Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:20 pm BST

PDB ID	:	2F3E
Title	:	Crystal Structure of the Bace complex with AXQ093, a macrocyclic inhibitor
Authors	:	Rondeau, J.-M.
Deposited on	:	2005-11-21
Resolution	:	2.11 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 following versions of software and data (see references ⓘ) were used in the production of this report:

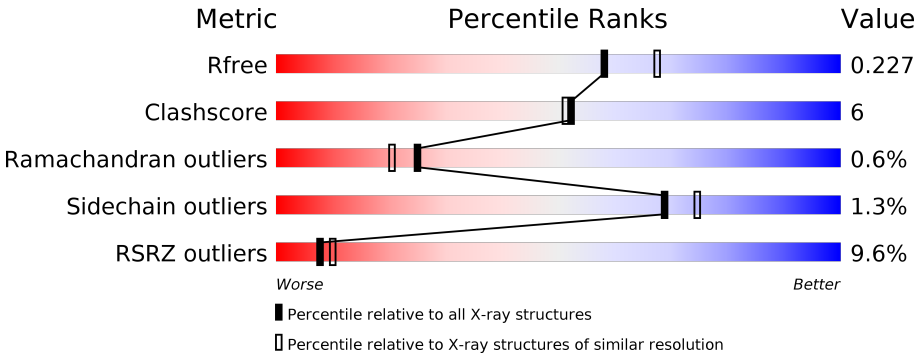
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 on 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	402	9% 81% 12% • 6%
1	B	402	12% 80% 13% • 6%
1	C	402	6% 81% 13% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9508 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.

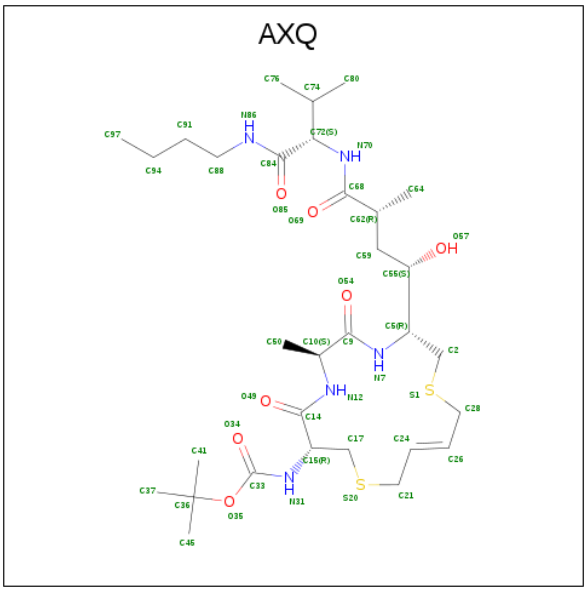
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2966	1898	493	561	14			
1	B	377	Total	C	N	O	S	0	0	0
			2966	1898	493	561	14			
1	C	381	Total	C	N	O	S	0	0	0
			2993	1917	497	565	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33P	GLY	-	CLONING ARTIFACT	UNP P56817
A	34P	PRO	-	CLONING ARTIFACT	UNP P56817
B	33P	GLY	-	CLONING ARTIFACT	UNP P56817
B	34P	PRO	-	CLONING ARTIFACT	UNP P56817
C	33P	GLY	-	CLONING ARTIFACT	UNP P56817
C	34P	PRO	-	CLONING ARTIFACT	UNP P56817

- Molecule 2 is {(E)-(3R,6S,9R)-3-[(1S,3R)-3-((S)-1 -BUTYLCARBAMOYL-2-METHYL-PROPYLCARB AMOYL)-1-HYDROXY-BUTYL]-6-METHYL-5, 8-DIOXO-1,11-DITHIA-4, 7-DIAZA-CYCLO PENTADEC-13-EN-9-YL}-CARBAMIC ACID TERT-BUTYL ESTER (three-letter code: AXQ) (formula: $C_{31}H_{55}N_5O_7S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O S 45 31 5 7 2	0	0
2	B	1	Total C N O S 45 31 5 7 2	0	0
2	C	1	Total C N O S 45 31 5 7 2	0	0

- Molecule 3 is water.

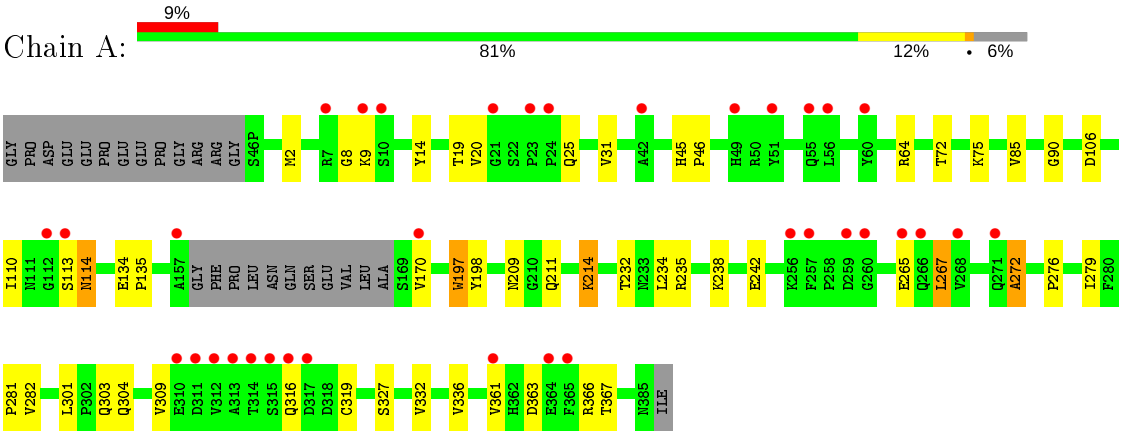
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	151	Total O 151 151	0	0
3	B	132	Total O 132 132	0	0
3	C	165	Total O 165 165	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

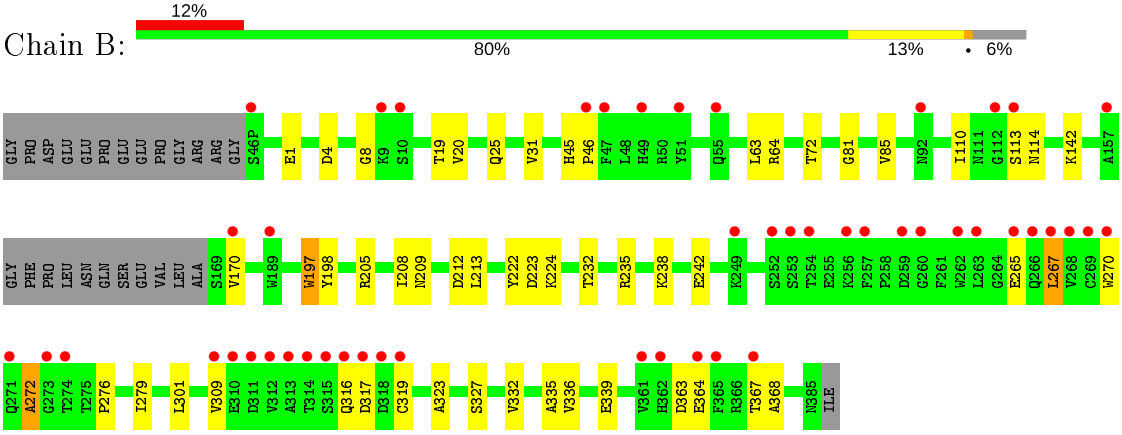
- Molecule 1: Beta-secretase 1

Chain A:



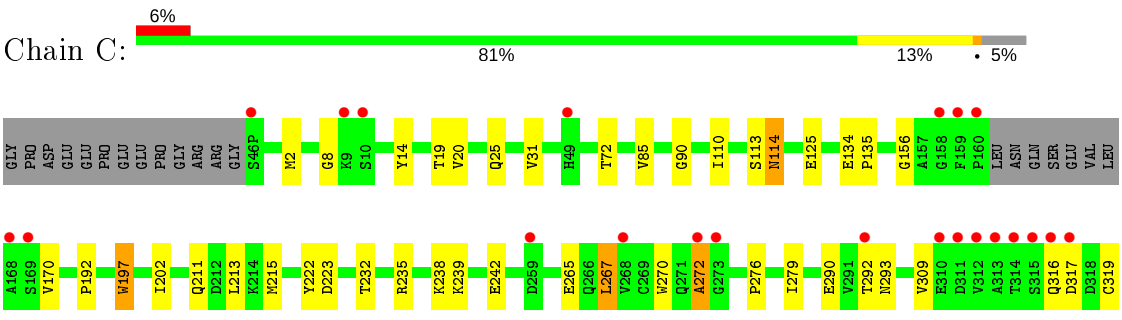
- Molecule 1: Beta-secretase 1

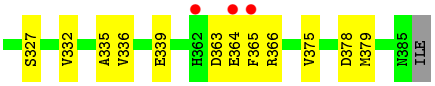
Chain B:



- Molecule 1: Beta-secretase 1

Chain C:




S327
V332
A335
V336
E339
H362
D363
E364
F365
R366
V375
D378
M379
N385
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.24Å 103.78Å 100.96Å 90.00° 103.04° 90.00°	Depositor
Resolution (Å)	63.42 – 2.11 63.42 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.7 (63.42-2.11) 98.8 (63.42-2.11)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.10Å)	Xtriage
Refinement program	CNS, CNX 2002	Depositor
R, R_{free}	0.206 , 0.237 0.197 , 0.227	Depositor DCC
R_{free} test set	4701 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9508	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: AXQ

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	A	0.34	0/3041	0.61	1/4133 (0.0%)
1	B	0.35	0/3041	0.61	0/4133
1	C	0.35	0/3070	0.62	0/4173
All	All	0.34	0/9152	0.61	1/12439 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	LEU	N-CA-C	-5.32	96.64	111.00

There are no chirality outliers.

There are no planarity outliers.

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	A	2966	0	2875	32	0
1	B	2966	0	2875	32	0
1	C	2993	0	2899	37	0
2	A	45	0	55	1	0
2	B	45	0	55	1	0
2	C	45	0	55	2	0
3	A	151	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	132	0	0	3	0
3	C	165	0	0	2	0
All	All	9508	0	8814	99	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 (99) 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:C:202:ILE:CD1	1:C:379:MET:HG3	2.14	0.77
1:C:363:ASP:HB3	1:C:366:ARG:O	1.94	0.67
1:B:301:LEU:HD11	1:B:367:THR:HA	1.78	0.66
1:B:323:ALA:HB1	1:B:336:VAL:HG11	1.77	0.66
1:C:202:ILE:HD11	1:C:379:MET:HG3	1.78	0.65
2:C:603:AXQ:H373	3:C:695:HOH:O	1.96	0.65
1:B:208:ILE:HD12	1:B:213:LEU:HD21	1.82	0.62
1:C:202:ILE:HD12	1:C:379:MET:HE2	1.81	0.62
1:A:232:THR:O	1:A:336:VAL:HG13	2.01	0.60
1:B:335:ALA:O	1:B:339:GLU:HG3	2.01	0.60
1:A:20:VAL:HG12	1:A:85:VAL:HG22	1.85	0.59
1:A:367:THR:H	1:C:211:GLN:HE22	1.51	0.58
1:A:276:PRO:O	1:A:279:ILE:HG12	2.03	0.58
1:C:20:VAL:HG12	1:C:85:VAL:HG22	1.86	0.58
1:B:276:PRO:O	1:B:279:ILE:HG12	2.04	0.56
1:C:276:PRO:O	1:C:279:ILE:HG12	2.07	0.55
1:A:363:ASP:HB3	1:A:366:ARG:O	2.08	0.54
1:B:20:VAL:HG12	1:B:85:VAL:HG22	1.90	0.54
1:A:214:LYS:HA	1:A:214:LYS:NZ	2.23	0.54
1:A:238:LYS:O	1:A:242:GLU:HG3	2.10	0.52
1:A:267:LEU:HD12	1:A:319:CYS:HB3	1.90	0.52
1:C:125:GLU:HG2	1:C:197:TRP:HB3	1.92	0.52
1:A:75:LYS:HD2	3:A:690:HOH:O	2.10	0.52
1:B:235:ARG:HB3	1:B:327:SER:HB2	1.91	0.52
1:B:205:ARG:NH2	1:B:212:ASP:HB2	2.24	0.52
1:B:267:LEU:HD12	1:B:319:CYS:HB3	1.92	0.52
1:C:267:LEU:HD12	1:C:319:CYS:HB3	1.92	0.52
1:A:8:GLY:C	1:A:170:VAL:HG22	2.29	0.51
1:C:215:MET:CE	1:C:239:LYS:HG2	2.41	0.50
1:A:304:GLN:HG3	1:A:361:VAL:HG21	1.94	0.49
1:B:209:ASN:HA	3:B:722:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ARG:HB3	1:C:327:SER:HB2	1.93	0.49
1:A:235:ARG:HB2	1:A:332:VAL:HB	1.95	0.49
1:A:235:ARG:HB3	1:A:327:SER:HB2	1.94	0.49
1:A:106:ASP:OD1	1:B:1:GLU:HG2	2.13	0.49
1:A:110:ILE:HB	1:A:113:SER:HB3	1.93	0.49
1:A:19:THR:HA	1:A:25:GLN:O	2.13	0.49
1:B:110:ILE:HB	1:B:113:SER:HB3	1.96	0.48
1:B:235:ARG:HB2	1:B:332:VAL:HB	1.95	0.48
1:C:19:THR:HA	1:C:25:GLN:O	2.14	0.48
1:B:272:ALA:HB2	1:B:316:GLN:O	2.14	0.48
1:C:238:LYS:O	1:C:242:GLU:HG3	2.14	0.48
1:C:272:ALA:HB2	1:C:316:GLN:O	2.13	0.48
1:B:31:VAL:O	1:B:31:VAL:HG23	2.13	0.48
1:C:110:ILE:HB	1:C:113:SER:HB3	1.96	0.48
1:A:367:THR:H	1:C:211:GLN:NE2	2.12	0.47
1:A:272:ALA:HB2	1:A:316:GLN:O	2.15	0.47
1:A:282:VAL:HG12	1:A:301:LEU:HD23	1.96	0.47
1:C:267:LEU:HD13	1:C:309:VAL:HG21	1.96	0.47
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.95	0.47
1:B:232:THR:O	1:B:336:VAL:HG13	2.15	0.47
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.97	0.47
1:B:368:ALA:HB3	3:B:713:HOH:O	2.14	0.46
1:A:303:GLN:HB2	1:A:361:VAL:HG11	1.98	0.46
1:B:64:ARG:HH11	1:B:64:ARG:HG2	1.81	0.46
1:B:63:LEU:HG	1:B:81:GLY:HA2	1.98	0.46
1:C:235:ARG:HB2	1:C:332:VAL:HB	1.96	0.46
1:C:202:ILE:CD1	1:C:379:MET:HE2	2.46	0.45
1:B:238:LYS:O	1:B:242:GLU:HG3	2.17	0.45
1:C:134:GLU:HA	1:C:135:PRO:HD3	1.89	0.45
1:A:267:LEU:HD13	1:A:309:VAL:HG21	1.99	0.45
1:A:8:GLY:O	1:A:170:VAL:HG22	2.17	0.44
1:B:267:LEU:HD13	1:B:309:VAL:HG21	1.98	0.44
1:C:293:ASN:HA	1:C:375:VAL:HA	1.99	0.44
1:C:14:TYR:O	1:C:31:VAL:HG22	2.17	0.44
1:B:19:THR:HA	1:B:25:GLN:O	2.17	0.44
1:C:364:GLU:HB3	1:C:365:PHE:HD1	1.83	0.44
1:B:363:ASP:CG	1:B:364:GLU:H	2.20	0.44
1:A:197:TRP:CG	1:A:198:TYR:N	2.86	0.43
1:C:31:VAL:O	1:C:31:VAL:HG23	2.18	0.43
1:A:134:GLU:HA	1:A:135:PRO:HD3	1.87	0.43
1:A:72:THR:HB	2:A:601:AXQ:O54	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:HE2	1:A:9:LYS:HB3	1.78	0.43
1:A:14:TYR:O	1:A:31:VAL:HG22	2.19	0.43
1:A:31:VAL:HG23	1:A:31:VAL:O	2.18	0.43
1:C:213:LEU:HD23	1:C:213:LEU:HA	1.82	0.43
1:C:72:THR:HB	2:C:603:AXQ:O54	2.19	0.43
1:B:72:THR:HB	2:B:602:AXQ:O54	2.20	0.42
1:C:215:MET:HE1	1:C:239:LYS:HG2	2.00	0.42
1:C:192:PRO:HG3	1:C:290:GLU:HA	2.02	0.42
1:B:142:LYS:HG3	3:B:677:HOH:O	2.20	0.42
1:B:222:TYR:HA	1:B:223:ASP:HA	1.58	0.42
1:B:8:GLY:C	1:B:170:VAL:HG22	2.39	0.42
1:C:232:THR:O	1:C:336:VAL:HG13	2.19	0.42
1:C:378:ASP:HB2	3:C:711:HOH:O	2.19	0.42
1:C:335:ALA:O	1:C:339:GLU:HG3	2.20	0.42
1:A:45:HIS:HA	1:A:46:PRO:HD3	1.94	0.41
1:B:198:TYR:CE2	1:B:224:LYS:HE3	2.55	0.41
1:B:270:TRP:O	1:B:317:ASP:HB3	2.21	0.41
1:B:45:HIS:HA	1:B:46:PRO:HD3	1.95	0.41
1:C:292:THR:HG21	1:C:378:ASP:HB3	2.02	0.41
1:B:323:ALA:CB	1:B:336:VAL:HG11	2.46	0.41
1:A:209:ASN:ND2	1:A:281:PRO:HB3	2.37	0.40
1:B:197:TRP:CG	1:B:198:TYR:N	2.88	0.40
1:A:114:ASN:HD22	1:A:114:ASN:HA	1.71	0.40
1:C:8:GLY:C	1:C:170:VAL:HG22	2.42	0.40
1:C:270:TRP:O	1:C:317:ASP:HB3	2.21	0.40
1:C:114:ASN:HD22	1:C:114:ASN:HA	1.71	0.40
1:C:222:TYR:HA	1:C:223:ASP:HA	1.63	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	A	373/402 (93%)	355 (95%)	16 (4%)	2 (0%)	29	25
1	B	373/402 (93%)	350 (94%)	21 (6%)	2 (0%)	29	25
1	C	377/402 (94%)	360 (96%)	14 (4%)	3 (1%)	19	14
All	All	1123/1206 (93%)	1065 (95%)	51 (4%)	7 (1%)	25	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	272	ALA
1	C	272	ALA
1	A	265	GLU
1	A	272	ALA
1	B	265	GLU
1	C	156	GLY
1	C	265	GLU

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	322/342 (94%)	316 (98%)	6 (2%)	57	61
1	B	322/342 (94%)	318 (99%)	4 (1%)	71	77
1	C	324/342 (95%)	321 (99%)	3 (1%)	78	83
All	All	968/1026 (94%)	955 (99%)	13 (1%)	69	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	114	ASN
1	A	197	TRP
1	A	211	GLN
1	A	214	LYS
1	A	267	LEU

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Mol	Chain	Res	Type
1	B	4	ASP
1	B	114	ASN
1	B	197	TRP
1	B	267	LEU
1	C	114	ASN
1	C	197	TRP
1	C	267	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	114	ASN
1	A	326	GLN
1	B	114	ASN
1	B	293	ASN
1	B	326	GLN
1	C	114	ASN
1	C	211	GLN

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 carbohydrates 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	AXQ	C	603	-	45,45,45	0.81	1 (2%)	55,60,60	1.47	7 (12%)
2	AXQ	B	602	-	45,45,45	0.85	1 (2%)	55,60,60	1.45	6 (10%)
2	AXQ	A	601	-	45,45,45	0.84	1 (2%)	55,60,60	1.46	7 (12%)

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	AXQ	C	603	-	-	5/65/65/65	0/0/1/1
2	AXQ	B	602	-	-	5/65/65/65	0/0/1/1
2	AXQ	A	601	-	-	5/65/65/65	0/0/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	AXQ	C55-C5	2.65	1.58	1.53
2	A	601	AXQ	C55-C5	2.21	1.57	1.53
2	C	603	AXQ	C55-C5	2.15	1.57	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	AXQ	C62-C59-C55	-5.08	105.73	114.74
2	B	602	AXQ	C62-C59-C55	-5.06	105.77	114.74
2	C	603	AXQ	C62-C59-C55	-5.04	105.80	114.74
2	A	601	AXQ	C36-O35-C33	-4.39	114.24	120.99
2	B	602	AXQ	C36-O35-C33	-4.35	114.31	120.99
2	C	603	AXQ	C36-O35-C33	-4.27	114.42	120.99
2	A	601	AXQ	C64-C62-C68	-2.78	104.95	109.42
2	C	603	AXQ	C88-N86-C84	-2.69	117.80	122.59
2	B	602	AXQ	C64-C62-C68	-2.67	105.12	109.42
2	A	601	AXQ	C88-N86-C84	-2.65	117.86	122.59
2	C	603	AXQ	C64-C62-C68	-2.59	105.25	109.42
2	B	602	AXQ	C17-C15-C14	-2.43	104.46	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	603	AXQ	C17-C15-C14	-2.25	104.84	109.73
2	A	601	AXQ	C17-C15-C14	-2.21	104.94	109.73
2	B	602	AXQ	C88-N86-C84	-2.17	118.71	122.59
2	A	601	AXQ	O57-C55-C59	-2.11	104.88	109.11
2	A	601	AXQ	C28-C26-C24	-2.10	119.82	125.24
2	C	603	AXQ	O57-C55-C59	-2.08	104.94	109.11
2	C	603	AXQ	C50-C10-C9	2.07	114.08	110.14
2	B	602	AXQ	C28-C26-C24	-2.05	119.95	125.24

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	603	AXQ	N12-C10-C9-O54
2	A	601	AXQ	N12-C10-C9-O54
2	B	602	AXQ	N12-C10-C9-O54
2	C	603	AXQ	N12-C10-C9-N7
2	A	601	AXQ	N12-C10-C9-N7
2	B	602	AXQ	N12-C10-C9-N7
2	C	603	AXQ	C55-C59-C62-C68
2	A	601	AXQ	C55-C59-C62-C68
2	B	602	AXQ	C55-C59-C62-C68
2	C	603	AXQ	C50-C10-C9-N7
2	C	603	AXQ	C50-C10-C9-O54
2	A	601	AXQ	C50-C10-C9-O54
2	B	602	AXQ	C50-C10-C9-O54
2	A	601	AXQ	C50-C10-C9-N7
2	B	602	AXQ	C50-C10-C9-N7

There are no ring outliers.

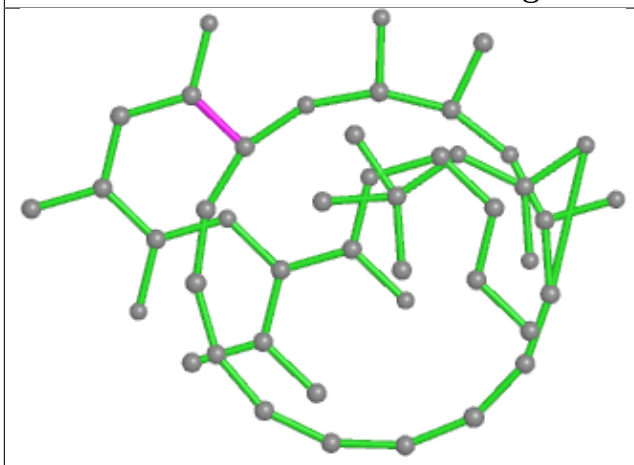
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	603	AXQ	2	0
2	B	602	AXQ	1	0
2	A	601	AXQ	1	0

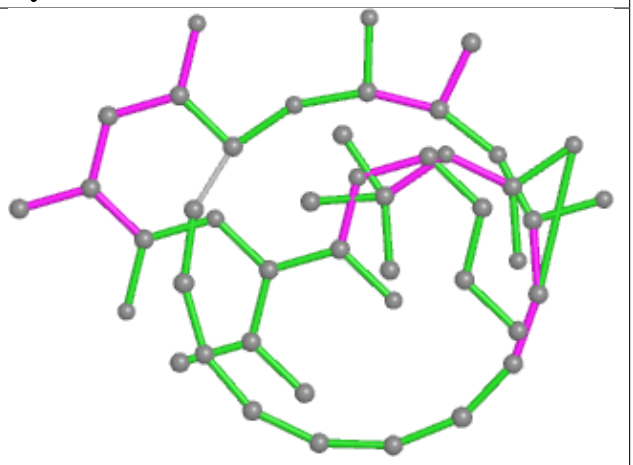
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

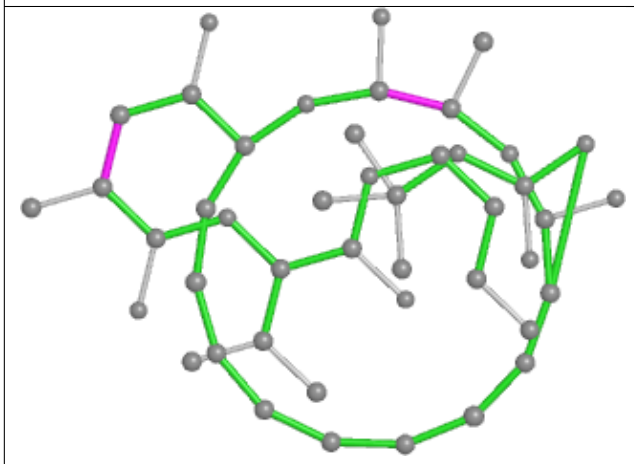
Ligand AXQ C 603



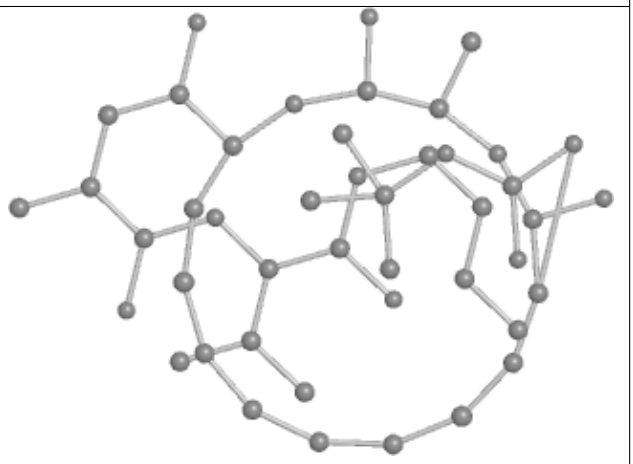
Bond lengths



Bond angles

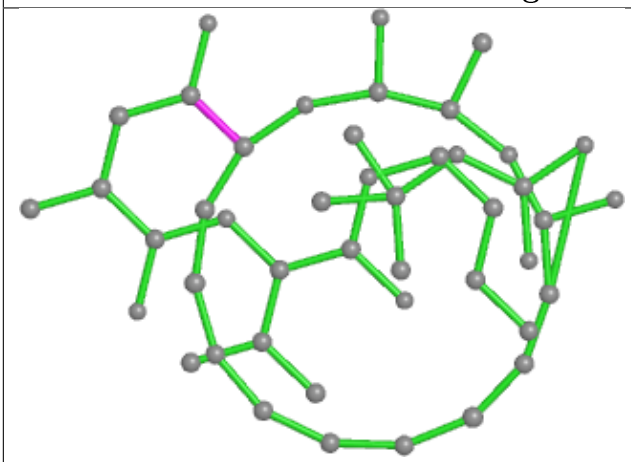


Torsions

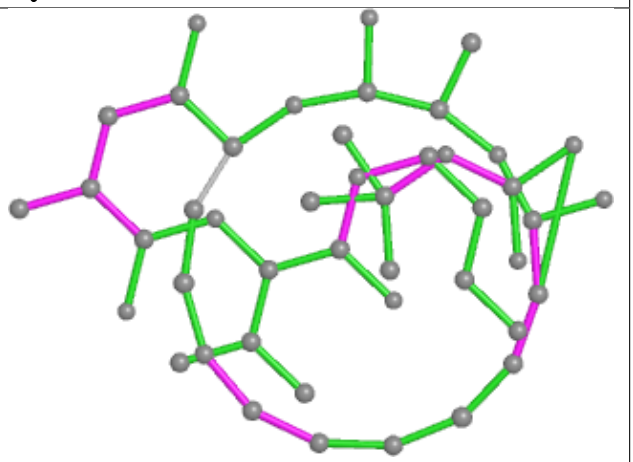


Rings

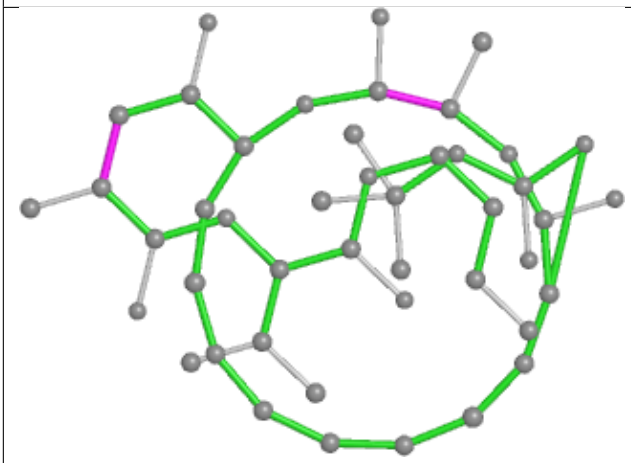
Ligand AXQ B 602



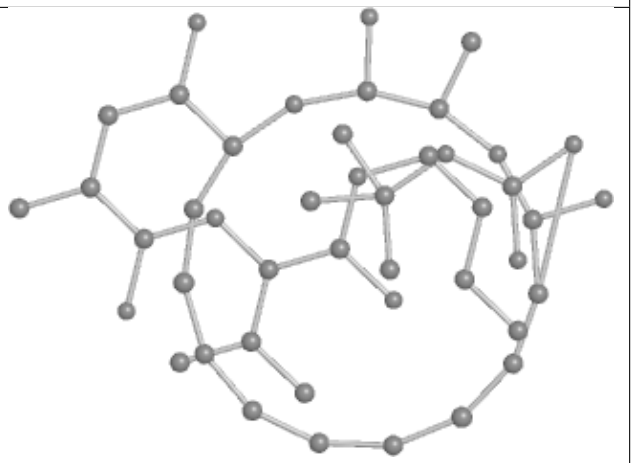
Bond lengths



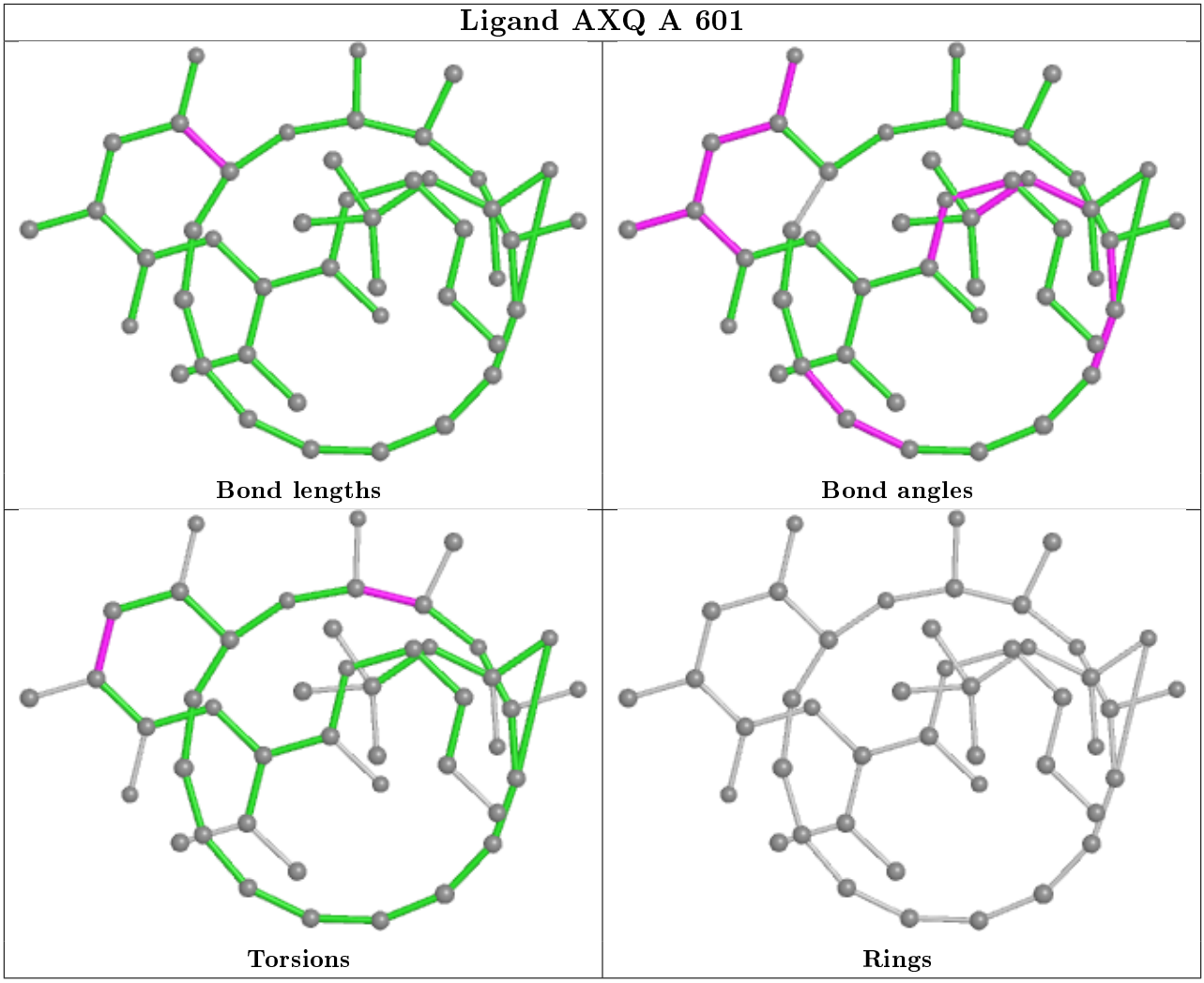
Bond angles



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	A	377/402 (93%)	0.79	35 (9%) 8 11	28, 49, 84, 119	0
1	B	377/402 (93%)	1.03	49 (12%) 3 4	27, 49, 89, 119	0
1	C	381/402 (94%)	0.73	25 (6%) 18 22	27, 47, 86, 118	0
All	All	1135/1206 (94%)	0.85	109 (9%) 8 10	27, 48, 87, 119	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	VAL	12.6
1	C	312	VAL	11.0
1	B	314	THR	10.6
1	B	315	SER	9.8
1	A	314	THR	8.7
1	C	158	GLY	8.4
1	A	313	ALA	8.0
1	A	312	VAL	7.1
1	C	313	ALA	6.9
1	B	313	ALA	6.6
1	A	311	ASP	6.5
1	C	314	THR	6.2
1	B	311	ASP	6.2
1	C	159	PHE	5.6
1	B	268	VAL	5.1
1	C	168	ALA	5.0
1	B	309	VAL	4.9
1	B	317	ASP	4.9
1	A	316	GLN	4.7
1	A	315	SER	4.6
1	C	315	SER	4.5
1	B	310	GLU	4.5
1	C	311	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	316	GLN	4.2
1	A	317	ASP	4.1
1	C	365	PHE	4.1
1	B	269	CYS	3.9
1	B	271	GLN	3.9
1	B	257	PHE	3.8
1	B	266	GLN	3.8
1	B	252	SER	3.6
1	B	256	LYS	3.6
1	B	157	ALA	3.6
1	C	160	PRO	3.6
1	B	253	SER	3.5
1	B	362	HIS	3.4
1	B	319	CYS	3.4
1	B	273	GLY	3.4
1	B	361	VAL	3.3
1	C	10	SER	3.2
1	B	274	THR	3.2
1	B	9	LYS	3.2
1	A	364	GLU	3.1
1	B	365	PHE	3.1
1	B	46(P)	SER	3.1
1	A	257	PHE	3.1
1	A	256	LYS	3.1
1	A	266	GLN	3.0
1	A	259	ASP	2.9
1	C	310	GLU	2.9
1	C	46(P)	SER	2.9
1	B	47	PHE	2.8
1	C	259	ASP	2.8
1	A	310	GLU	2.8
1	A	265	GLU	2.8
1	A	112	GLY	2.8
1	A	157	ALA	2.8
1	B	265	GLU	2.8
1	B	113	SER	2.8
1	B	318	ASP	2.7
1	C	49	HIS	2.7
1	A	10	SER	2.7
1	C	273	GLY	2.7
1	C	268	VAL	2.7
1	B	259	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	364	GLU	2.6
1	B	267	LEU	2.6
1	B	51	TYR	2.6
1	A	21	GLY	2.6
1	B	364	GLU	2.6
1	C	9	LYS	2.5
1	B	55	GLN	2.5
1	A	365	PHE	2.5
1	B	49	HIS	2.5
1	B	262	TRP	2.5
1	A	113	SER	2.5
1	C	316	GLN	2.4
1	A	170	VAL	2.4
1	C	169	SER	2.4
1	A	24	PRO	2.4
1	B	249	LYS	2.4
1	C	292	THR	2.4
1	A	49	HIS	2.3
1	B	260	GLY	2.3
1	B	263	LEU	2.3
1	B	270	TRP	2.3
1	A	271	GLN	2.3
1	A	361	VAL	2.3
1	B	112	GLY	2.3
1	A	9	LYS	2.3
1	A	23	PRO	2.3
1	B	254	THR	2.2
1	A	51	TYR	2.2
1	C	362	HIS	2.2
1	B	10	SER	2.2
1	B	170	VAL	2.2
1	C	317	ASP	2.2
1	B	92	ASN	2.2
1	A	55	GLN	2.1
1	A	60	TYR	2.1
1	A	56	LEU	2.1
1	B	189	TRP	2.1
1	A	7	ARG	2.1
1	B	46	PRO	2.1
1	C	272	ALA	2.1
1	A	260	GLY	2.1
1	B	367	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	268	VAL	2.0
1	A	42	ALA	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 carbohydrates in this entry.

6.4 Ligands (i)

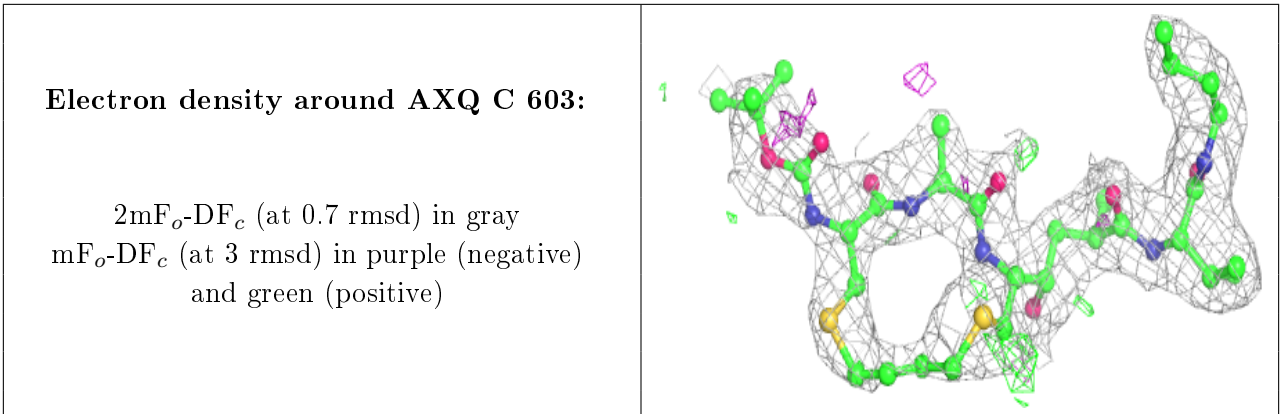
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

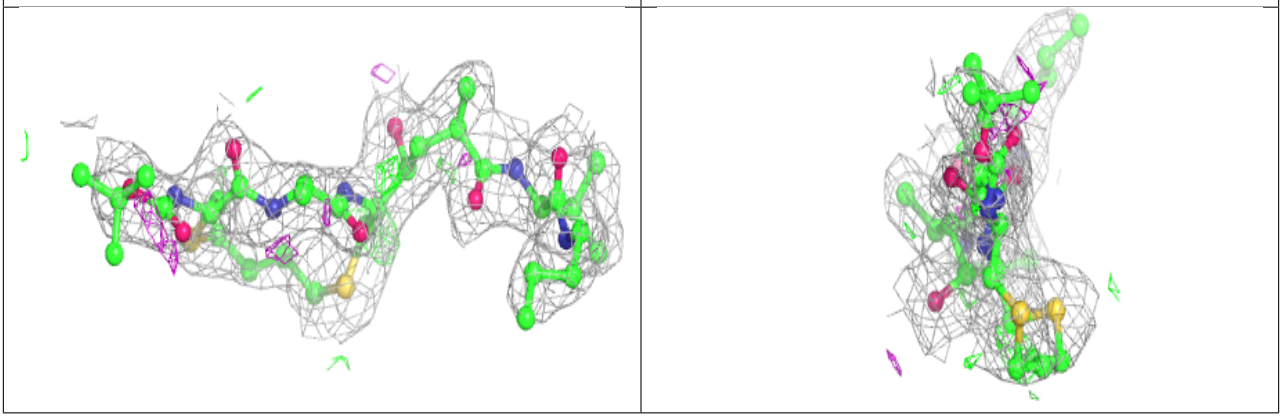
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AXQ	C	603	45/45	0.86	0.20	37,61,89,90	0
2	AXQ	A	601	45/45	0.86	0.24	42,67,91,94	0
2	AXQ	B	602	45/45	0.87	0.23	37,63,91,93	0

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 AXQ C 603:

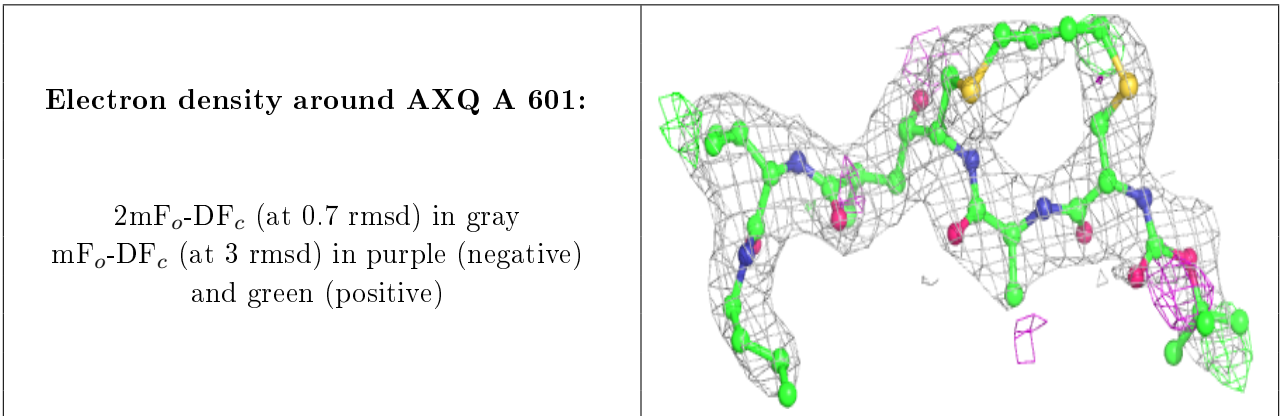
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

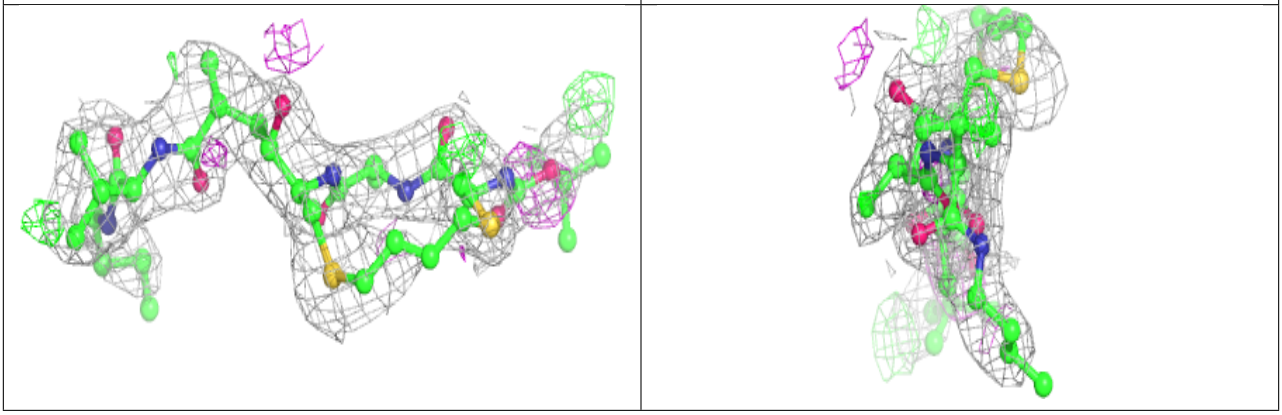




Electron density around AXQ A 601:

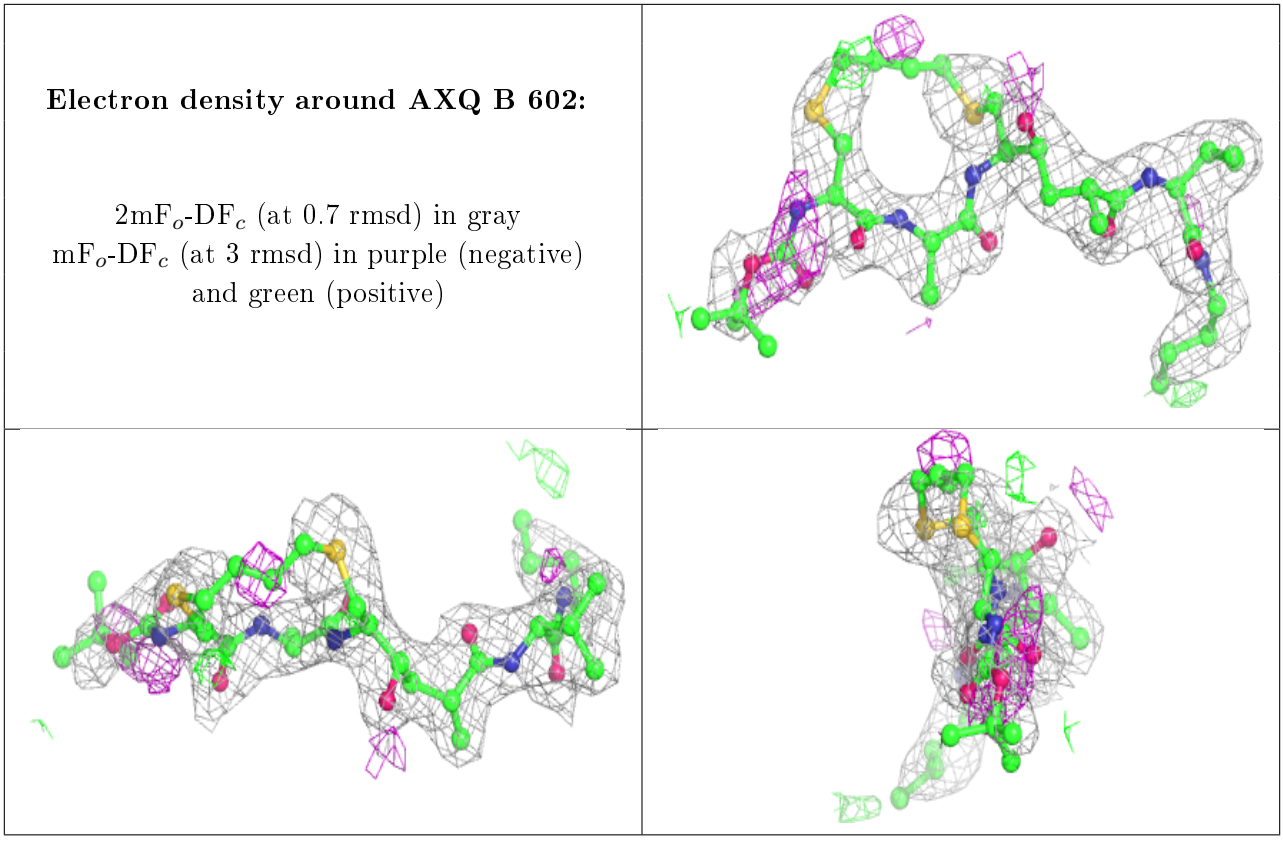
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around AXQ B 602:

$2mF_o$-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.