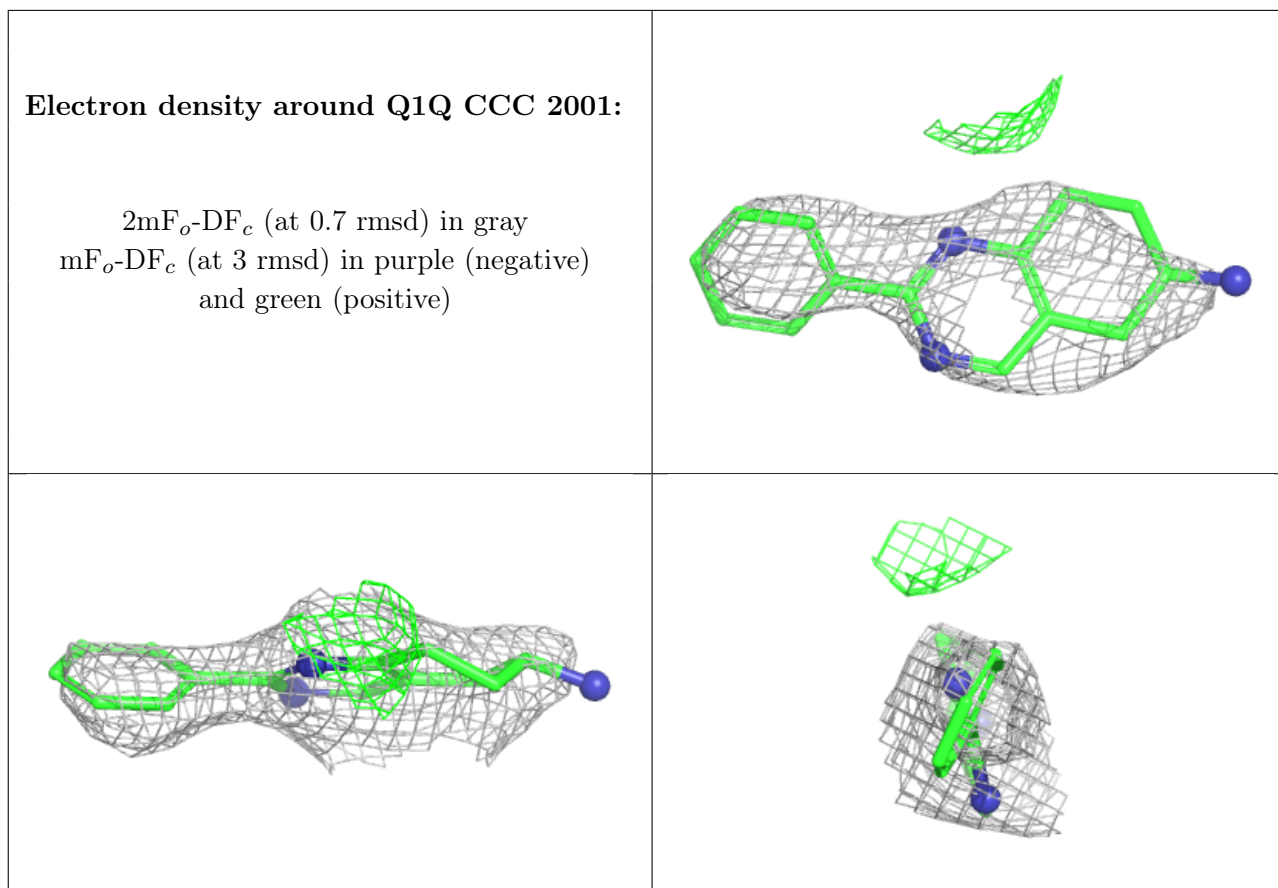
There are no oligosaccharides in this entry.

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.

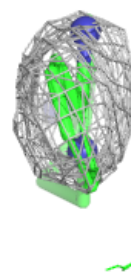
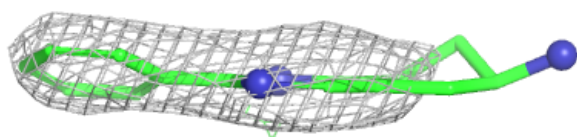
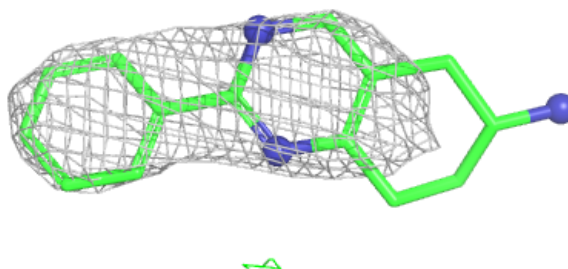
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	Q1Q	CCC	2001	17/17	0.88	0.13	100,110,113,115	0
2	Q1Q	BBB	2001	17/17	0.92	0.10	84,97,110,110	0
2	Q1Q	AAA	2001	17/17	0.92	0.11	91,94,97,98	0

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.

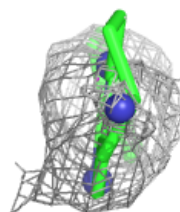
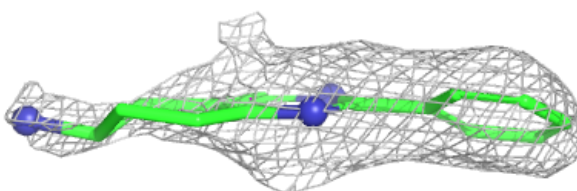
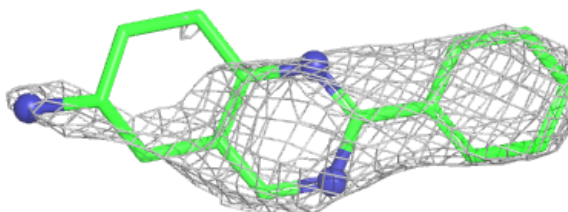


Electron density around Q1Q BBB 2001:

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

**Electron density around Q1Q AAA 2001:**

$2mF_o-DF_c$ (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.