



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:14 AM UTC

PDB ID : 5OTL / pdb_00005otl
Title : The crystal structure of CK2alpha in complex with compound 29
Authors : Brear, P.; De Fusco, C.; Iegre, J.; Yoshida, M.; Mitchell, S.; Rossmann, M.; Carro, L.; Sore, H.; Hyvonen, M.; Spring, D.
Deposited on : 2017-08-22
Resolution : 1.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

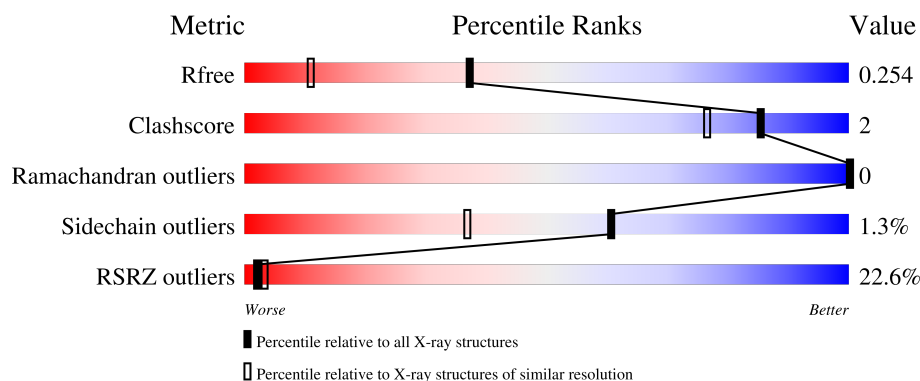
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	A	352	31% 86% 5% 9%
1	B	352	10% 85% 8% 7%

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
5	PEG	B	406	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5941 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	3	0
			2725	1744	479	491	11			
1	B	326	Total	C	N	O	S	0	5	0
			2788	1785	489	502	12			

There are 50 discrepancies between the modelled and reference sequences:

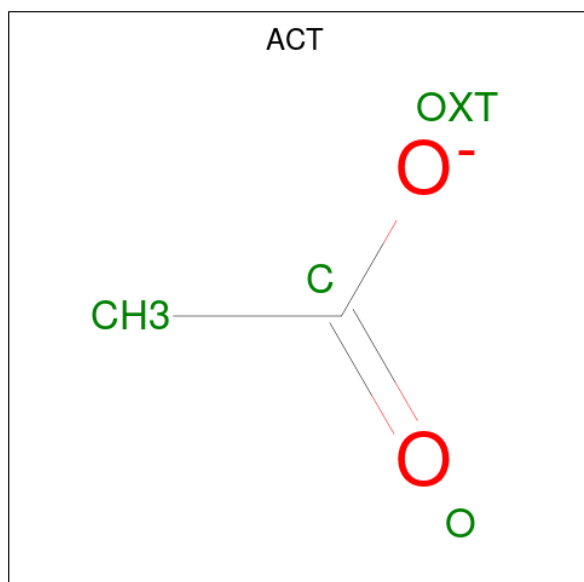
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP P68400
A	-21	SER	-	expression tag	UNP P68400
A	-20	MET	-	expression tag	UNP P68400
A	-19	ASP	-	expression tag	UNP P68400
A	-18	ILE	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	PHE	-	expression tag	UNP P68400
A	-15	ASP	-	expression tag	UNP P68400
A	-14	ASP	-	expression tag	UNP P68400
A	-13	ASP	-	expression tag	UNP P68400
A	-12	ALA	-	expression tag	UNP P68400
A	-11	ASP	-	expression tag	UNP P68400
A	-10	ASP	-	expression tag	UNP P68400
A	-9	ASP	-	expression tag	UNP P68400
A	-8	GLY	-	expression tag	UNP P68400
A	-7	SER	-	expression tag	UNP P68400
A	-6	GLY	-	expression tag	UNP P68400
A	-5	SER	-	expression tag	UNP P68400
A	-4	GLY	-	expression tag	UNP P68400
A	-3	SER	-	expression tag	UNP P68400
A	-2	GLY	-	expression tag	UNP P68400
A	-1	SER	-	expression tag	UNP P68400
A	0	GLY	-	expression tag	UNP P68400
A	1	SER	-	expression tag	UNP P68400
A	21	SER	ARG	engineered mutation	UNP P68400

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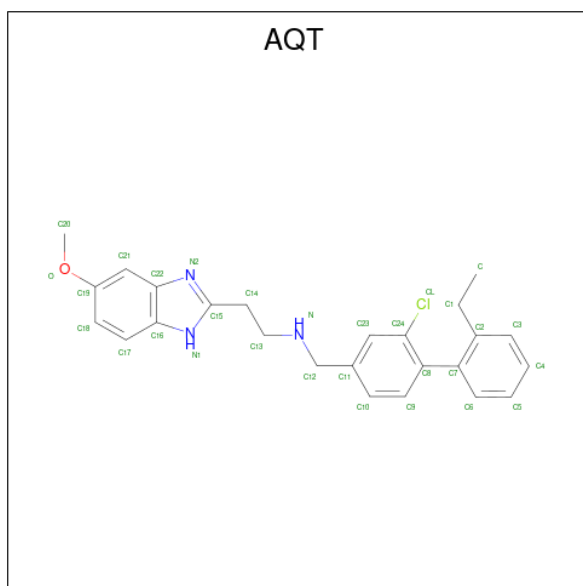
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P68400
B	-21	SER	-	expression tag	UNP P68400
B	-20	MET	-	expression tag	UNP P68400
B	-19	ASP	-	expression tag	UNP P68400
B	-18	ILE	-	expression tag	UNP P68400
B	-17	GLU	-	expression tag	UNP P68400
B	-16	PHE	-	expression tag	UNP P68400
B	-15	ASP	-	expression tag	UNP P68400
B	-14	ASP	-	expression tag	UNP P68400
B	-13	ASP	-	expression tag	UNP P68400
B	-12	ALA	-	expression tag	UNP P68400
B	-11	ASP	-	expression tag	UNP P68400
B	-10	ASP	-	expression tag	UNP P68400
B	-9	ASP	-	expression tag	UNP P68400
B	-8	GLY	-	expression tag	UNP P68400
B	-7	SER	-	expression tag	UNP P68400
B	-6	GLY	-	expression tag	UNP P68400
B	-5	SER	-	expression tag	UNP P68400
B	-4	GLY	-	expression tag	UNP P68400
B	-3	SER	-	expression tag	UNP P68400
B	-2	GLY	-	expression tag	UNP P68400
B	-1	SER	-	expression tag	UNP P68400
B	0	GLY	-	expression tag	UNP P68400
B	1	SER	-	expression tag	UNP P68400
B	21	SER	ARG	engineered mutation	UNP P68400

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



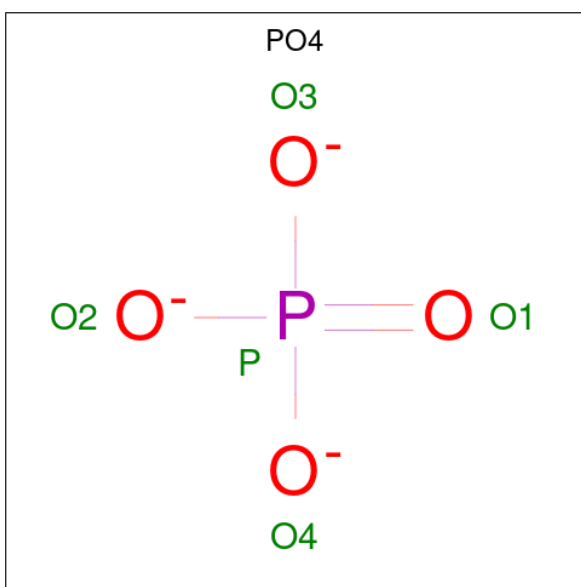
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is {N}-[[3-chloranyl-4-(2-ethylphenyl)phenyl]methyl]-2-(5-methoxy-1 {H}-benzimidazol-2-yl)ethanamine (CCD ID: AQT) (formula: C₂₅H₂₆ClN₃O) (labeled as "Ligand of Interest" by depositor).



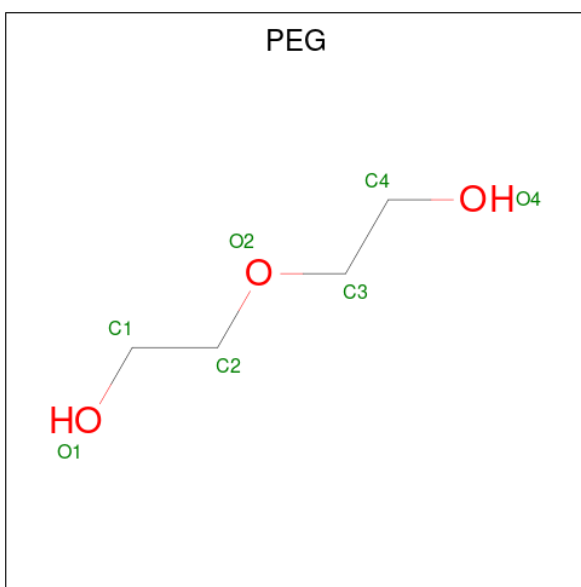
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			30	25	1	3	1		
3	B	1	Total	C	Cl	N	O	0	1
			60	50	2	6	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



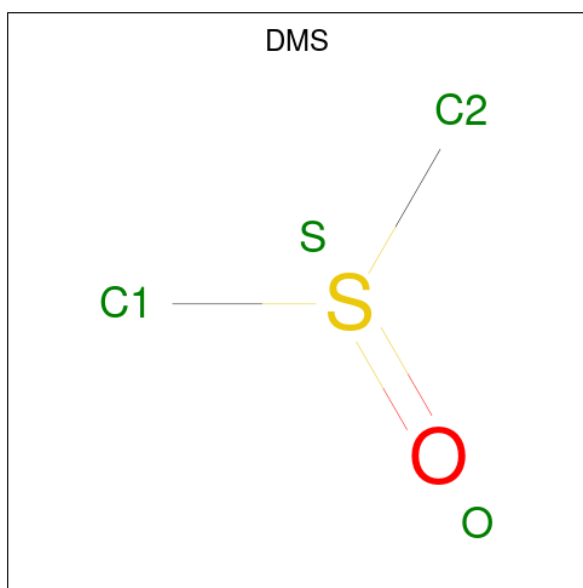
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	80	Total	O	0	0
			80	80		
7	B	216	Total	O	0	0
			216	216		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.66Å 67.83Å 332.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.22 – 1.57 83.22 – 1.57	Depositor EDS
% Data completeness (in resolution range)	95.6 (83.22-1.57) 95.6 (83.22-1.57)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.57Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.225 , 0.244 0.234 , 0.254	Depositor DCC
R_{free} test set	5184 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.096 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5941	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, PEG, AQT, PO4, DMS

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	0.77	0/2798	1.10	2/3784 (0.1%)
1	B	0.92	1/2863 (0.0%)	1.08	5/3873 (0.1%)
All	All	0.85	1/5661 (0.0%)	1.09	7/7657 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	137	MET	SD-CE	-6.03	1.64	1.79

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	314	THR	N-CA-C	-5.44	103.51	110.53
1	A	55	GLU	N-CA-C	-5.25	101.14	109.96
1	B	124	LEU	CA-C-N	5.13	128.10	120.31
1	B	124	LEU	C-N-CA	5.13	128.10	120.31
1	B	216	TRP	N-CA-C	-5.12	105.61	111.14
1	A	205	ASP	CA-CB-CG	5.03	117.63	112.60

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	2725	0	2660	7	0
1	B	2788	0	2726	16	0
2	A	8	0	6	0	0
2	B	8	0	6	0	0
3	A	30	0	0	0	0
3	B	60	0	0	1	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
5	B	7	0	10	6	0
6	B	4	0	6	1	0
7	A	80	0	0	0	0
7	B	216	0	0	4	0
All	All	5941	0	5414	24	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 2.

All (24) 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:A:163:MET:HE2	1:A:174:ILE:HG21	1.64	0.79
1:B:197:PHE:HE2	5:B:406:PEG:H11	1.52	0.73
1:B:231:PRO:HA	5:B:406:PEG:H42	1.76	0.68
1:B:197:PHE:CE2	5:B:406:PEG:H11	2.35	0.58
1:B:286:HIS:HE1	7:B:687:HOH:O	1.89	0.55
1:B:47:ARG:HG3	1:B:52:GLU:HG2	1.90	0.54
1:B:236:HIS:HE1	7:B:675:HOH:O	1.92	0.52
1:B:91:GLY:HA3	1:B:146:TYR:CE2	2.49	0.48
1:B:114:GLU:O	1:B:114:GLU:HG3	2.13	0.48
1:A:91:GLY:HA3	1:A:146:TYR:CE2	2.50	0.47
1:B:203:LEU:O	6:B:407:DMS:H11	2.15	0.46
1:A:163:MET:HE2	1:A:174:ILE:CG2	2.42	0.45
1:A:316:ARG:HH21	1:A:320:GLU:HG3	1.84	0.43
1:B:59:ILE:HD11	7:B:525:HOH:O	2.18	0.43
1:B:285:VAL:HG22	1:B:293:VAL:HG11	2.01	0.42
1:B:316:ARG:HH21	1:B:320:GLU:HG3	1.85	0.42
1:B:230:GLU:HG3	5:B:406:PEG:H41	2.01	0.41
1:A:5:VAL:HB	1:A:261:TYR:HA	2.01	0.41
5:B:406:PEG:H12	7:B:653:HOH:O	2.20	0.41
1:B:231:PRO:HA	5:B:406:PEG:C4	2.48	0.41
1:A:114:GLU:O	1:A:114:GLU:HG3	2.21	0.41
1:B:221:MET:HE1	3:B:403[A]:AQT:CL	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:VAL:HG22	1:A:293:VAL:HG11	2.02	0.40
1:B:72:PRO:HA	1:B:78:ILE:HD11	2.04	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	319/352 (91%)	310 (97%)	9 (3%)	0	100	100
1	B	329/352 (94%)	322 (98%)	7 (2%)	0	100	100
All	All	648/704 (92%)	632 (98%)	16 (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	298/319 (93%)	294 (99%)	4 (1%)	61	37
1	B	305/319 (96%)	301 (99%)	4 (1%)	61	37
All	All	603/638 (94%)	595 (99%)	8 (1%)	61	37

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	66	VAL
1	A	70	LEU
1	A	73	VAL
1	B	70	LEU
1	B	73	VAL
1	B	265	LEU
1	B	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	186	GLN
1	A	207	GLN
1	A	270	ASN
1	B	168	HIS
1	B	186	GLN
1	B	236	HIS
1	B	262	ASN
1	B	270	ASN
1	B	286	HIS

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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
4	PO4	A	404	-	4,4,4	2.58	3 (75%)	6,6,6	0.66	0
2	ACT	B	402	-	3,3,3	1.25	0	3,3,3	1.44	0
5	PEG	B	406	-	6,6,6	0.44	0	5,5,5	0.53	0
2	ACT	B	401	-	3,3,3	1.54	0	3,3,3	0.99	0
3	AQT	B	403[B]	-	33,33,33	0.23	0	44,45,45	0.41	0
3	AQT	B	403[A]	-	33,33,33	0.26	0	44,45,45	0.60	1 (2%)
2	ACT	A	401	-	3,3,3	1.29	0	3,3,3	1.11	0
4	PO4	B	404	-	4,4,4	2.64	2 (50%)	6,6,6	0.95	0
2	ACT	A	402	-	3,3,3	1.44	0	3,3,3	0.87	0
4	PO4	B	405	-	4,4,4	2.58	2 (50%)	6,6,6	0.85	0
3	AQT	A	403	-	33,33,33	0.28	0	44,45,45	0.50	0
6	DMS	B	407	-	3,3,3	0.30	0	3,3,3	0.49	0

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	AQT	B	403[B]	-	-	2/15/15/15	0/4/4/4
3	AQT	A	403	-	-	1/15/15/15	0/4/4/4
3	AQT	B	403[A]	-	-	1/15/15/15	0/4/4/4
5	PEG	B	406	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	404	PO4	P-O1	4.44	1.60	1.50
4	A	404	PO4	P-O1	4.29	1.60	1.50
4	B	405	PO4	P-O1	4.28	1.60	1.50
4	B	405	PO4	P-O2	2.08	1.60	1.54
4	B	404	PO4	P-O4	2.02	1.60	1.54
4	A	404	PO4	P-O4	2.00	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	PO4	P-O2	2.00	1.60	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403[A]	AQT	C14-C13-N	-2.52	104.19	112.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403[B]	AQT	N-C13-C14-C15
5	B	406	PEG	O1-C1-C2-O2
5	B	406	PEG	O2-C3-C4-O4
3	A	403	AQT	C14-C13-N-C12
3	B	403[B]	AQT	C14-C13-N-C12
3	B	403[A]	AQT	C13-C14-C15-N2

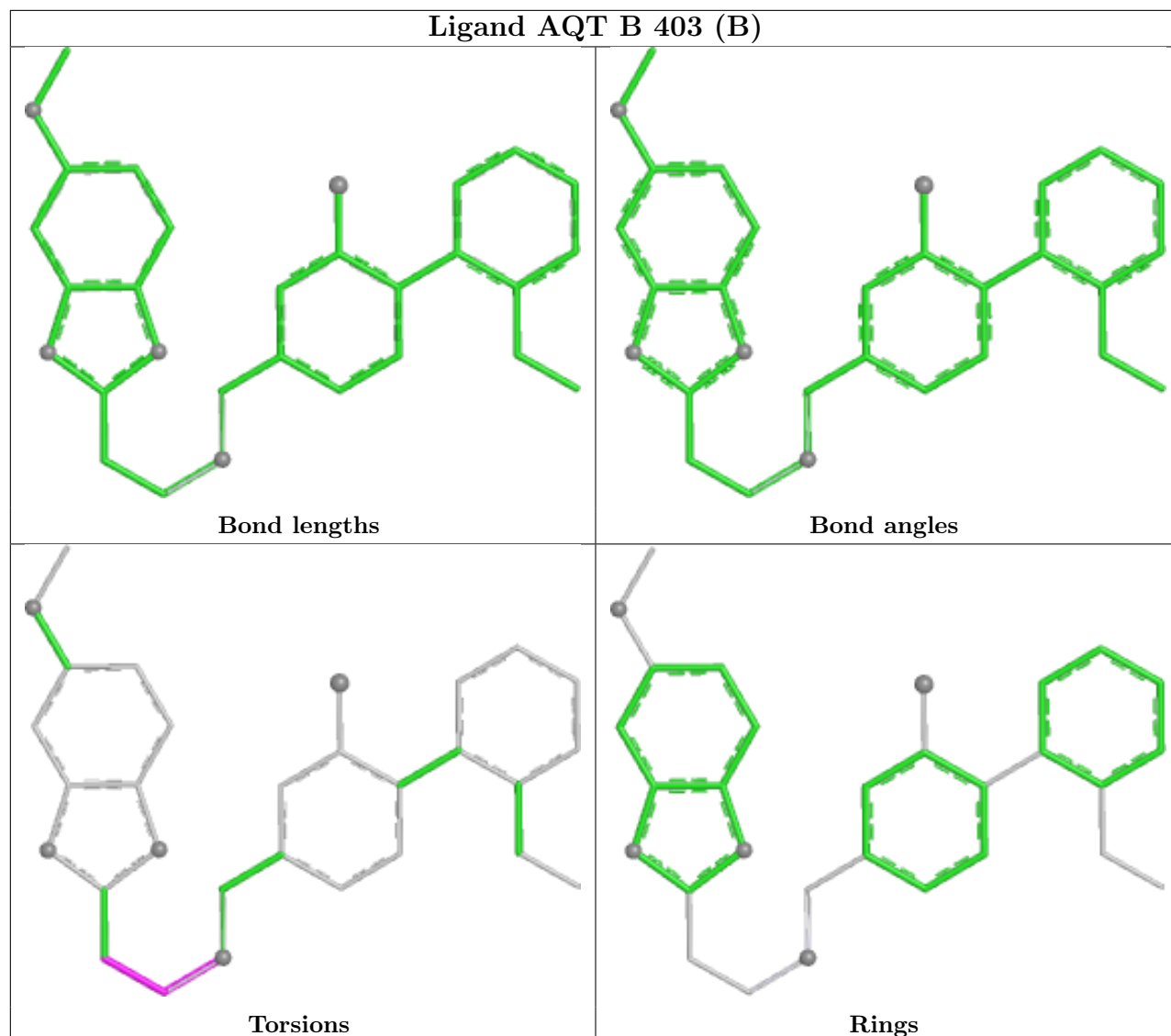
There are no ring outliers.

3 monomers are involved in 8 short contacts:

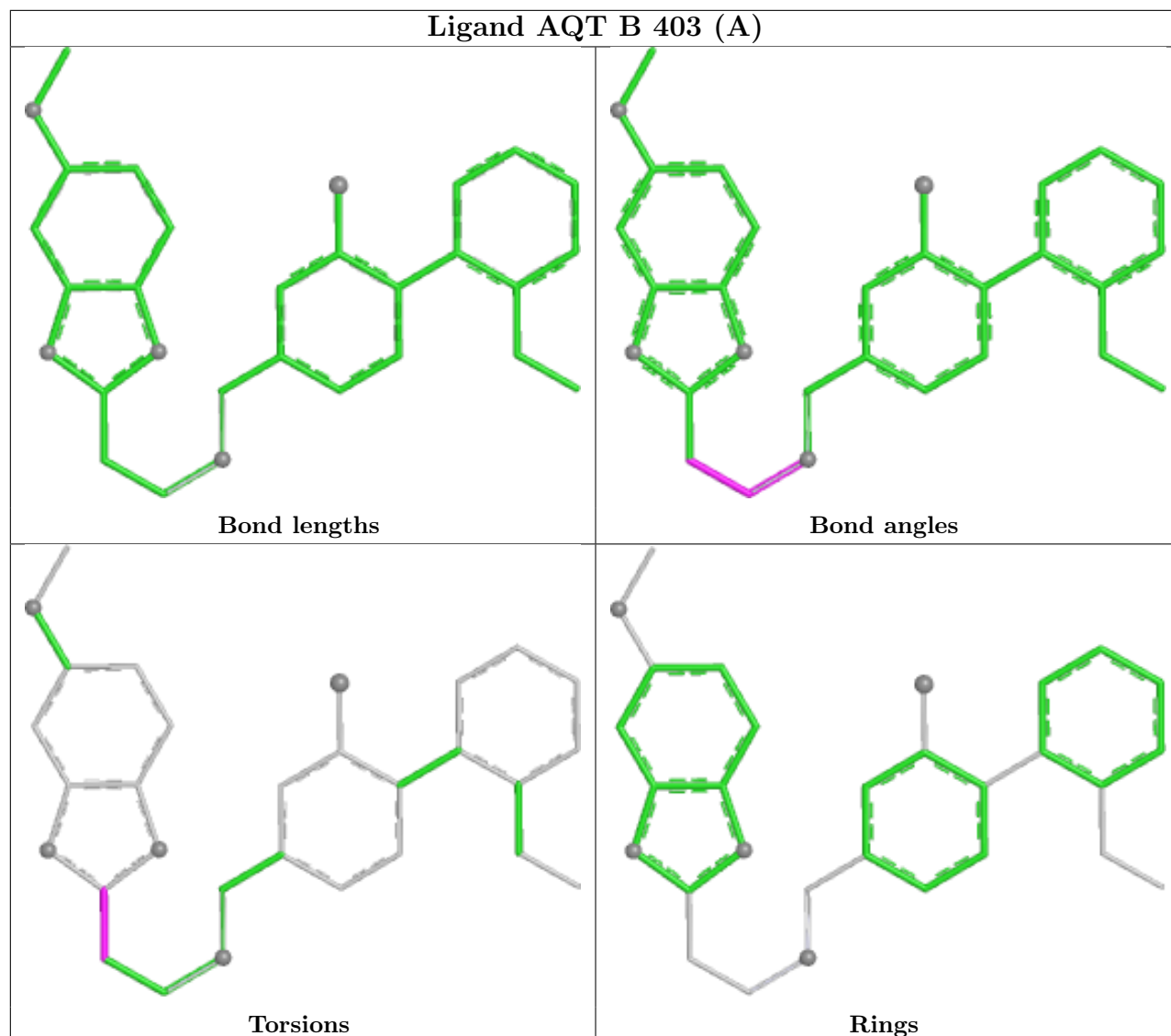
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	406	PEG	6	0
3	B	403[A]	AQT	1	0
6	B	407	DMS	1	0

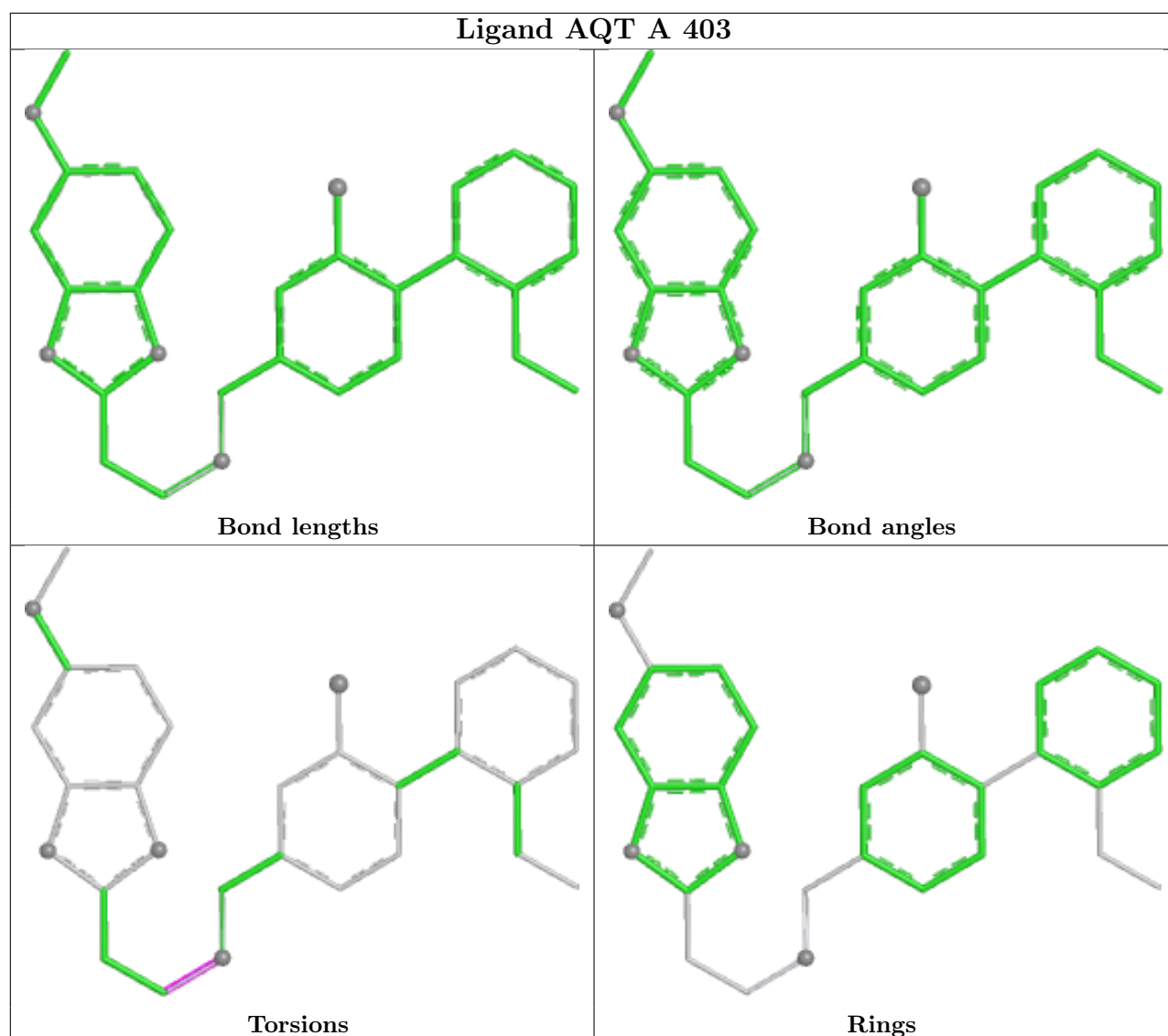
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AQT B 403 (B)



Ligand AQT B 403 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/352 (90%)	1.68	110 (34%) 1 1	17, 53, 88, 108	3 (0%)
1	B	326/352 (92%)	0.60	36 (11%) 10 17	8, 26, 59, 88	5 (1%)
All	All	646/704 (91%)	1.14	146 (22%) 2 3	8, 39, 80, 108	8 (1%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	PHE	9.4
1	B	50	TYR	6.7
1	B	125	TYR	6.2
1	B	328	VAL	6.1
1	A	50	TYR	6.1
1	A	45	LEU	6.0
1	B	124	LEU	5.7
1	A	327	VAL	5.7
1	B	33	TRP	5.5
1	B	121	PHE	5.2
1	A	42	VAL	5.0
1	A	73	VAL	5.0
1	A	128	LEU	4.7
1	A	30	VAL	4.4
1	A	72	PRO	4.2
1	A	258	ILE	4.1
1	A	46	GLY	4.1
1	B	49	LYS	4.0
1	A	74	LYS	4.0
1	A	48	GLY	4.0
1	A	5	VAL	3.8
1	A	53	VAL	3.8
1	A	116	VAL	3.7
1	B	73	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	33	TRP	3.7
1	A	31	VAL	3.6
1	A	54	PHE	3.6
1	A	325	TYR	3.5
1	A	273	LEU	3.5
1	A	282	GLU	3.5
1	A	18	HIS	3.5
1	A	49	LYS	3.5
1	A	57	ILE	3.4
1	B	74	LYS	3.4
1	A	70	LEU	3.4
1	A	288	GLU	3.4
1	A	284	PHE	3.3
1	A	4	PRO	3.3
1	A	51	SER	3.3
1	A	28	SER	3.3
1	B	118	ASN	3.2
1	A	43	ARG	3.2
1	B	105	VAL	3.2
1	A	269	PHE	3.1
1	A	41	LEU	3.1
1	A	47	ARG	3.1
1	A	249	LEU	3.0
1	A	19[A]	ARG	3.0
1	B	117	ASN	3.0
1	A	255	TYR	3.0
1	B	128	LEU	3.0
1	A	265	LEU	2.9
1	A	59	ILE	2.9
1	A	226	ILE	2.9
1	B	31	VAL	2.9
1	A	117	ASN	2.9
1	A	69	ILE	2.9
1	A	267	PRO	2.8
1	B	122	LYS	2.8
1	A	75	LYS	2.8
1	A	225	MET	2.8
1	B	71	LYS	2.8
1	A	105	VAL	2.7
1	A	17	THR	2.7
1	A	263	ILE	2.7
1	B	72	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	280	ARG	2.7
1	A	204	VAL	2.6
1	A	118	ASN	2.6
1	A	44	LYS	2.6
1	A	261	TYR	2.6
1	A	66	VAL	2.6
1	A	239	TYR	2.5
1	A	304	LEU	2.5
1	A	115	HIS	2.5
1	B	104	PRO	2.5
1	A	129	THR	2.5
1	B	69	ILE	2.5
1	A	71	LYS	2.5
1	A	119	THR	2.5
1	B	107	ARG	2.5
1	A	307	TYR	2.5
1	B	123	GLN	2.5
1	B	126	GLN	2.5
1	A	127	THR	2.5
1	B	36	GLN	2.4
1	B	100	ILE	2.4
1	A	146	TYR	2.4
1	A	206	TYR	2.4
1	A	216	TRP	2.4
1	A	281	TRP	2.4
1	A	297	ALA	2.4
1	A	52	GLU	2.4
1	A	316	ARG	2.4
1	A	11	VAL	2.4
1	A	65	VAL	2.4
1	A	55	GLU	2.4
1	A	168	HIS	2.4
1	A	60	THR	2.4
1	A	268	ARG	2.4
1	B	47	ARG	2.4
1	A	131	TYR	2.4
1	A	126	GLN	2.3
1	A	184	PRO	2.3
1	B	116	VAL	2.3
1	B	34	GLY	2.3
1	A	78	ILE	2.3
1	A	89	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	102	LYS	2.3
1	A	120	ASP	2.3
1	A	283	ARG	2.3
1	A	64	LYS	2.3
1	A	27	GLU	2.3
1	A	285	VAL	2.2
1	B	76	LYS	2.2
1	A	292	LEU	2.2
1	A	305	LEU	2.2
1	B	59	ILE	2.2
1	A	98	ALA	2.2
1	A	169	ARG	2.2
1	A	320	GLU	2.2
1	B	283	ARG	2.2
1	A	190	VAL	2.2
1	B	27	GLU	2.2
1	A	109	PRO	2.1
1	A	272	ILE	2.1
1	A	228	ARG	2.1
1	A	275	ARG	2.1
1	A	205	ASP	2.1
1	B	103	ASP	2.1
1	B	271	ASP	2.1
1	A	113	PHE	2.1
1	A	138	TYR	2.1
1	B	280	ARG	2.1
1	B	114	GLU	2.1
1	A	77	LYS	2.0
1	A	233	PHE	2.0
1	A	326	THR	2.0
1	A	254	LEU	2.0
1	A	188	TYR	2.0
1	A	256	ASP	2.0
1	A	250	GLY	2.0
1	A	274	GLY	2.0
1	A	135	PHE	2.0
1	A	266	ASP	2.0
1	A	257	TYR	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

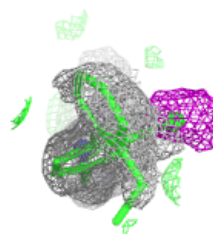
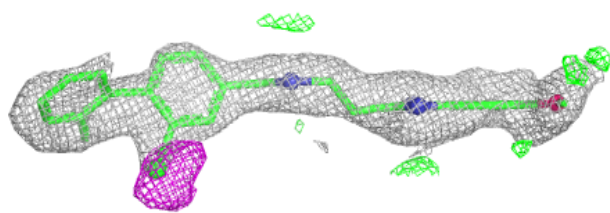
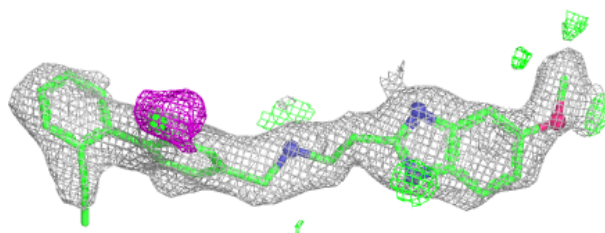
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	DMS	B	407	4/4	0.73	0.24	47,52,52,56	0
3	AQT	A	403	30/30	0.75	0.19	54,63,67,77	0
3	AQT	B	403[B]	30/30	0.82	0.13	66,71,77,83	30
4	PO4	A	404	5/5	0.82	0.13	55,55,59,60	0
5	PEG	B	406	7/7	0.82	0.15	26,37,42,42	0
3	AQT	B	403[A]	30/30	0.82	0.13	12,23,33,35	30
2	ACT	A	402	4/4	0.89	0.12	29,30,33,34	0
2	ACT	A	401	4/4	0.90	0.12	35,39,39,40	0
4	PO4	B	405	5/5	0.90	0.09	40,48,50,53	0
4	PO4	B	404	5/5	0.93	0.09	31,35,37,41	0
2	ACT	B	401	4/4	0.93	0.08	20,20,22,25	0
2	ACT	B	402	4/4	0.95	0.10	25,30,30,32	0

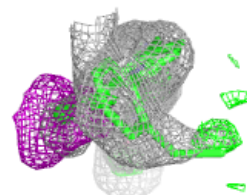
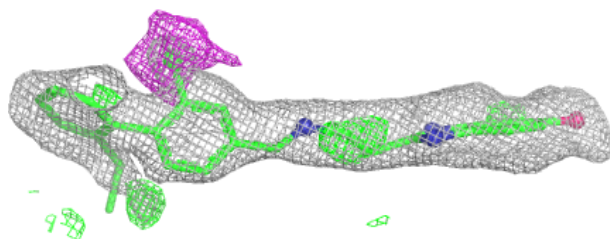
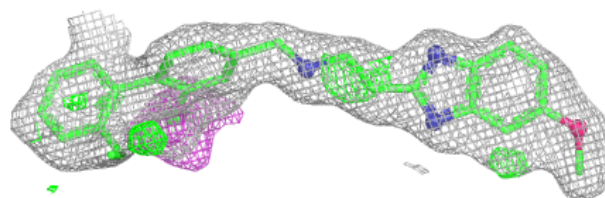
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

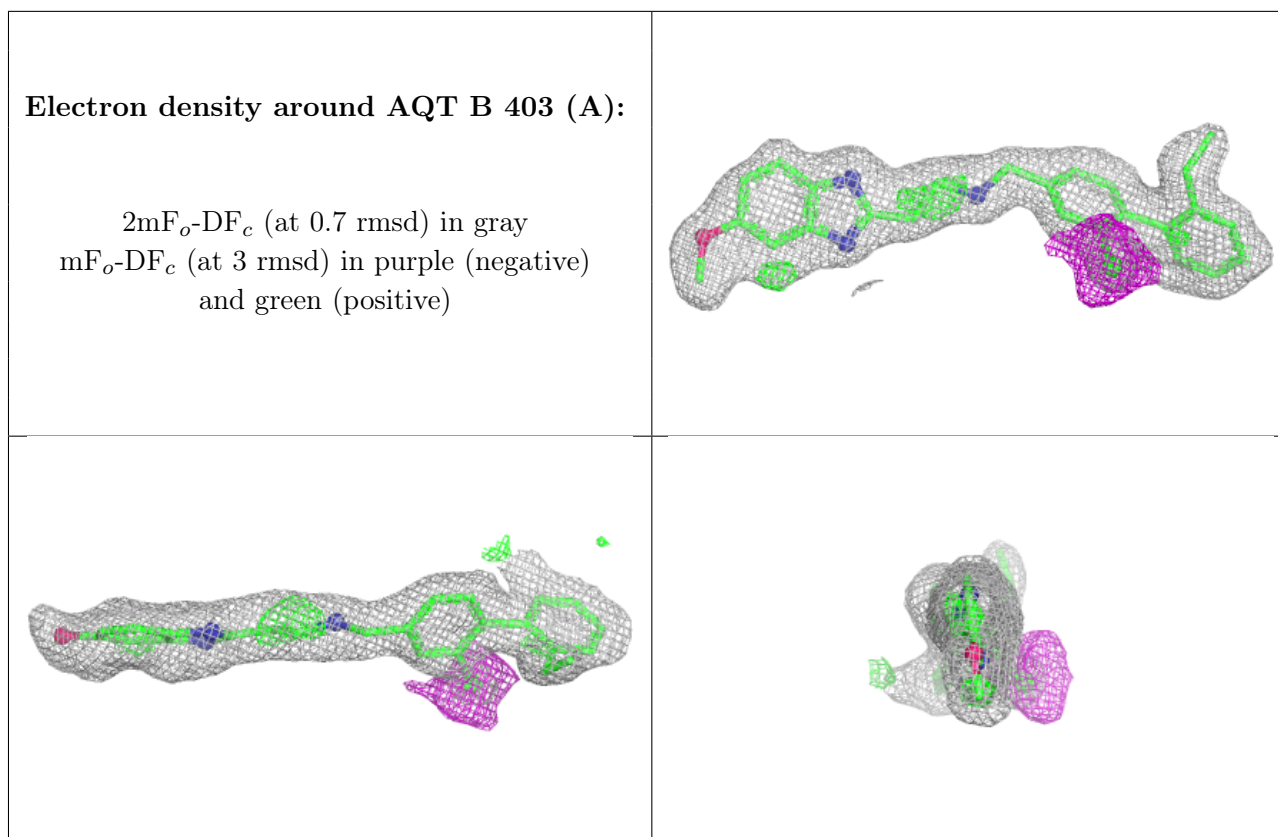
Electron density around AQT A 403:

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

**Electron density around AQT B 403 (B):**

$2mF_o-DF_c$ (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.