



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:46 AM UTC

PDB ID : 8BI5 / pdb_00008bi5
Title : Crystal structure of human Choline Kinase A in complex with UNC0737
Authors : Diaz-Saez, L.; Ward, J.; Kennedy, E.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Huber, K.; Structural Genomics Consortium (SGC)
Deposited on : 2022-11-01
Resolution : 2.50 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

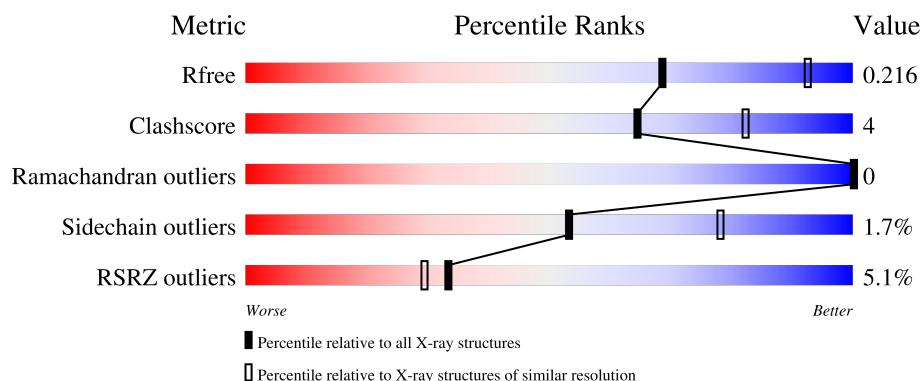
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	A	457	
1	B	457	

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.

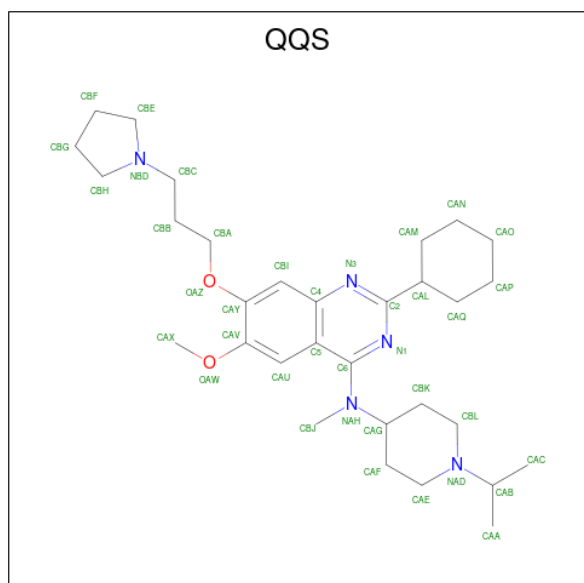
- Molecule 1 is a protein called Choline kinase alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total 2993	C 1942	N 498	O 536	S 17	4	7	0
1	B	354	Total 2980	C 1930	N 495	O 538	S 17	4	7	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is 2-cyclohexyl-6-methoxy- {N}-methyl- {N}-(1-propan-2-ylpiperidin-4-yl)-7-(3-pyrrolidin-1-ylpropoxy)quinazolin-4-amine (CCD ID: QQS) (formula: C₃₁H₄₉N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			76	62	10	4		
3	B	1	Total	C	N	O	0	0
			38	31	5	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Cl	0	0
			2	2		
6	B	3	Total	Cl	0	0
			3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	169	Total	O	0	0
			169	169		
7	B	165	Total	O	0	0
			165	165		

- Molecule 1: Choline kinase alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.49Å 131.49Å 168.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.53 – 2.50 46.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.53-2.50) 100.0 (46.53-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.23 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.187 , 0.213 0.190 , 0.216	Depositor DCC
R_{free} test set	2633 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6483	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: CL, QQS, EDO, MG, PO4

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	0.92	0/3092	1.33	1/4161 (0.0%)
1	B	0.93	0/3078	1.32	0/4143
All	All	0.93	0/6170	1.33	1/8304 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	ARG	CG-CD-NE	5.54	124.18	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2993	0	2976	19	0
1	B	2980	0	2955	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	76	0	0	6	0
3	B	38	0	0	3	0
4	A	12	0	18	0	0
4	B	28	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	0	0
5	B	10	0	0	0	0
6	A	2	0	0	0	0
6	B	3	0	0	0	0
7	A	169	0	0	3	0
7	B	165	0	0	1	0
All	All	6483	0	5991	47	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 4.

All (47) 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)
3:A:501[B]:QQS:CAU	3:A:501[B]:QQS:CBJ	2.35	1.03
3:A:501[A]:QQS:CBJ	3:A:501[A]:QQS:CAU	2.59	0.81
1:A:183:MET:HE1	1:A:331[A]:PHE:CD1	2.17	0.80
1:B:235:PHE:CE1	1:B:331[B]:PHE:CE1	2.70	0.80
3:A:501[A]:QQS:CBH	3:A:501[A]:QQS:CAX	2.65	0.74
1:A:195:LYS:H	1:A:207:GLN:HE21	1.35	0.72
1:B:183:MET:HE1	1:B:331[B]:PHE:HB2	1.71	0.72
3:A:501[A]:QQS:N1	3:A:501[A]:QQS:CAF	2.53	0.71
1:A:178:VAL:HG12	1:B:178:VAL:HG12	1.72	0.71
1:A:339:ARG:CZ	1:A:405:MET:HE2	2.23	0.69
1:B:387:GLN:HG2	1:B:389:ASP:OD1	1.93	0.68
1:A:177[A]:MET:HA	1:A:177[A]:MET:HE3	1.80	0.64
1:B:183:MET:HE1	1:B:331[A]:PHE:CD1	2.34	0.62
1:A:383:LEU:HD21	1:A:405:MET:HE1	1.84	0.59
1:B:235:PHE:HE1	1:B:331[B]:PHE:CE1	2.21	0.59
3:A:501[A]:QQS:CAX	3:A:501[A]:QQS:OAZ	2.50	0.59
1:B:309:GLU:OE2	7:B:601:HOH:O	2.17	0.58
1:B:84:GLU:HB3	1:B:85:PRO:HD2	1.87	0.57
1:B:304:HIS:HD2	1:B:331[B]:PHE:CE1	2.23	0.57
1:B:183:MET:HE1	1:B:331[A]:PHE:HB2	1.87	0.56
3:A:501[B]:QQS:CAF	3:A:501[B]:QQS:N1	2.68	0.56
3:B:501:QQS:CBJ	3:B:501:QQS:CAU	2.85	0.53
1:A:183:MET:HE1	1:A:331[B]:PHE:HB2	1.89	0.53
1:B:235:PHE:CZ	1:B:331[B]:PHE:CD1	2.97	0.52
1:B:131:ASP:N	1:B:131:ASP:OD1	2.44	0.50
1:A:183:MET:HG3	1:A:240:MET:HE2	1.93	0.50
1:A:183:MET:HE1	1:A:331[A]:PHE:CG	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:LEU:HD21	1:A:405:MET:CE	2.45	0.47
1:A:339:ARG:NH2	1:A:405:MET:HE2	2.30	0.47
1:A:174:ALA:CB	7:A:761:HOH:O	2.61	0.46
1:B:84:GLU:HB3	1:B:85:PRO:CD	2.47	0.44
1:B:304:HIS:CD2	1:B:331[B]:PHE:CE1	3.05	0.44
1:A:174:ALA:HB1	7:A:761:HOH:O	2.18	0.44
1:B:149:GLY:O	1:B:150:ALA:C	2.60	0.44
1:A:207:GLN:NE2	7:A:608:HOH:O	2.50	0.43
1:A:282:LEU:N	1:A:283:PRO:CD	2.81	0.43
1:B:387:GLN:CG	1:B:389:ASP:OD1	2.66	0.42
1:A:425:ILE:O	1:A:428:ALA:HB3	2.20	0.42
1:A:183:MET:HE2	1:A:183:MET:HB3	1.78	0.42
1:A:178:VAL:HG11	1:B:177[A]:MET:SD	2.61	0.41
1:B:282:LEU:N	1:B:283:PRO:CD	2.84	0.41
3:B:501:QQS:OAW	3:B:501:QQS:CBA	2.69	0.41
1:B:304:HIS:CD2	1:B:331[B]:PHE:CD1	3.09	0.41
1:B:364:ALA:HB1	4:B:502:EDO:H12	2.03	0.41
1:A:126:GLN:OE1	1:A:142:LYS:HD3	2.21	0.41
3:B:501:QQS:N1	3:B:501:QQS:CAF	2.85	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	358/457 (78%)	353 (99%)	5 (1%)	0	100	100
1	B	357/457 (78%)	351 (98%)	6 (2%)	0	100	100
All	All	715/914 (78%)	704 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	325/400 (81%)	318 (98%)	7 (2%)	45	73
1	B	324/400 (81%)	316 (98%)	8 (2%)	42	69
All	All	649/800 (81%)	634 (98%)	15 (2%)	53	72

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177[A]	MET
1	A	177[B]	MET
1	A	178	VAL
1	A	331[A]	PHE
1	A	331[B]	PHE
1	A	357	GLU
1	A	451	GLN
1	B	81	GLU
1	B	89	ARG
1	B	131	ASP
1	B	177[A]	MET
1	B	177[B]	MET
1	B	178	VAL
1	B	331[A]	PHE
1	B	331[B]	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	207	GLN
1	A	387	GLN
1	A	392	ASN
1	A	442	GLN
1	A	451	GLN
1	B	122	ASN

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Mol	Chain	Res	Type
1	B	410	ASN
1	B	442	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 7 are monoatomic - leaving 16 for Mogul analysis.

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	EDO	A	504	-	3,3,3	0.13	0	2,2,2	0.30	0
5	PO4	B	509	-	4,4,4	0.64	0	6,6,6	0.49	0
4	EDO	A	502	-	3,3,3	0.12	0	2,2,2	0.25	0
4	EDO	B	505	-	3,3,3	0.11	0	2,2,2	0.16	0
3	QQS	B	501	-	40,42,42	1.08	4 (10%)	51,58,58	2.30	17 (33%)
4	EDO	B	506	-	3,3,3	0.14	0	2,2,2	0.19	0
4	EDO	B	503	-	3,3,3	0.13	0	2,2,2	0.22	0
4	EDO	B	507	-	3,3,3	0.14	0	2,2,2	0.27	0
4	EDO	B	508	-	3,3,3	0.17	0	2,2,2	0.32	0
4	EDO	A	503	-	3,3,3	0.34	0	2,2,2	0.39	0
4	EDO	B	504	-	3,3,3	0.13	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	QQS	A	501[A]	-	40,42,42	0.91	2 (5%)	51,58,58	2.81	20 (39%)
5	PO4	B	510	-	4,4,4	0.84	0	6,6,6	0.44	0
5	PO4	A	505	-	4,4,4	0.87	0	6,6,6	0.42	0
4	EDO	B	502	-	3,3,3	0.13	0	2,2,2	0.25	0
3	QQS	A	501[B]	-	40,42,42	1.04	4 (10%)	51,58,58	2.69	23 (45%)

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
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	A	502	-	-	0/1/1/1	-
4	EDO	B	505	-	-	1/1/1/1	-
3	QQS	B	501	-	-	9/25/62/62	0/5/5/5
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	B	507	-	-	1/1/1/1	-
4	EDO	B	508	-	-	1/1/1/1	-
4	EDO	A	503	-	-	1/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
3	QQS	A	501[A]	-	-	10/25/62/62	0/5/5/5
4	EDO	B	502	-	-	0/1/1/1	-
3	QQS	A	501[B]	-	-	14/25/62/62	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501[B]	QQS	C4-N3	-2.67	1.33	1.37
3	B	501	QQS	CBI-C4	-2.61	1.37	1.41
3	B	501	QQS	CAU-CAV	2.49	1.41	1.36
3	B	501	QQS	C4-N3	-2.42	1.33	1.37
3	A	501[A]	QQS	CAM-CAL	-2.41	1.47	1.53
3	A	501[B]	QQS	CBI-C4	-2.31	1.38	1.41
3	A	501[B]	QQS	C6-N1	2.30	1.34	1.32
3	A	501[B]	QQS	CAU-CAV	2.20	1.40	1.36
3	B	501	QQS	CBL-NAD	2.06	1.51	1.47
3	A	501[A]	QQS	C6-C5	-2.03	1.40	1.43

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501[B]	QQS	C2-N3-C4	7.22	121.28	116.50
3	A	501[A]	QQS	CAE-NAD-CAB	-6.88	102.03	113.01
3	A	501[A]	QQS	CAF-CAE-NAD	-6.71	101.08	111.42
3	A	501[A]	QQS	CAN-CAM-CAL	-5.99	100.98	111.56
3	A	501[B]	QQS	CBA-OAZ-CAY	-5.81	103.67	117.69
3	A	501[A]	QQS	CBK-CAG-NAH	-5.66	108.58	111.91
3	A	501[B]	QQS	CBK-CAG-NAH	-5.62	108.60	111.91
3	A	501[A]	QQS	CAF-CAG-NAH	-5.58	108.63	111.91
3	B	501	QQS	C2-N3-C4	5.36	120.06	116.50
3	A	501[B]	QQS	N1-C6-NAH	5.35	123.60	115.64
3	B	501	QQS	OAZ-CAY-CBI	-5.32	116.46	125.20
3	A	501[A]	QQS	CBL-NAD-CAB	-4.96	105.10	113.01
3	B	501	QQS	CBK-CAG-NAH	4.83	114.76	111.91
3	B	501	QQS	N3-C2-N1	-4.76	119.62	126.21
3	A	501[B]	QQS	CBL-CBK-CAG	-4.73	102.12	110.78
3	A	501[A]	QQS	C2-N3-C4	4.65	119.58	116.50
3	A	501[A]	QQS	CBK-CBL-NAD	-4.63	104.29	111.42
3	A	501[B]	QQS	OAZ-CAY-CBI	-4.24	118.25	125.20
3	A	501[B]	QQS	CBG-CBH-NBD	-4.19	98.97	103.90
3	A	501[B]	QQS	CAN-CAM-CAL	-4.19	104.17	111.56
3	A	501[B]	QQS	CBK-CBL-NAD	-4.10	105.11	111.42
3	B	501	QQS	CAN-CAM-CAL	-4.09	104.35	111.56
3	B	501	QQS	CBF-CBE-NBD	3.91	108.51	103.90
3	A	501[A]	QQS	C6-C5-C4	3.79	117.98	115.47
3	B	501	QQS	OAZ-CAY-CAV	3.78	123.55	115.75
3	A	501[B]	QQS	N3-C2-N1	-3.74	121.02	126.21
3	A	501[A]	QQS	CAX-OAW-CAV	-3.67	112.13	117.51
3	A	501[A]	QQS	CBA-OAZ-CAY	-3.62	108.95	117.69
3	A	501[A]	QQS	N3-C2-N1	-3.51	121.34	126.21
3	B	501	QQS	CBL-CBK-CAG	-3.43	104.50	110.78
3	B	501	QQS	CBC-NBD-CBH	3.41	121.31	113.25
3	A	501[B]	QQS	CBC-CBB-CBA	-3.28	101.38	112.77
3	A	501[B]	QQS	C6-C5-C4	3.28	117.64	115.47
3	A	501[A]	QQS	CBF-CBE-NBD	3.18	107.66	103.90
3	B	501	QQS	CBA-OAZ-CAY	3.15	125.28	117.69
3	B	501	QQS	CAP-CAQ-CAL	-3.10	106.09	111.56
3	B	501	QQS	CBC-NBD-CBE	-2.89	106.39	113.25
3	A	501[A]	QQS	C5-C4-N3	-2.88	119.75	122.80
3	B	501	QQS	C2-N1-C6	2.70	124.06	114.99
3	A	501[A]	QQS	CBG-CBF-CBE	-2.68	97.69	105.10
3	B	501	QQS	CAE-NAD-CBL	2.66	114.20	109.13
3	A	501[B]	QQS	C5-C4-N3	-2.64	120.00	122.80
3	A	501[B]	QQS	CBB-CBC-NBD	-2.60	106.63	113.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501[B]	QQS	CAE-NAD-CBL	2.53	113.96	109.13
3	B	501	QQS	CBC-CBB-CBA	-2.49	104.11	112.77
3	A	501[B]	QQS	CBC-NBD-CBH	-2.44	107.47	113.25
3	A	501[A]	QQS	N1-C6-NAH	2.44	119.27	115.64
3	A	501[B]	QQS	CBF-CBE-NBD	2.35	106.67	103.90
3	B	501	QQS	C5-C6-N1	-2.31	117.97	122.44
3	A	501[B]	QQS	CAQ-CAL-C2	-2.29	107.05	111.85
3	A	501[B]	QQS	OAZ-CAY-CAV	2.29	120.48	115.75
3	A	501[B]	QQS	CAO-CAP-CAQ	-2.28	106.74	111.42
3	A	501[A]	QQS	CAE-CAF-CAG	-2.27	106.62	110.78
3	A	501[B]	QQS	OAW-CAV-CAY	2.26	118.47	115.40
3	A	501[A]	QQS	CAP-CAQ-CAL	-2.18	107.72	111.56
3	A	501[B]	QQS	CBC-NBD-CBE	-2.14	108.17	113.25
3	A	501[A]	QQS	OAW-CAV-CAU	-2.05	122.57	125.16
3	A	501[A]	QQS	C2-N1-C6	2.04	121.86	114.99
3	A	501[B]	QQS	OAW-CAV-CAU	-2.04	122.58	125.16
3	B	501	QQS	OAZ-CBA-CBB	-2.01	100.90	108.30

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501[A]	QQS	CBB-CBC-NBD-CBE
3	A	501[A]	QQS	CBK-CAG-NAH-CBJ
3	A	501[A]	QQS	CAF-CAG-NAH-CBJ
3	A	501[B]	QQS	CBB-CBC-NBD-CBE
3	A	501[B]	QQS	CAF-CAG-NAH-C6
3	A	501[B]	QQS	CAF-CAG-NAH-CBJ
3	A	501[B]	QQS	CAA-CAB-NAD-CBL
3	B	501	QQS	CBB-CBC-NBD-CBH
3	B	501	QQS	CBK-CAG-NAH-CBJ
3	B	501	QQS	CAF-CAG-NAH-CBJ
3	B	501	QQS	CBI-CAY-OAZ-CBA
3	B	501	QQS	CAV-CAY-OAZ-CBA
3	A	501[B]	QQS	CAY-CAV-OAW-CAX
3	B	501	QQS	CBA-CBB-CBC-NBD
3	B	501	QQS	OAZ-CBA-CBB-CBC
3	A	501[A]	QQS	CAU-CAV-OAW-CAX
3	A	501[B]	QQS	CAU-CAV-OAW-CAX
3	A	501[A]	QQS	CAY-CAV-OAW-CAX
3	A	501[B]	QQS	OAZ-CBA-CBB-CBC
3	A	501[A]	QQS	OAZ-CBA-CBB-CBC

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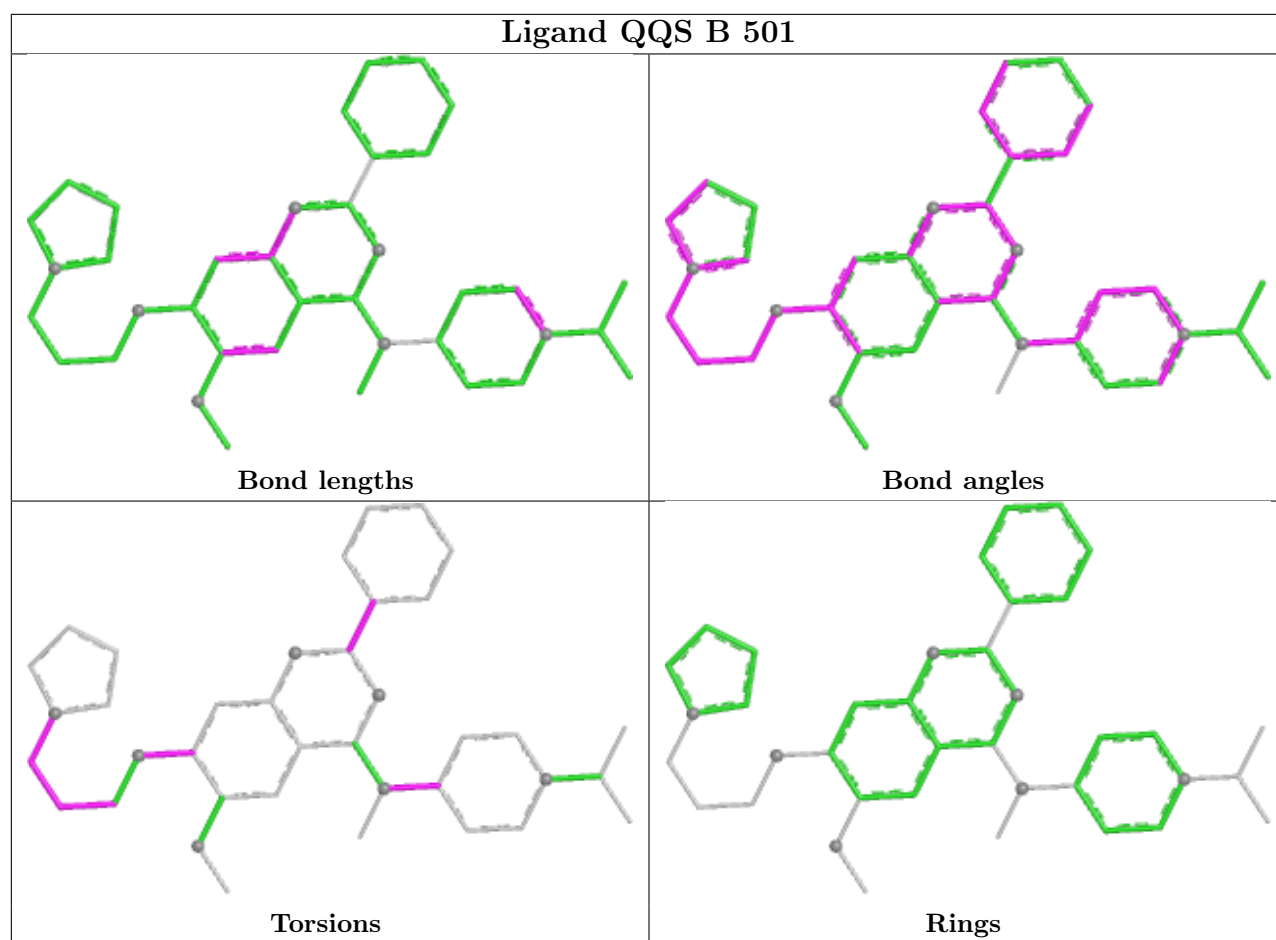
Mol	Chain	Res	Type	Atoms
3	A	501[A]	QQS	N1-C2-CAL-CAM
4	B	505	EDO	O1-C1-C2-O2
3	A	501[B]	QQS	CAV-CAY-OAZ-CBA
3	A	501[B]	QQS	CBB-CBA-OAZ-CAY
3	A	501[A]	QQS	CBA-CBB-CBC-NBD
3	A	501[B]	QQS	N1-C6-NAH-CAG
3	A	501[B]	QQS	CBI-CAY-OAZ-CBA
4	A	503	EDO	O1-C1-C2-O2
4	B	507	EDO	O1-C1-C2-O2
4	B	508	EDO	O1-C1-C2-O2
3	B	501	QQS	N1-C2-CAL-CAM
3	A	501[B]	QQS	CAC-CAB-NAD-CBL
4	B	504	EDO	O1-C1-C2-O2
3	A	501[A]	QQS	CBB-CBC-NBD-CBH
3	A	501[B]	QQS	CBB-CBC-NBD-CBH
3	B	501	QQS	CBB-CBC-NBD-CBE
3	A	501[A]	QQS	N1-C6-NAH-CAG
4	A	504	EDO	O1-C1-C2-O2
4	B	506	EDO	O1-C1-C2-O2
3	A	501[B]	QQS	N3-C2-CAL-CAM

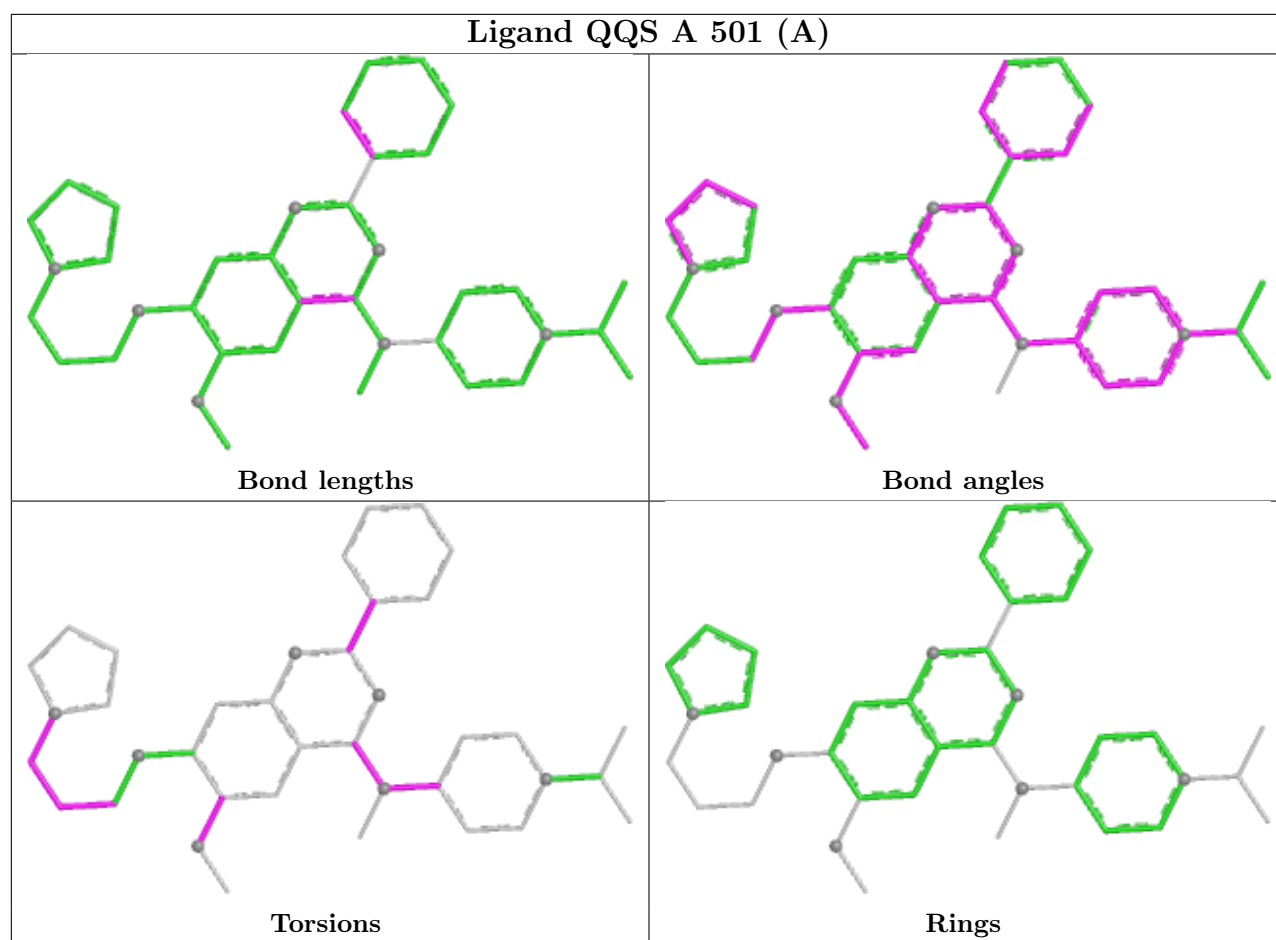
There are no ring outliers.

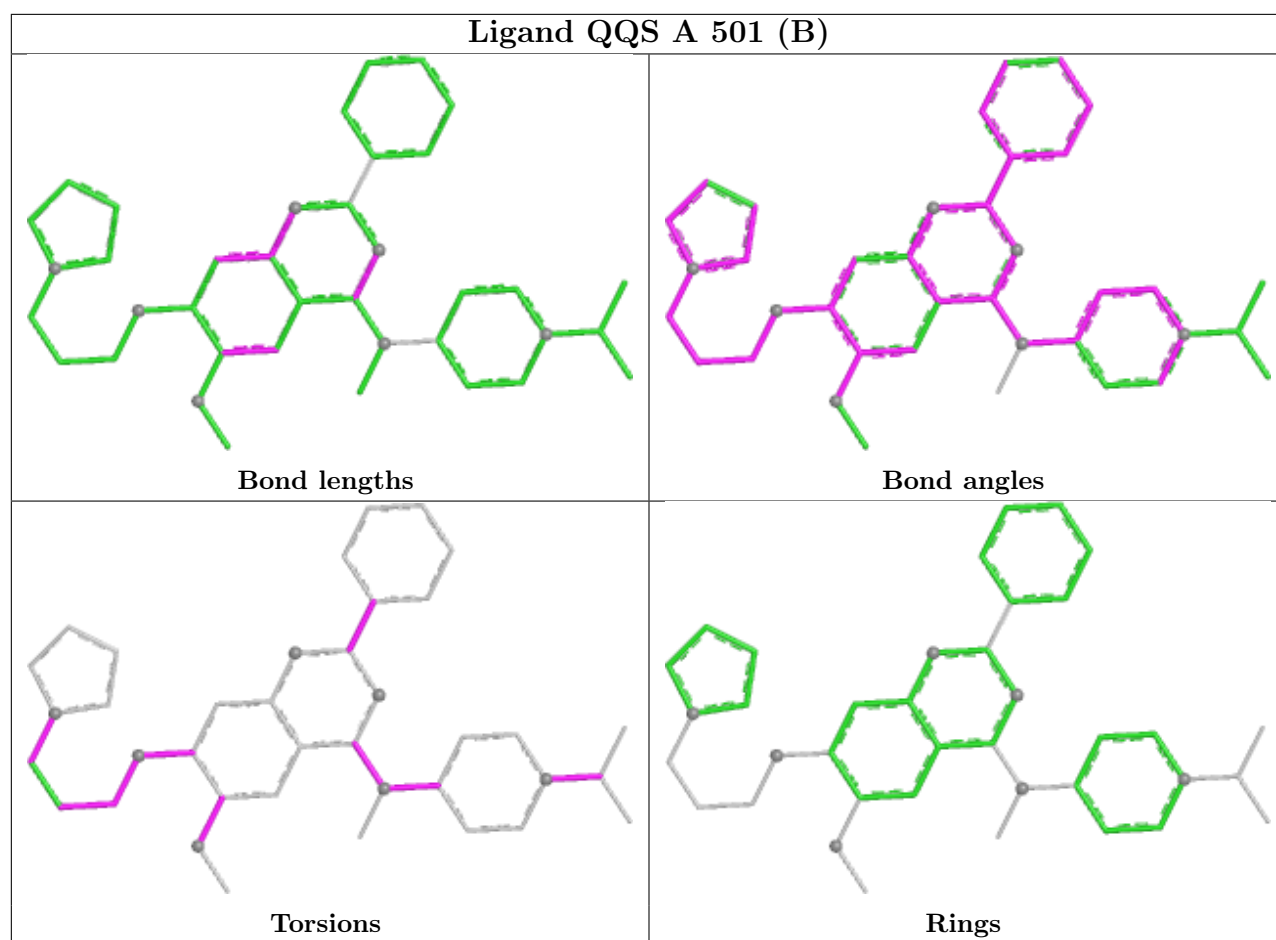
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	QQS	3	0
3	A	501[A]	QQS	4	0
4	B	502	EDO	1	0
3	A	501[B]	QQS	2	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.







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	355/457 (77%)	0.21	14 (3%) 43 38	23, 50, 94, 123	8 (2%)
1	B	354/457 (77%)	0.33	22 (6%) 26 23	31, 50, 105, 140	8 (2%)
All	All	709/914 (77%)	0.27	36 (5%) 33 29	23, 50, 100, 140	16 (2%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	LEU	7.5
1	B	150	ALA	7.3
1	B	174	ALA	6.6
1	A	174	ALA	6.2
1	A	176	ALA	4.7
1	A	175	GLU	4.6
1	A	151	ILE	4.5
1	B	175	GLU	3.8
1	B	117	ARG	3.6
1	B	176	ALA	3.6
1	A	120	LEU	3.6
1	B	118	GLY	3.3
1	A	271	ILE	3.2
1	A	263	ILE	3.0
1	B	85	PRO	2.9
1	B	81	GLU	2.8
1	A	357	GLU	2.8
1	A	177[A]	MET	2.7
1	B	132	THR	2.7
1	A	264	LYS	2.6
1	B	177[A]	MET	2.5
1	B	111	PHE	2.4
1	B	113	ILE	2.4
1	A	429	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	123	MET	2.4
1	A	121	SER	2.3
1	B	235	PHE	2.3
1	B	121	SER	2.2
1	B	148	TYR	2.2
1	B	149	GLY	2.2
1	A	266	THR	2.1
1	B	116	ILE	2.1
1	A	278	LEU	2.1
1	B	397	GLU	2.1
1	B	84	GLU	2.0
1	B	87	THR	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 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(Å ²)	Q<0.9
5	PO4	B	509	5/5	0.61	0.14	115,123,125,136	0
4	EDO	B	505	4/4	0.76	0.31	85,85,87,88	0
4	EDO	B	507	4/4	0.79	0.29	85,91,92,94	0
3	QQS	A	501[B]	38/38	0.84	0.28	53,61,81,82	38
3	QQS	A	501[A]	38/38	0.84	0.28	51,56,86,88	38
4	EDO	A	502	4/4	0.85	0.22	69,78,79,80	0
4	EDO	B	503	4/4	0.85	0.24	68,72,78,82	0
4	EDO	B	504	4/4	0.85	0.24	68,72,76,77	0
4	EDO	B	508	4/4	0.86	0.22	68,78,81,82	0
4	EDO	A	503	4/4	0.86	0.21	59,68,69,71	0
4	EDO	B	506	4/4	0.89	0.20	57,71,73,76	0

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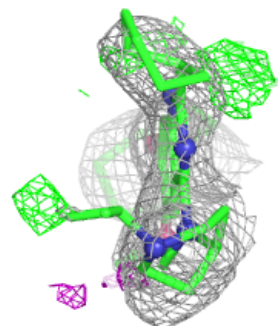
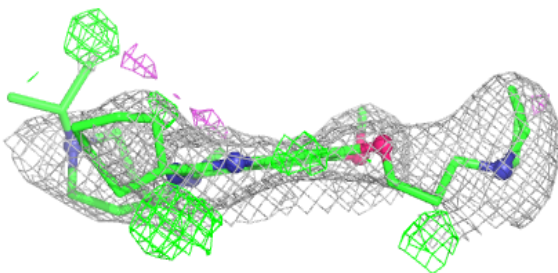
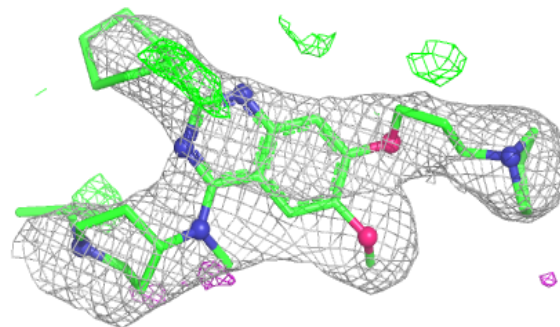
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	504	4/4	0.90	0.18	61,68,70,76	0
6	CL	B	512	1/1	0.90	0.15	82,82,82,82	0
6	CL	B	511	1/1	0.91	0.17	75,75,75,75	0
6	CL	A	507	1/1	0.91	0.18	88,88,88,88	0
6	CL	A	506	1/1	0.92	0.23	101,101,101,101	0
5	PO4	A	505	5/5	0.93	0.09	85,87,92,93	0
6	CL	B	513	1/1	0.93	0.22	87,87,87,87	0
4	EDO	B	502	4/4	0.94	0.14	46,51,53,58	0
3	QQS	B	501	38/38	0.94	0.14	45,62,82,83	0
5	PO4	B	510	5/5	0.97	0.11	54,57,62,68	0
2	MG	B	500	1/1	0.98	0.12	42,42,42,42	0
2	MG	A	500	1/1	0.98	0.10	43,43,43,43	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.

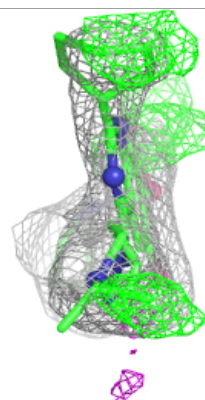
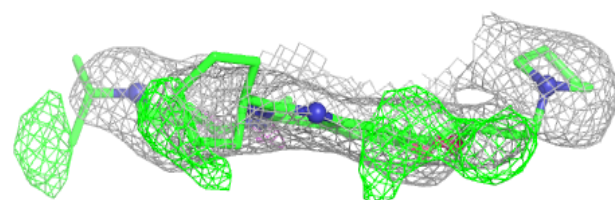
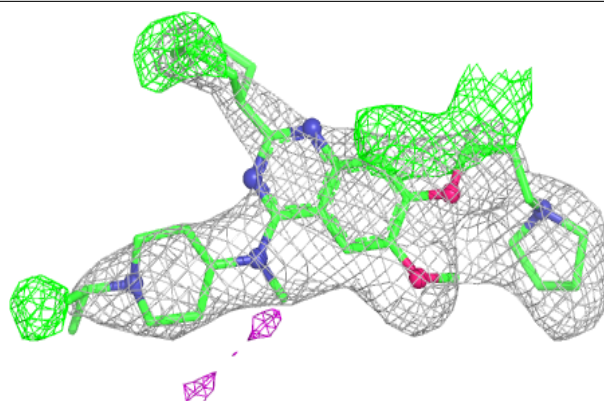
Electron density around QQS A 501 (B):

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

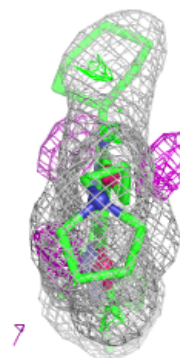
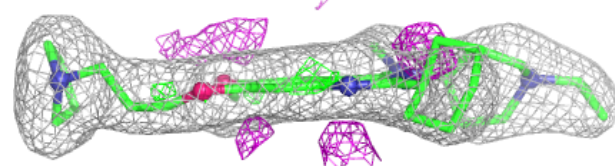
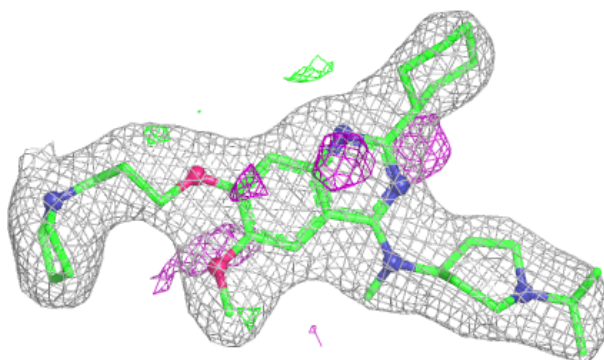


Electron density around QQS A 501 (A):

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

**Electron density around QQS B 501:**

$2mF_o-DF_c$ (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.