Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2022 – 12:53 pm GMT

PDB ID	:	6YYQ
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 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 (i)) were used in the production of this report:

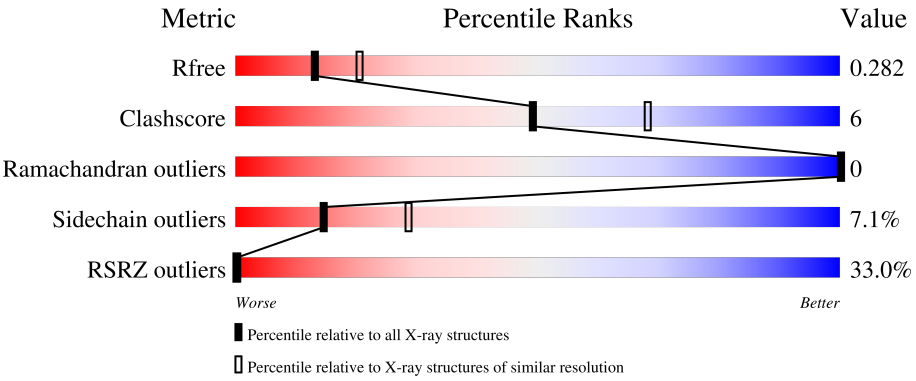
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	28% 84% 12%
1	BBB	225	30% 84% 13%
1	CCC	225	31% 82% 16%
1	DDD	225	41% 78% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	Q1Q	CCC	2001	-	-	-	X

2 Entry composition (i)

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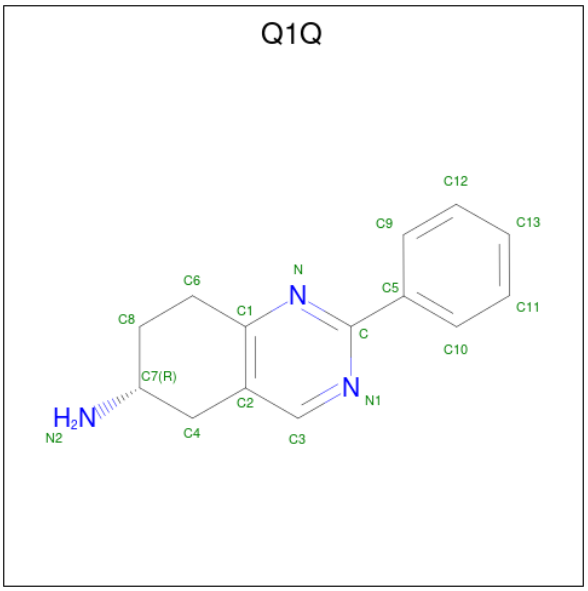
Chain	Residue	Modelled	Actual	Comment	Reference
DDD	221	HIS	-	expression tag	UNP P25774
DDD	222	HIS	-	expression tag	UNP P25774
DDD	223	HIS	-	expression tag	UNP P25774

- Molecule 2 is (6 {R})-2-phenyl-5,6,7,8-tetrahydroquinazolin-6-amine (three-letter code: Q1Q) (formula: $C_{14}H_{15}N_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is water.

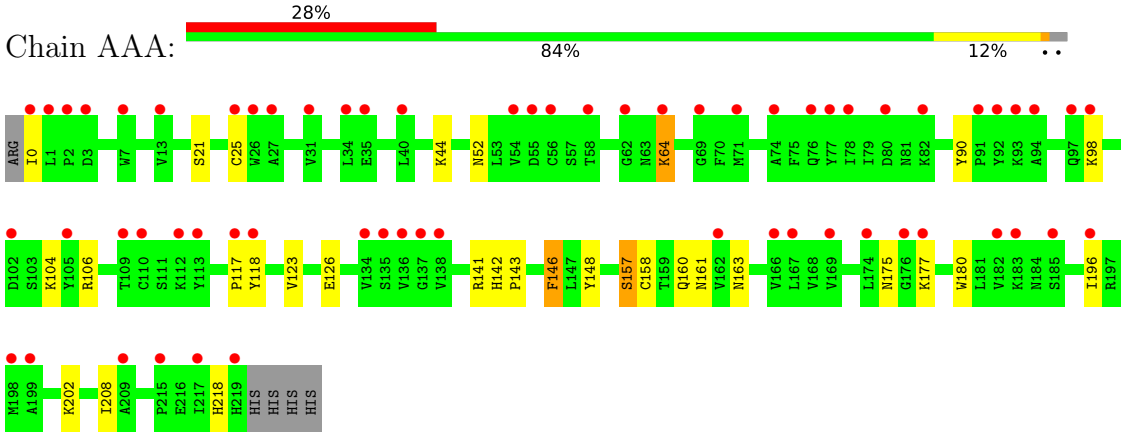
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	53	Total O 53 53	0	0
3	BBB	51	Total O 51 51	0	0
3	CCC	59	Total O 59 59	0	0
3	DDD	38	Total O 38 38	0	0

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.

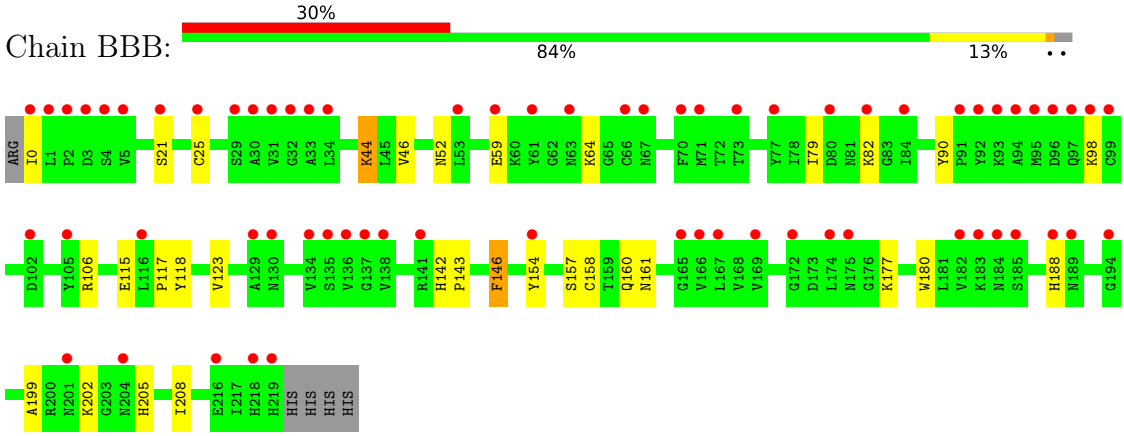
• Molecule 1: Cathepsin S

Chain AAA:



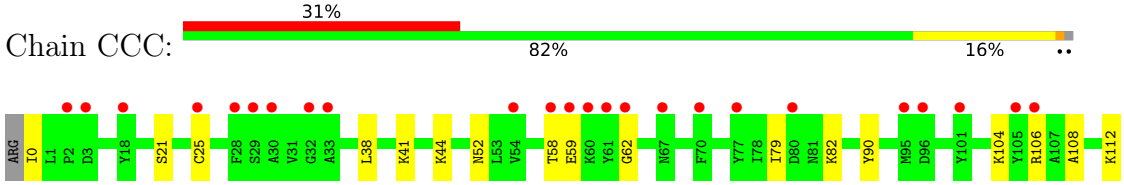
• Molecule 1: Cathepsin S

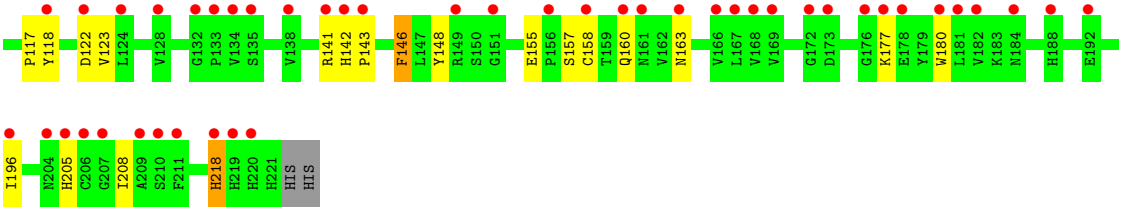
Chain BBB:



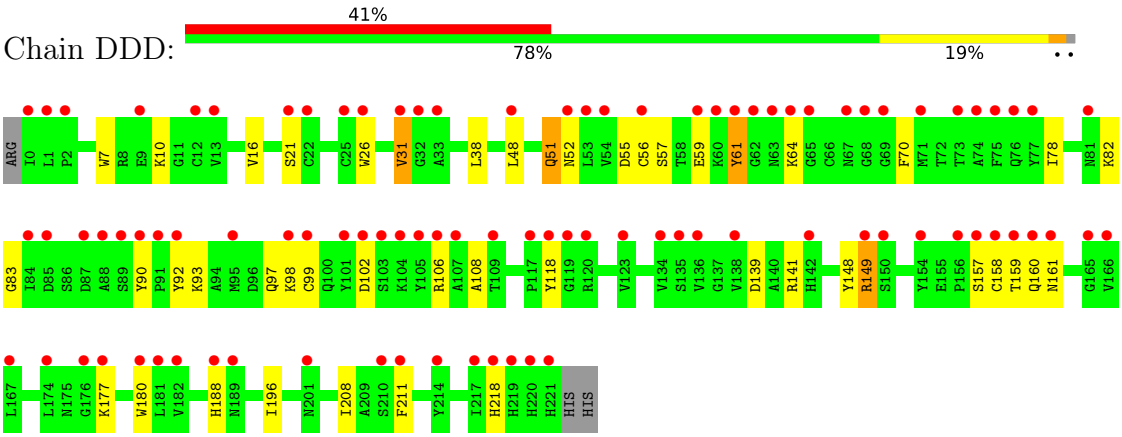
• Molecule 1: Cathepsin S

Chain CCC:





• Molecule 1: Cathepsin S



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	92.77Å 92.77Å 182.89Å 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) 99.8 (28.82-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.51Å)	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 (5.03%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	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.*

[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: 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	0.73	0/1757	0.85	1/2376 (0.0%)
1	BBB	0.69	0/1768	0.85	1/2391 (0.0%)
1	CCC	0.69	0/1779	0.86	3/2406 (0.1%)
1	DDD	0.70	0/1790	0.89	2/2421 (0.1%)
All	All	0.70	0/7094	0.86	7/9594 (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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	146	PHE	CB-CA-C	-6.23	97.94	110.40
1	CCC	218	HIS	CA-CB-CG	6.09	123.96	113.60
1	CCC	218	HIS	CB-CA-C	5.90	122.20	110.40
1	CCC	146	PHE	CB-CA-C	-5.54	99.32	110.40
1	BBB	146	PHE	CB-CA-C	-5.40	99.60	110.40
1	DDD	51	GLN	CB-CG-CD	-5.25	97.96	111.60
1	DDD	149	ARG	CG-CD-NE	-5.05	101.20	111.80

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 (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	1713	0	1632	13	0
1	BBB	1720	0	1639	19	0
1	CCC	1733	0	1646	16	0
1	DDD	1740	0	1655	37	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	2	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.

All (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
1:BBB:25:CYS:SG	3:BBB:2139:HOH:O	2.17	1.03
1:DDD:51:GLN:HE21	1:DDD:92:TYR:HA	1.33	0.93
1:DDD:31:VAL:HG22	1:DDD:48:LEU:HB2	1.51	0.92
1:DDD:26:TRP:CH2	3:DDD:307:HOH:O	2.23	0.91
1:AAA:142:HIS:ND1	1:DDD:21:SER:HB2	1.90	0.86
1:DDD:55:ASP:OD2	1:DDD:97:GLN:HG3	1.81	0.80
1:DDD:57:SER:HB3	3:DDD:307:HOH:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:83:GLY:O	3:DDD:301:HOH:O	1.99	0.80
1:AAA:25:CYS:SG	3:AAA:2134:HOH:O	2.43	0.77
1:DDD:56:CYS:HG	1:DDD:99:CYS:HG	0.75	0.73
1:DDD:26:TRP:HH2	3:DDD:307:HOH:O	1.62	0.72
1:AAA:161:ASN:HD21	1:BBB:161:ASN:HD21	1.39	0.70
1:DDD:188[B]:HIS:CE1	3:DDD:303:HOH:O	2.48	0.67
1:BBB:79:ILE:O	1:BBB:82:LYS:HD2	1.95	0.66
1:BBB:44:LYS:HE3	1:BBB:46:VAL:HG21	1.78	0.65
1:DDD:99:CYS:HB2	3:DDD:318:HOH:O	1.96	0.65
1:CCC:25:CYS:SG	3:CCC:2123:HOH:O	2.55	0.64
1:DDD:51:GLN:HE22	1:DDD:92:TYR:HA	0.84	0.64
1:DDD:149:ARG:NH2	3:DDD:304:HOH:O	2.30	0.63
1:CCC:62:GLY:HA3	3:CCC:2153:HOH:O	1.98	0.62
1:DDD:26:TRP:CZ3	3:DDD:307:HOH:O	2.49	0.60
1:DDD:139:ASP:OD1	1:DDD:141:ARG:HG3	2.02	0.60
1:BBB:115:GLU:O	1:DDD:93:LYS:NZ	2.35	0.59
1:AAA:180:TRP:CD1	1:AAA:208:ILE:HD13	2.37	0.59
1:DDD:157:SER:O	3:DDD:302:HOH:O	2.16	0.59
1:AAA:141:ARG:NH2	1:AAA:163:ASN:HD22	2.00	0.58
1:CCC:180:TRP:CD1	1:CCC:208:ILE:HD13	2.40	0.57
1:DDD:16:VAL:O	3:DDD:303:HOH:O	2.17	0.57
1:BBB:180:TRP:CD1	1:BBB:208:ILE:HD13	2.40	0.57
1:CCC:141:ARG:NH1	1:CCC:163:ASN:HD22	2.03	0.57
1:BBB:21:SER:CB	1:CCC:142:HIS:HD1	2.15	0.56
1:DDD:98:LYS:N	1:DDD:98:LYS:HD3	2.21	0.55
1:DDD:188[B]:HIS:NE2	3:DDD:303:HOH:O	2.33	0.55
1:CCC:79:ILE:O	1:CCC:82:LYS:HD2	2.06	0.55
1:DDD:180:TRP:CD1	1:DDD:208:ILE:HD13	2.42	0.55
1:BBB:142:HIS:ND1	1:CCC:21:SER:HB2	2.23	0.54
1:AAA:64:LYS:NZ	3:AAA:2104:HOH:O	2.40	0.54
1:DDD:55:ASP:CG	1:DDD:97:GLN:HG3	2.28	0.53
1:BBB:117:PRO:HD2	1:BBB:123:VAL:HG11	1.95	0.49
1:CCC:117:PRO:HD2	1:CCC:123:VAL:HG11	1.94	0.49
1:AAA:141:ARG:HH21	1:AAA:163:ASN:HD22	1.61	0.48
1:AAA:157:SER:O	1:AAA:157:SER:OG	2.32	0.48
1:CCC:143:PRO:HA	1:CCC:146:PHE:CD2	2.48	0.48
1:BBB:21:SER:CB	1:CCC:142:HIS:ND1	2.76	0.48
1:DDD:93:LYS:CE	1:DDD:97:GLN:OE1	2.62	0.47
1:AAA:143:PRO:HA	1:AAA:146:PHE:CD2	2.49	0.47
1:DDD:7:TRP:HA	1:DDD:10:LYS:HD2	1.97	0.46
1:AAA:141:ARG:NH2	1:AAA:163:ASN:ND2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:199:ALA:HB1	1:BBB:202:LYS:HE3	1.98	0.45
1:AAA:148:TYR:CE2	1:AAA:196:ILE:HA	2.52	0.45
1:DDD:38:LEU:HD13	1:DDD:108:ALA:HB2	1.99	0.45
1:DDD:51:GLN:HE22	1:DDD:92:TYR:CB	2.27	0.44
1:DDD:148:TYR:CE2	1:DDD:196:ILE:HA	2.51	0.44
1:CCC:112:LYS:NZ	3:CCC:2106:HOH:O	2.50	0.44
1:BBB:44:LYS:CE	1:BBB:46:VAL:CG2	2.96	0.44
1:BBB:157:SER:O	1:BBB:157:SER:OG	2.31	0.43
1:CCC:148:TYR:CE2	1:CCC:196:ILE:HA	2.53	0.43
1:CCC:58:THR:OG1	1:CCC:59:GLU:OE2	2.33	0.43
1:BBB:188[B]:HIS:CE1	3:BBB:2116:HOH:O	2.70	0.43
1:DDD:218:HIS:HB2	3:DDD:319:HOH:O	2.19	0.43
1:AAA:117:PRO:HD2	1:AAA:123:VAL:HG11	2.00	0.43
1:BBB:44:LYS:CE	1:BBB:46:VAL:HG21	2.46	0.43
1:BBB:143:PRO:HA	1:BBB:146:PHE:CD2	2.54	0.43
1:DDD:118:TYR:OH	1:DDD:160:GLN:HB3	2.18	0.43
1:DDD:56:CYS:CB	1:DDD:99:CYS:HG	2.28	0.43
1:CCC:118:TYR:OH	1:CCC:160:GLN:HB3	2.20	0.42
1:DDD:31:VAL:CG2	1:DDD:48:LEU:HB2	2.36	0.42
1:BBB:154:TYR:HA	1:BBB:205:HIS:CE1	2.55	0.41
1:BBB:118:TYR:OH	1:BBB:160:GLN:HB3	2.20	0.41
1:BBB:142:HIS:HB3	3:CCC:2124:HOH:O	2.20	0.41
1:AAA:118:TYR:OH	1:AAA:160:GLN:HB3	2.21	0.41
1:CCC:38:LEU:HD13	1:CCC:108:ALA:HB2	2.02	0.41
1:CCC:155:GLU:H	1:CCC:205:HIS:CE1	2.39	0.41
1:DDD:51:GLN:CD	1:DDD:93:LYS:H	2.24	0.41

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%)	10	19
1	BBB	182/186 (98%)	172 (94%)	10 (6%)	21	41
1	CCC	183/186 (98%)	171 (93%)	12 (7%)	16	32
1	DDD	184/186 (99%)	170 (92%)	14 (8%)	13	25
All	All	730/744 (98%)	678 (93%)	52 (7%)	14	28

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	0	ILE
1	AAA	21	SER
1	AAA	44	LYS
1	AAA	52	ASN
1	AAA	64	LYS
1	AAA	90	TYR
1	AAA	98	LYS
1	AAA	104	LYS
1	AAA	106	ARG
1	AAA	126	GLU
1	AAA	157	SER
1	AAA	158	CYS
1	AAA	175	ASN

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Mol	Chain	Res	Type
1	AAA	177	LYS
1	AAA	202	LYS
1	AAA	218	HIS
1	BBB	0	ILE
1	BBB	44	LYS
1	BBB	52	ASN
1	BBB	59	GLU
1	BBB	64	LYS
1	BBB	90	TYR
1	BBB	98	LYS
1	BBB	106	ARG
1	BBB	158	CYS
1	BBB	177	LYS
1	CCC	0	ILE
1	CCC	41	LYS
1	CCC	44	LYS
1	CCC	52	ASN
1	CCC	90	TYR
1	CCC	104	LYS
1	CCC	106	ARG
1	CCC	122	ASP
1	CCC	157	SER
1	CCC	158	CYS
1	CCC	177	LYS
1	CCC	218	HIS
1	DDD	31	VAL
1	DDD	52	ASN
1	DDD	59	GLU
1	DDD	61	TYR
1	DDD	64	LYS
1	DDD	70	PHE
1	DDD	82	LYS
1	DDD	90	TYR
1	DDD	102	ASP
1	DDD	106	ARG
1	DDD	158	CYS
1	DDD	161	ASN
1	DDD	177	LYS
1	DDD	211	PHE

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 monosaccharides 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%)	23,26,26	1.91	8 (34%)
2	Q1Q	CCC	2001	-	19,19,19	1.30	3 (15%)	23,26,26	2.05	5 (21%)
2	Q1Q	AAA	2001	-	19,19,19	1.66	5 (26%)	23,26,26	2.27	6 (26%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	2001	Q1Q	C-N1	4.01	1.40	1.34
2	AAA	2001	Q1Q	C1-N	3.83	1.41	1.34
2	CCC	2001	Q1Q	C-N1	3.63	1.40	1.34
2	AAA	2001	Q1Q	C-N1	3.21	1.39	1.34
2	AAA	2001	Q1Q	C3-N1	2.75	1.40	1.34
2	BBB	2001	Q1Q	C1-N	2.60	1.38	1.34
2	BBB	2001	Q1Q	C-N	2.56	1.40	1.34
2	CCC	2001	Q1Q	C1-N	2.52	1.38	1.34
2	BBB	2001	Q1Q	C3-N1	2.32	1.39	1.34
2	AAA	2001	Q1Q	C6-C1	2.15	1.54	1.50
2	AAA	2001	Q1Q	C-N	2.04	1.38	1.34
2	CCC	2001	Q1Q	C-N	2.01	1.38	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	2001	Q1Q	N1-C-N	-7.20	118.20	125.25
2	CCC	2001	Q1Q	N1-C-N	-6.07	119.30	125.25
2	BBB	2001	Q1Q	N1-C-N	-4.54	120.81	125.25
2	CCC	2001	Q1Q	C3-N1-C	4.17	121.73	116.22
2	AAA	2001	Q1Q	C3-N1-C	4.07	121.59	116.22
2	BBB	2001	Q1Q	C5-C-N1	3.86	121.56	117.41
2	AAA	2001	Q1Q	C5-C-N1	3.63	121.32	117.41
2	AAA	2001	Q1Q	C2-C1-N	-3.46	120.26	122.81
2	BBB	2001	Q1Q	C2-C1-N	-3.21	120.45	122.81
2	CCC	2001	Q1Q	C5-C-N1	3.06	120.70	117.41
2	CCC	2001	Q1Q	C4-C2-C3	-3.03	117.12	121.91
2	BBB	2001	Q1Q	C3-N1-C	2.62	119.69	116.22
2	CCC	2001	Q1Q	C2-C3-N1	-2.61	119.47	123.82
2	BBB	2001	Q1Q	C6-C8-C7	-2.37	106.59	111.63
2	BBB	2001	Q1Q	C6-C1-N	2.35	118.99	115.85
2	BBB	2001	Q1Q	C2-C3-N1	-2.28	120.01	123.82
2	AAA	2001	Q1Q	C6-C1-N	2.16	118.73	115.85
2	AAA	2001	Q1Q	C-N-C1	2.06	121.15	117.02
2	BBB	2001	Q1Q	C2-C4-C7	2.00	115.50	112.08

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

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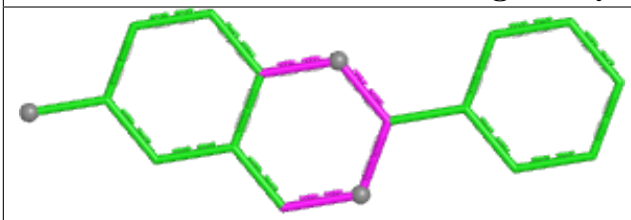
Mol	Chain	Res	Type	Atoms
2	CCC	2001	Q1Q	N1-C-C5-C9
2	CCC	2001	Q1Q	N1-C-C5-C10
2	AAA	2001	Q1Q	N-C-C5-C10

There are no ring outliers.

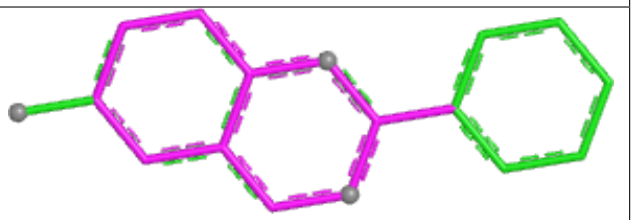
No monomer is involved in short contacts.

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 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.

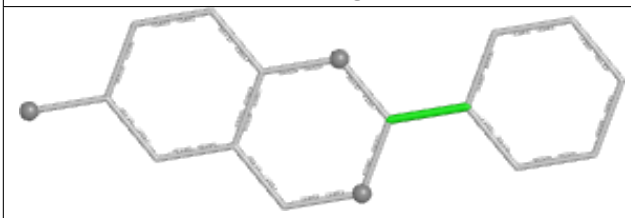
Ligand Q1Q BBB 2001



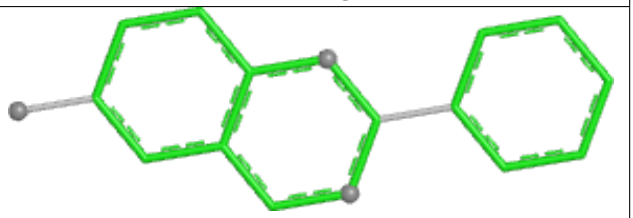
Bond lengths



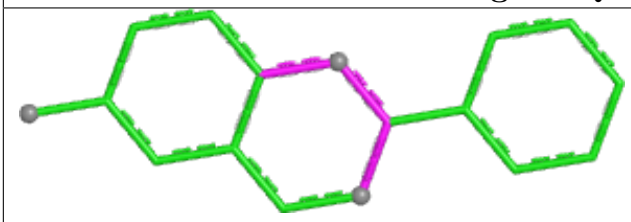
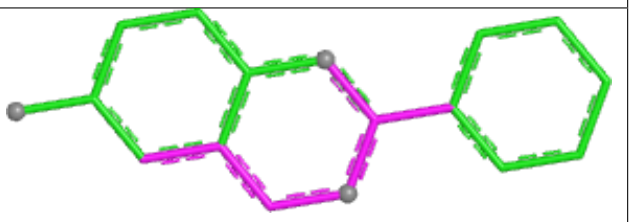
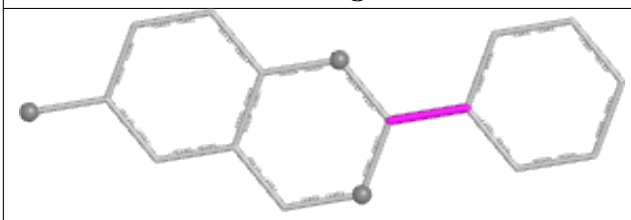
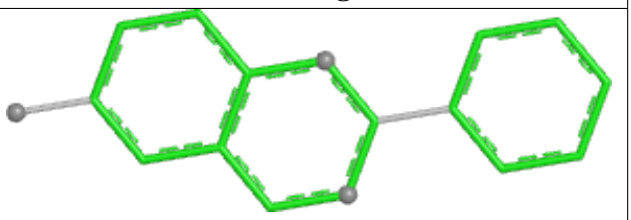
Bond angles

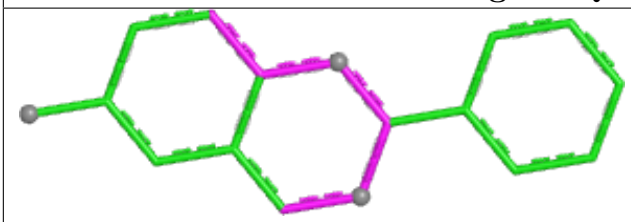
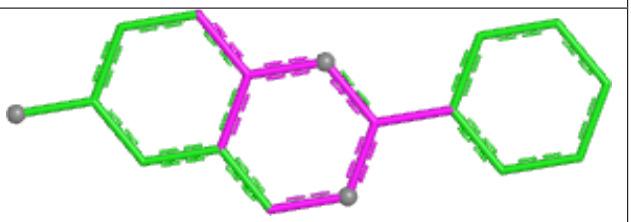
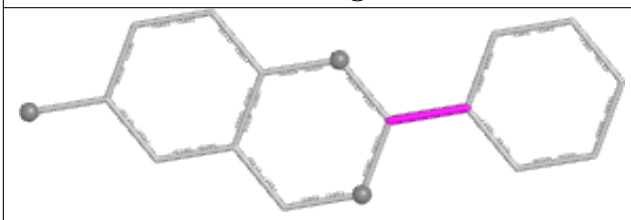
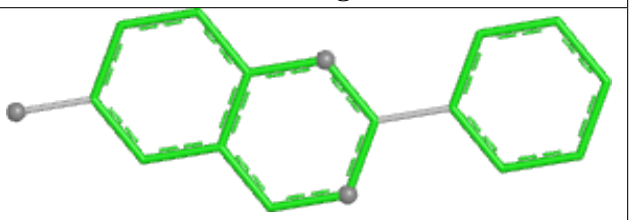


Torsions



Rings

Ligand Q1Q CCC 2001	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand Q1Q AAA 2001	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	220/225 (97%)	1.52	63 (28%)	0	0	54, 72, 95, 132	0
1	BBB	220/225 (97%)	1.61	67 (30%)	0	0	46, 75, 109, 137	0
1	CCC	222/225 (98%)	1.60	69 (31%)	0	0	44, 76, 106, 137	0
1	DDD	222/225 (98%)	2.07	93 (41%)	0	0	53, 91, 128, 148	0
All	All	884/900 (98%)	1.70	292 (33%)	0	0	44, 77, 117, 148	0

All (292) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	102	ASP	9.7
1	DDD	101	TYR	8.4
1	DDD	60	LYS	8.3
1	CCC	105	TYR	7.9
1	DDD	61	TYR	7.6
1	DDD	117	PRO	7.3
1	CCC	61	TYR	6.7
1	DDD	62	GLY	6.7
1	DDD	26	TRP	6.4
1	DDD	91	PRO	6.4
1	DDD	118	TYR	6.3
1	DDD	104	LYS	6.2
1	AAA	219	HIS	6.1
1	AAA	117	PRO	6.0
1	DDD	105	TYR	6.0
1	BBB	91	PRO	5.8
1	BBB	218	HIS	5.7
1	BBB	98	LYS	5.7
1	AAA	136	VAL	5.2
1	CCC	59	GLU	5.2
1	BBB	105	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	0	ILE	5.1
1	DDD	52	ASN	5.0
1	DDD	63	ASN	5.0
1	DDD	54	VAL	4.9
1	DDD	107	ALA	4.8
1	CCC	134	VAL	4.8
1	DDD	167	LEU	4.8
1	CCC	166	VAL	4.7
1	DDD	67	ASN	4.7
1	DDD	65	GLY	4.6
1	AAA	0	ILE	4.6
1	CCC	158	CYS	4.5
1	DDD	33	ALA	4.5
1	AAA	77	TYR	4.4
1	DDD	89	SER	4.4
1	DDD	188[A]	HIS	4.4
1	DDD	1	LEU	4.4
1	DDD	219	HIS	4.4
1	BBB	95	MET	4.4
1	BBB	59	GLU	4.4
1	BBB	61	TYR	4.4
1	AAA	138	VAL	4.4
1	DDD	221	HIS	4.3
1	DDD	218	HIS	4.3
1	CCC	33	ALA	4.3
1	BBB	5	VAL	4.3
1	AAA	166	VAL	4.2
1	BBB	93	LYS	4.2
1	DDD	211	PHE	4.2
1	BBB	30	ALA	4.2
1	BBB	166	VAL	4.2
1	CCC	58	THR	4.2
1	DDD	120	ARG	4.2
1	DDD	88	ALA	4.2
1	BBB	4	SER	4.1
1	DDD	103	SER	4.1
1	DDD	59	GLU	4.1
1	DDD	154	TYR	4.1
1	AAA	110	CYS	4.1
1	DDD	177	LYS	4.1
1	AAA	74	ALA	4.1
1	CCC	62	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	CCC	188	HIS	4.0
1	BBB	1	LEU	4.0
1	BBB	219	HIS	4.0
1	CCC	219	HIS	4.0
1	BBB	138	VAL	3.9
1	AAA	1	LEU	3.9
1	AAA	82	LYS	3.9
1	DDD	73	THR	3.9
1	DDD	81	ASN	3.8
1	BBB	167	LEU	3.8
1	BBB	175	ASN	3.7
1	DDD	64	LYS	3.7
1	AAA	135	SER	3.7
1	DDD	85	ASP	3.7
1	AAA	109	THR	3.7
1	BBB	201	ASN	3.6
1	AAA	167	LEU	3.6
1	DDD	174	LEU	3.6
1	CCC	77	TYR	3.6
1	CCC	167	LEU	3.6
1	DDD	71	MET	3.6
1	BBB	136	VAL	3.5
1	AAA	64	LYS	3.5
1	CCC	128	VAL	3.5
1	BBB	102	ASP	3.5
1	DDD	159	THR	3.4
1	BBB	2	PRO	3.4
1	AAA	174	LEU	3.4
1	AAA	54	VAL	3.4
1	DDD	136	VAL	3.4
1	DDD	182	VAL	3.4
1	AAA	56	CYS	3.3
1	DDD	25	CYS	3.3
1	DDD	123	VAL	3.3
1	BBB	174	LEU	3.3
1	BBB	32	GLY	3.3
1	CCC	180	TRP	3.3
1	DDD	161	ASN	3.3
1	DDD	176	GLY	3.3
1	DDD	92	TYR	3.3
1	CCC	177	LYS	3.3
1	CCC	160	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	189	ASN	3.2
1	CCC	118	TYR	3.2
1	DDD	217	ILE	3.2
1	CCC	96	ASP	3.2
1	CCC	29	SER	3.2
1	DDD	2	PRO	3.2
1	DDD	220	HIS	3.2
1	AAA	93	LYS	3.2
1	AAA	76	GLN	3.2
1	DDD	189	ASN	3.2
1	BBB	97	GLN	3.1
1	BBB	182	VAL	3.1
1	CCC	218	HIS	3.1
1	DDD	69	GLY	3.1
1	DDD	106	ARG	3.1
1	CCC	122	ASP	3.1
1	CCC	182	VAL	3.1
1	BBB	154	TYR	3.1
1	CCC	2	PRO	3.1
1	BBB	84	ILE	3.0
1	DDD	22	CYS	3.0
1	DDD	32	GLY	3.0
1	CCC	18	TYR	3.0
1	CCC	54	VAL	3.0
1	DDD	181	LEU	2.9
1	BBB	94	ALA	2.9
1	BBB	130	ASN	2.9
1	AAA	183	LYS	2.9
1	BBB	77	TYR	2.9
1	CCC	168	VAL	2.9
1	DDD	95	MET	2.9
1	CCC	143	PRO	2.9
1	CCC	149	ARG	2.9
1	CCC	60	LYS	2.9
1	AAA	31	VAL	2.8
1	AAA	94	ALA	2.8
1	BBB	134	VAL	2.8
1	DDD	98	LYS	2.8
1	CCC	209	ALA	2.8
1	AAA	13	VAL	2.8
1	AAA	78	ILE	2.8
1	CCC	30	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	AAA	198	MET	2.8
1	AAA	98	LYS	2.8
1	CCC	192	GLU	2.8
1	BBB	33	ALA	2.8
1	CCC	151	GLY	2.8
1	DDD	56	CYS	2.8
1	CCC	101	TYR	2.8
1	DDD	138	VAL	2.7
1	CCC	161	ASN	2.7
1	DDD	87	ASP	2.7
1	DDD	99	CYS	2.7
1	AAA	182	VAL	2.7
1	BBB	73	THR	2.7
1	DDD	158	CYS	2.7
1	CCC	135	SER	2.7
1	CCC	207	GLY	2.7
1	AAA	177	LYS	2.7
1	AAA	25	CYS	2.7
1	AAA	134	VAL	2.7
1	BBB	34	LEU	2.7
1	DDD	119	GLY	2.6
1	DDD	68	GLY	2.6
1	BBB	216	GLU	2.6
1	AAA	71	MET	2.6
1	DDD	77	TYR	2.6
1	CCC	205	HIS	2.6
1	DDD	165	GLY	2.6
1	CCC	67	ASN	2.6
1	DDD	166	VAL	2.6
1	BBB	172	GLY	2.6
1	CCC	172	GLY	2.6
1	CCC	176	GLY	2.6
1	DDD	13	VAL	2.5
1	DDD	156	PRO	2.5
1	DDD	160	GLN	2.5
1	BBB	70	PHE	2.5
1	DDD	74	ALA	2.5
1	CCC	206	CYS	2.5
1	DDD	135	SER	2.5
1	CCC	106	ARG	2.5
1	DDD	53	LEU	2.5
1	CCC	28	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	AAA	40	LEU	2.5
1	AAA	162	VAL	2.5
1	CCC	169	VAL	2.5
1	CCC	181	LEU	2.5
1	DDD	31	VAL	2.5
1	CCC	156	PRO	2.5
1	BBB	137	GLY	2.5
1	AAA	97	GLN	2.5
1	BBB	185	SER	2.5
1	DDD	84	ILE	2.5
1	BBB	3	ASP	2.5
1	BBB	188[A]	HIS	2.4
1	DDD	210	SER	2.4
1	CCC	3	ASP	2.4
1	AAA	209	ALA	2.4
1	DDD	12	CYS	2.4
1	BBB	96	ASP	2.4
1	BBB	71	MET	2.4
1	CCC	142	HIS	2.4
1	BBB	29	SER	2.4
1	AAA	169	VAL	2.4
1	BBB	31	VAL	2.4
1	CCC	138	VAL	2.4
1	CCC	220	HIS	2.4
1	DDD	142	HIS	2.4
1	BBB	129	ALA	2.4
1	CCC	184	ASN	2.4
1	BBB	82	LYS	2.4
1	AAA	92	TYR	2.4
1	AAA	113	TYR	2.4
1	CCC	32	GLY	2.3
1	CCC	133	PRO	2.3
1	AAA	58	THR	2.3
1	BBB	21	SER	2.3
1	BBB	184	ASN	2.3
1	DDD	75	PHE	2.3
1	BBB	165	GLY	2.3
1	AAA	102	ASP	2.3
1	DDD	180	TRP	2.3
1	AAA	2	PRO	2.3
1	AAA	215	PRO	2.3
1	DDD	0	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	DDD	150	SER	2.3
1	AAA	112	LYS	2.3
1	DDD	76	GLN	2.3
1	CCC	95	MET	2.3
1	CCC	132	GLY	2.3
1	DDD	214	TYR	2.3
1	AAA	137	GLY	2.3
1	AAA	26	TRP	2.3
1	AAA	55	ASP	2.3
1	AAA	80	ASP	2.3
1	BBB	25	CYS	2.3
1	AAA	196	ILE	2.2
1	CCC	196	ILE	2.2
1	DDD	149	ARG	2.2
1	BBB	53	LEU	2.2
1	AAA	91	PRO	2.2
1	CCC	25	CYS	2.2
1	CCC	124	LEU	2.2
1	BBB	92	TYR	2.2
1	CCC	141	ARG	2.2
1	DDD	157	SER	2.2
1	BBB	99	CYS	2.2
1	CCC	178	GLU	2.2
1	DDD	9	GLU	2.2
1	CCC	70	PHE	2.2
1	CCC	163	ASN	2.2
1	AAA	34	LEU	2.2
1	AAA	118	TYR	2.2
1	CCC	210	SER	2.2
1	DDD	90	TYR	2.2
1	AAA	176	GLY	2.2
1	AAA	105	TYR	2.1
1	DDD	109	THR	2.1
1	DDD	48	LEU	2.1
1	BBB	63	ASN	2.1
1	DDD	134	VAL	2.1
1	AAA	35	GLU	2.1
1	AAA	62	GLY	2.1
1	DDD	21	SER	2.1
1	BBB	80	ASP	2.1
1	AAA	69	GLY	2.1
1	CCC	80	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	BBB	67	ASN	2.1
1	DDD	201	ASN	2.1
1	AAA	27	ALA	2.1
1	AAA	199	ALA	2.1
1	BBB	141	ARG	2.1
1	AAA	3	ASP	2.1
1	AAA	217	ILE	2.1
1	AAA	185	SER	2.1
1	BBB	66	CYS	2.1
1	BBB	135	SER	2.1
1	CCC	211	PHE	2.1
1	AAA	7	TRP	2.1
1	BBB	194	GLY	2.1
1	BBB	183	LYS	2.0
1	BBB	204	ASN	2.0
1	CCC	173	ASP	2.0
1	BBB	169	VAL	2.0
1	CCC	204	ASN	2.0
1	BBB	116	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)

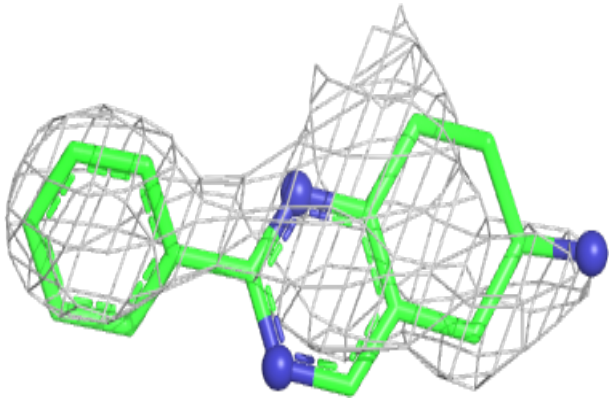
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

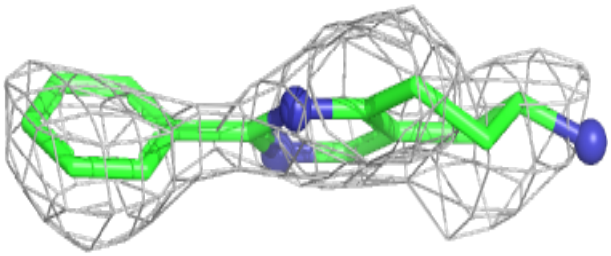
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	Q1Q	CCC	2001	17/17	0.51	0.44	100,110,113,115	0
2	Q1Q	AAA	2001	17/17	0.68	0.37	91,94,97,98	0
2	Q1Q	BBB	2001	17/17	0.82	0.27	84,97,110,110	0

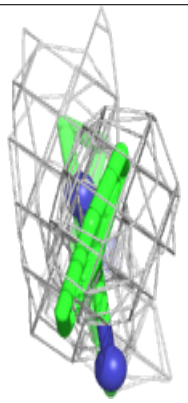
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Q1Q CCC 2001:

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

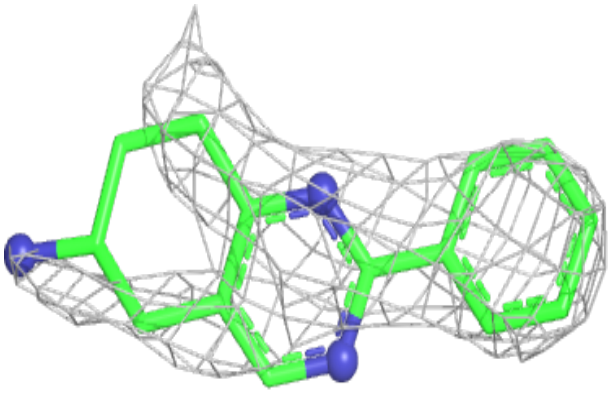


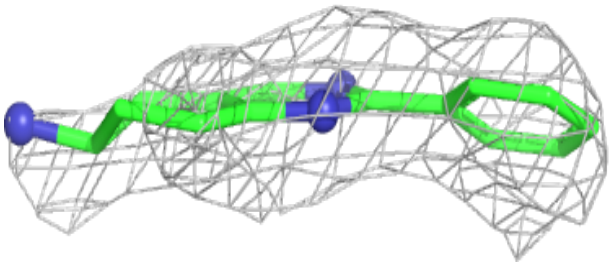


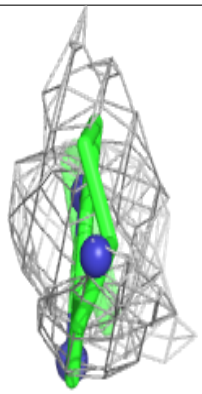


Electron density around Q1Q AAA 2001:

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

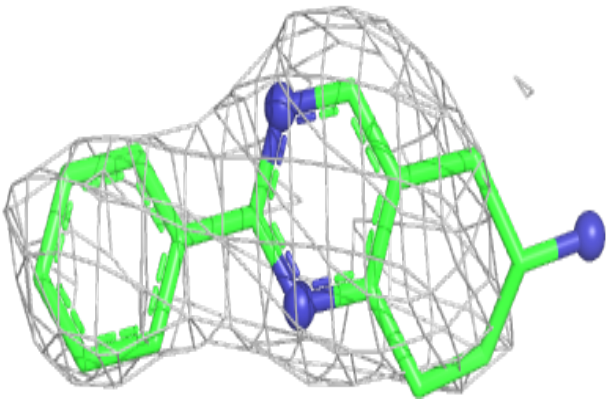


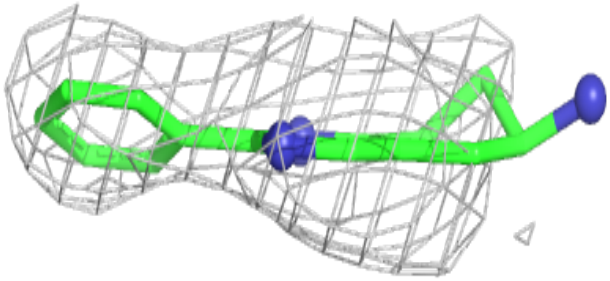


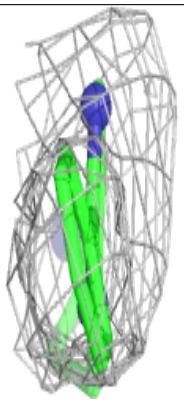


Electron density around Q1Q BBB 2001:

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







6.5 Other polymers (i)

There are no such residues in this entry.