



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:43 AM UTC

PDB ID : 6YQC / pdb_00006yqc
Title : Taka-amylase in complex with alpha-glucosyl epi-cyclophellitol epoxide inhibitor
Authors : Armstrong, Z.; Chen, Y.; Artola, M.; Overkleeft, H.; Davies, G.
Deposited on : 2020-04-16
Resolution : 1.35 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

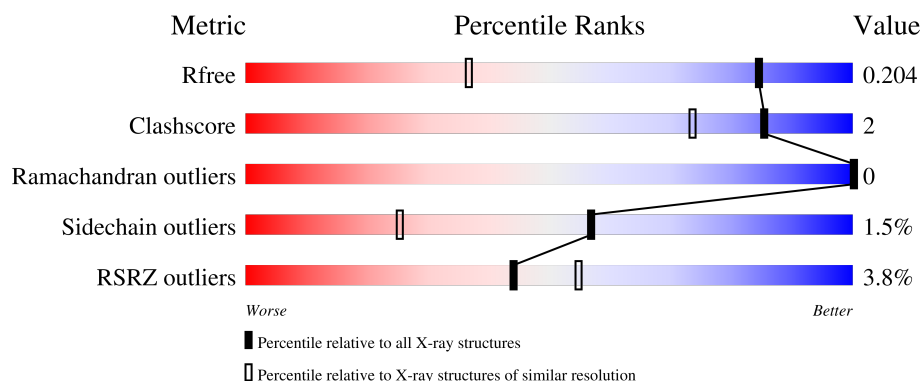
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	499	5% 89% 6% 5%
1	BBB	499	2% 89% 6% 5%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15544 atoms, of which 7236 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 Alpha-amylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	476	Total	C	H	N	O	S	219	8	0
			7259	2362	3521	606	750	20			
1	BBB	476	Total	C	H	N	O	S	217	7	0
			7251	2360	3521	602	749	19			

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



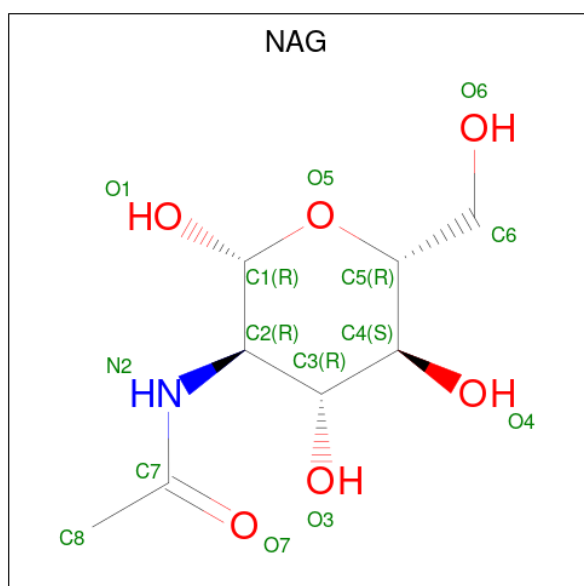
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		

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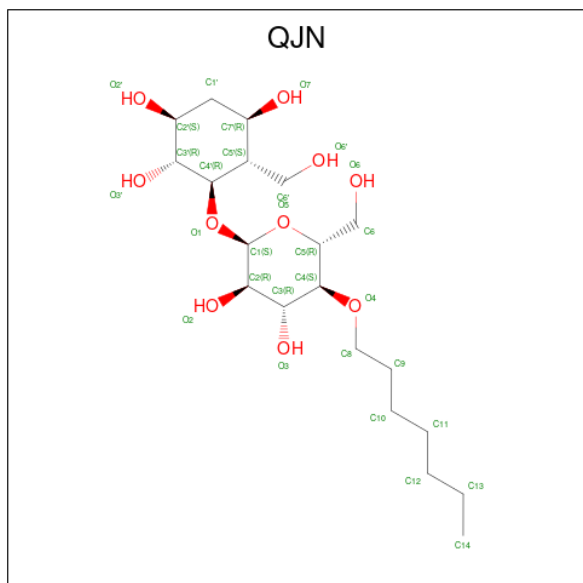
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	BBB	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 4 is (1 {R},2 {S},4 {R},5 {S},6 {R})-6-[(2 {S},3 {R},4 {R},5 {S},6 {R})-5-heptoxy-6-(hydroxymethyl)-3,4-bis(oxidanyl)oxan-2-yl]oxy-5-(hydroxymethyl)cyclohexane-1,2,4-triol (CCD ID: QJN) (formula: C₂₀H₃₈O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	7	0
			63	19	34	10		
4	BBB	1	Total	C	H	O	7	0
			66	20	36	10		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total	Ca	0	0
			1	1		
5	BBB	1	Total	Ca	0	0
			1	1		

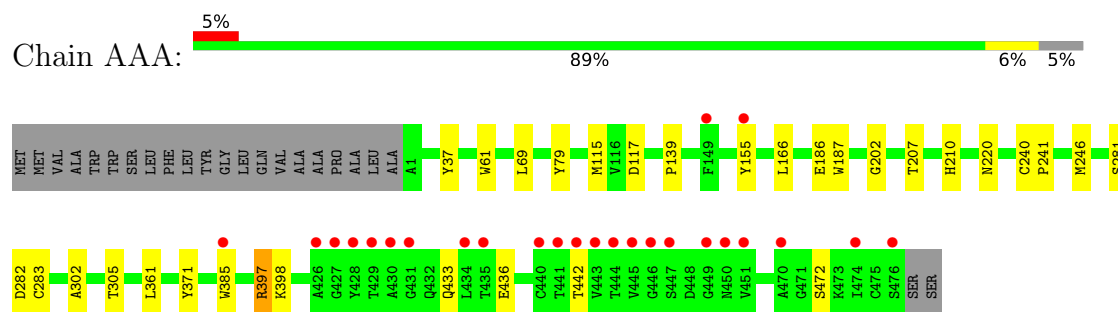
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	312	Total 312	O 312	0	0
6	BBB	375	Total 375	O 375	0	0

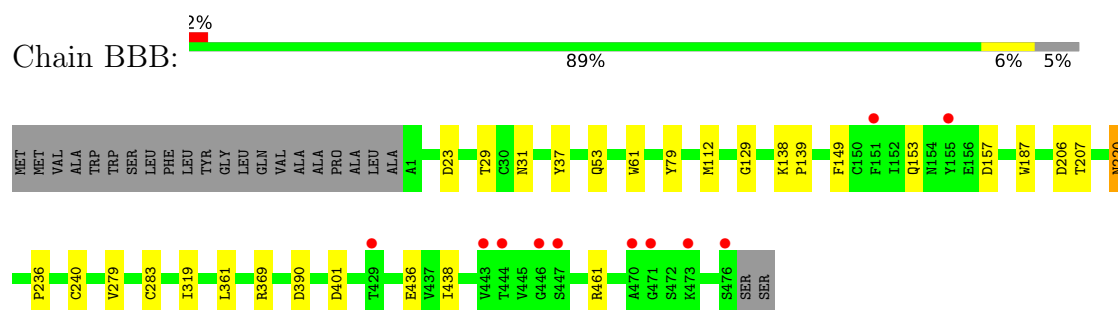
3 Residue-property plots [i](#)

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: Alpha-amylase



• Molecule 1: Alpha-amylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.77Å 98.99Å 75.45Å 90.00° 103.60° 90.00°	Depositor
Resolution (Å)	73.33 – 1.35 73.33 – 1.35	Depositor EDS
% Data completeness (in resolution range)	95.3 (73.33-1.35) 95.3 (73.33-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.177 , 0.204 0.177 , 0.204	Depositor DCC
R_{free} test set	9489 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	1.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15544	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: CA, NAG, QJN, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AAA	1.05	0/3838	1.17	1/5243 (0.0%)
1	BBB	1.05	2/3830 (0.1%)	1.14	6/5231 (0.1%)
All	All	1.05	2/7668 (0.0%)	1.16	7/10474 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	206	ASP	CG-OD1	5.33	1.35	1.25
1	BBB	236	PRO	C-O	-5.12	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	220	ASN	CA-CB-CG	5.76	118.36	112.60
1	BBB	23	ASP	CA-CB-CG	5.57	118.17	112.60
1	BBB	401	ASP	CB-CA-C	5.53	118.53	109.90
1	BBB	390	ASP	CA-CB-CG	5.47	118.07	112.60
1	AAA	117	ASP	CA-CB-CG	5.37	117.97	112.60
1	BBB	157	ASP	CA-CB-CG	5.20	117.80	112.60
1	BBB	29	THR	CA-CB-OG1	-5.08	101.98	109.60

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	AAA	3738	3521	3509	21	0
1	BBB	3730	3521	3511	11	1
2	AAA	24	36	36	1	0
2	BBB	40	60	60	0	0
3	AAA	14	14	13	0	0
3	BBB	14	14	13	0	0
4	AAA	29	34	0	0	0
4	BBB	30	36	0	0	0
5	AAA	1	0	0	0	0
5	BBB	1	0	0	0	0
6	AAA	312	0	0	0	0
6	BBB	375	0	0	2	0
All	All	8308	7236	7142	32	1

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 (32) 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:AAA:397[B]:ARG:HH21	1:AAA:397[B]:ARG:HG2	1.41	0.84
1:BBB:31[A]:ASN:OD1	6:BBB:601:HOH:O	1.94	0.83
1:AAA:397[B]:ARG:HH21	1:AAA:397[B]:ARG:CG	1.99	0.76
1:AAA:397[B]:ARG:HG2	1:AAA:397[B]:ARG:NH2	2.02	0.71
1:AAA:397[A]:ARG:HD3	1:AAA:397[A]:ARG:C	2.21	0.65
1:BBB:240:CYS:HB3	1:BBB:283[B]:CYS:HA	1.85	0.57
1:AAA:433:GLN:HE21	1:AAA:442:THR:HG21	1.70	0.56
1:BBB:53:GLN:HG3	1:BBB:112:MET:SD	2.49	0.52
1:AAA:302:ALA:HA	1:AAA:305:THR:O	2.11	0.49
1:BBB:240:CYS:HB3	1:BBB:283[A]:CYS:HA	1.95	0.49
1:AAA:281[B]:SER:OG	1:AAA:282:ASP:OD1	2.30	0.46
1:AAA:139:PRO:HG3	1:AAA:186[B]:GLU:HG2	1.98	0.45
1:AAA:139:PRO:HG3	1:AAA:186[B]:GLU:CG	2.47	0.44
1:AAA:361:LEU:C	1:AAA:361:LEU:HD13	2.42	0.44
1:BBB:279:VAL:HG13	1:BBB:283[A]:CYS:SG	2.57	0.44
1:AAA:155:TYR:O	2:AAA:505:EDO:H21	2.18	0.43
1:AAA:385:TRP:CZ3	1:AAA:397[B]:ARG:NH2	2.87	0.43
1:AAA:37:TYR:CE1	1:AAA:79:TYR:HA	2.54	0.42
1:AAA:69:LEU:HD12	1:AAA:69:LEU:C	2.45	0.42
1:AAA:397[A]:ARG:HD3	1:AAA:398:LYS:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:319[B]:ILE:O	1:BBB:369:ARG:HD2	2.19	0.42
1:BBB:361:LEU:HD13	1:BBB:361:LEU:C	2.45	0.42
1:AAA:397[A]:ARG:C	1:AAA:397[A]:ARG:CD	2.92	0.41
1:BBB:37:TYR:CE1	1:BBB:79:TYR:HA	2.55	0.41
1:BBB:129:GLY:HA3	1:BBB:149:PHE:CE1	2.55	0.41
1:AAA:240[B]:CYS:N	1:AAA:241:PRO:CD	2.84	0.41
1:AAA:246:MET:HE3	1:AAA:246:MET:HB2	1.95	0.41
1:BBB:138:LYS:HA	1:BBB:139:PRO:HA	1.92	0.41
1:BBB:461:ARG:NH1	6:BBB:616:HOH:O	2.53	0.41
1:AAA:166:LEU:HD21	1:AAA:210:HIS:CE1	2.56	0.40
1:AAA:371:TYR:CE1	1:AAA:472:SER:HB3	2.56	0.40
1:AAA:115:MET:HA	1:AAA:202:GLY:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:153:GLN:HE22	1:BBB:438:ILE:O[2_554]	1.57	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	482/499 (97%)	467 (97%)	15 (3%)	0	100	100
1	BBB	481/499 (96%)	470 (98%)	11 (2%)	0	100	100
All	All	963/998 (96%)	937 (97%)	26 (3%)	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	AAA	404/414 (98%)	395 (98%)	9 (2%)	45	14
1	BBB	404/414 (98%)	399 (99%)	5 (1%)	63	32
All	All	808/828 (98%)	794 (98%)	14 (2%)	57	20

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	61	TRP
1	AAA	187	TRP
1	AAA	207	THR
1	AAA	220	ASN
1	AAA	283[A]	CYS
1	AAA	283[B]	CYS
1	AAA	397[A]	ARG
1	AAA	397[B]	ARG
1	AAA	436	GLU
1	BBB	61	TRP
1	BBB	187	TRP
1	BBB	207	THR
1	BBB	220	ASN
1	BBB	436	GLU

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	$\# Z > 2$
3	NAG	BBB	504	1	14,14,15	0.68	0	17,19,21	1.29	4 (23%)
2	EDO	BBB	507	-	3,3,3	0.29	0	2,2,2	0.24	0
2	EDO	BBB	509	-	3,3,3	0.23	0	2,2,2	0.29	0
2	EDO	AAA	505	-	3,3,3	0.05	0	2,2,2	0.38	0
4	QJN	BBB	512	1	31,31,31	0.88	2 (6%)	38,42,42	1.07	2 (5%)
2	EDO	AAA	508	-	3,3,3	0.42	0	2,2,2	0.31	0
2	EDO	BBB	502	-	3,3,3	0.28	0	2,2,2	0.23	0
2	EDO	BBB	511	-	3,3,3	0.26	0	2,2,2	0.51	0
2	EDO	AAA	506	-	3,3,3	0.42	0	2,2,2	0.26	0
2	EDO	AAA	504	-	3,3,3	0.17	0	2,2,2	0.47	0
2	EDO	BBB	508	-	3,3,3	0.21	0	2,2,2	0.08	0
2	EDO	BBB	510	-	3,3,3	0.42	0	2,2,2	0.61	0
2	EDO	BBB	505	-	3,3,3	0.31	0	2,2,2	0.14	0
2	EDO	BBB	501	-	3,3,3	0.34	0	2,2,2	0.54	0
2	EDO	BBB	506	-	3,3,3	0.32	0	2,2,2	0.11	0
4	QJN	AAA	507	1	30,30,31	0.92	1 (3%)	37,41,42	1.14	4 (10%)
3	NAG	AAA	502	1	14,14,15	0.80	1 (7%)	17,19,21	0.91	1 (5%)
2	EDO	AAA	501	-	3,3,3	0.38	0	2,2,2	0.43	0
2	EDO	AAA	503	-	3,3,3	0.29	0	2,2,2	0.18	0
2	EDO	BBB	503	-	3,3,3	0.21	0	2,2,2	0.80	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	NAG	BBB	504	1	-	0/6/23/26	0/1/1/1
2	EDO	BBB	507	-	-	1/1/1/1	-
2	EDO	BBB	509	-	-	0/1/1/1	-
2	EDO	AAA	505	-	-	0/1/1/1	-
4	QJN	BBB	512	1	-	1/16/56/56	0/2/2/2
2	EDO	AAA	508	-	-	0/1/1/1	-
2	EDO	BBB	502	-	-	0/1/1/1	-
2	EDO	BBB	511	-	-	1/1/1/1	-
2	EDO	AAA	506	-	-	0/1/1/1	-
2	EDO	AAA	504	-	-	0/1/1/1	-
2	EDO	BBB	508	-	-	1/1/1/1	-
2	EDO	BBB	510	-	-	0/1/1/1	-
2	EDO	BBB	505	-	-	0/1/1/1	-
2	EDO	BBB	501	-	-	0/1/1/1	-
2	EDO	BBB	506	-	-	0/1/1/1	-
4	QJN	AAA	507	1	-	0/15/55/56	0/2/2/2
3	NAG	AAA	502	1	-	0/6/23/26	0/1/1/1
2	EDO	AAA	501	-	-	0/1/1/1	-
2	EDO	AAA	503	-	-	0/1/1/1	-
2	EDO	BBB	503	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	507	QJN	C6'-C5'	2.41	1.56	1.52
4	BBB	512	QJN	C1'-C7'	-2.32	1.48	1.52
4	BBB	512	QJN	C2'-C3'	2.23	1.55	1.52
3	AAA	502	NAG	C1-C2	-2.10	1.49	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BBB	512	QJN	C7'-C1'-C2'	4.02	116.16	111.50
4	AAA	507	QJN	C1-C2-C3	3.26	116.86	110.01
3	BBB	504	NAG	C3-C4-C5	-2.89	105.00	110.23
4	BBB	512	QJN	C1-C2-C3	2.60	115.47	110.01
3	AAA	502	NAG	C1-O5-C5	-2.41	108.95	112.19
4	AAA	507	QJN	C1-O5-C5	-2.28	109.27	113.72
4	AAA	507	QJN	C1'-C2'-C3'	2.13	113.74	110.67
3	BBB	504	NAG	C8-C7-N2	-2.11	112.62	116.12
4	AAA	507	QJN	C5'-C4'-C3'	-2.10	107.72	112.26
3	BBB	504	NAG	C2-N2-C7	2.06	125.66	122.90
3	BBB	504	NAG	O5-C1-C2	-2.05	108.12	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

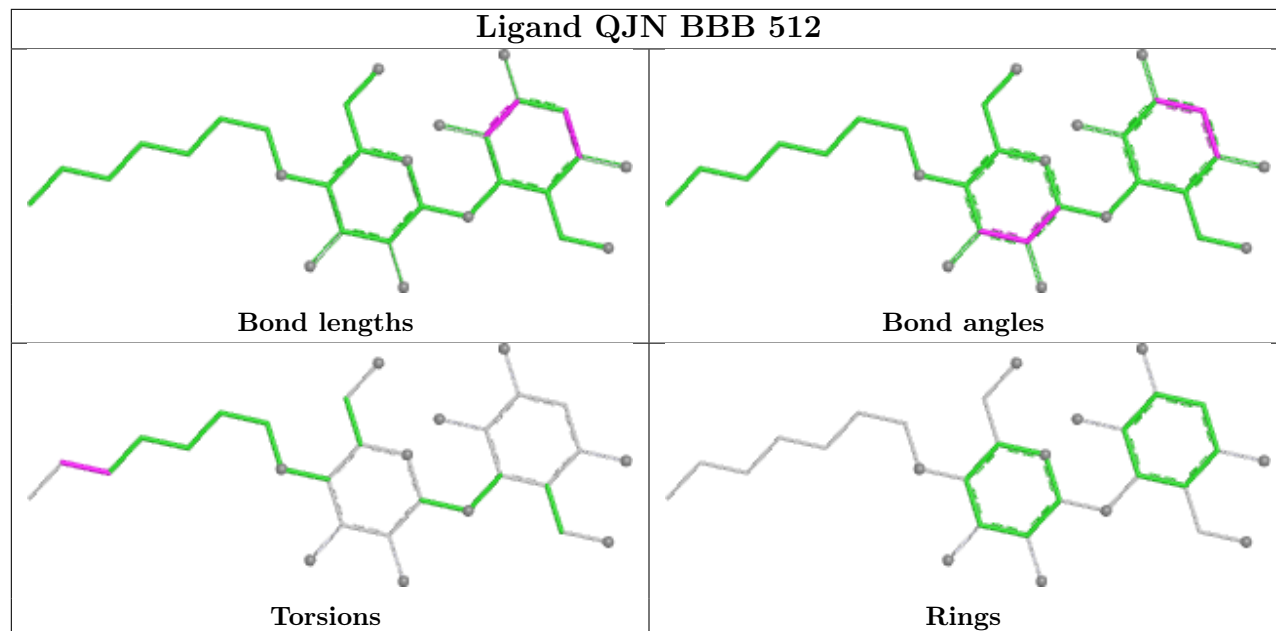
Mol	Chain	Res	Type	Atoms
4	BBB	512	QJN	C11-C12-C13-C14
2	BBB	508	EDO	O1-C1-C2-O2
2	BBB	503	EDO	O1-C1-C2-O2
2	BBB	507	EDO	O1-C1-C2-O2
2	BBB	511	EDO	O1-C1-C2-O2

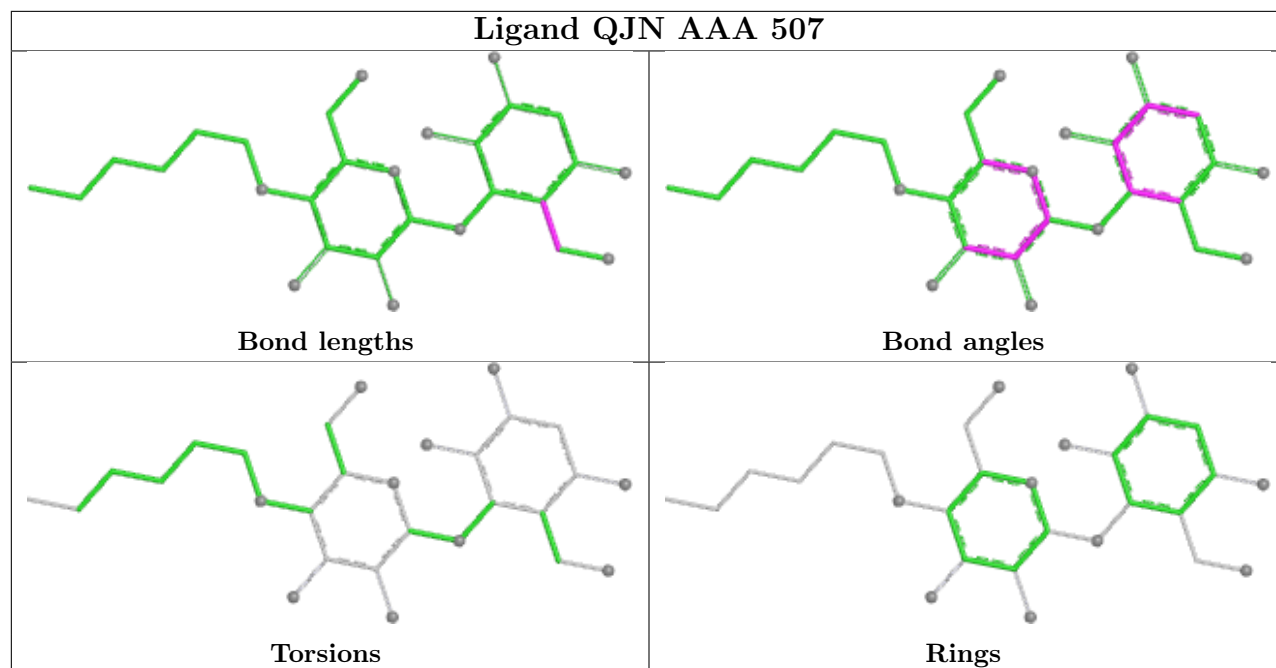
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	505	EDO	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.





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	AAA	476/499 (95%)	0.34	25 (5%)	32 42	8, 17, 34, 56	8 (1%)
1	BBB	476/499 (95%)	0.06	11 (2%)	61 71	6, 15, 28, 48	8 (1%)
All	All	952/998 (95%)	0.20	36 (3%)	44 55	6, 16, 32, 56	16 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	476	SER	3.5
1	AAA	470	ALA	3.5
1	AAA	430	ALA	3.4
1	AAA	428	TYR	3.2
1	AAA	442	THR	3.2
1	BBB	443	VAL	3.2
1	AAA	149	PHE	3.1
1	AAA	443	VAL	3.0
1	BBB	155	TYR	3.0
1	AAA	476	SER	2.9
1	AAA	449	GLY	2.8
1	AAA	444	THR	2.8
1	AAA	431	GLY	2.8
1	AAA	446	GLY	2.8
1	AAA	445	VAL	2.7
1	AAA	385	TRP	2.7
1	AAA	451	VAL	2.6
1	BBB	151	PHE	2.6
1	AAA	429	THR	2.6
1	AAA	426	ALA	2.6
1	AAA	447	SER	2.5
1	BBB	447	SER	2.5
1	AAA	434	LEU	2.5
1	BBB	470	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	474	ILE	2.3
1	BBB	473	LYS	2.3
1	BBB	446	GLY	2.2
1	BBB	471	GLY	2.2
1	AAA	450	ASN	2.2
1	AAA	441	THR	2.2
1	AAA	427	GLY	2.2
1	BBB	429	THR	2.1
1	AAA	435	THR	2.1
1	BBB	444	THR	2.0
1	AAA	440	CYS	2.0
1	AAA	155	TYR	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
2	EDO	BBB	507	4/4	0.84	0.13	38,38,40,40	1
2	EDO	AAA	504	4/4	0.90	0.10	21,22,25,25	1
2	EDO	BBB	501	4/4	0.91	0.10	23,23,24,24	1
2	EDO	AAA	505	4/4	0.91	0.12	21,23,33,33	1
2	EDO	BBB	509	4/4	0.92	0.10	29,30,36,36	1
3	NAG	AAA	502	14/15	0.92	0.08	23,27,33,35	3
3	NAG	BBB	504	14/15	0.92	0.08	23,25,28,31	3
2	EDO	BBB	508	4/4	0.93	0.10	27,32,37,37	1
2	EDO	BBB	503	4/4	0.93	0.10	25,29,29,29	1
2	EDO	BBB	510	4/4	0.94	0.09	20,25,28,28	1
2	EDO	AAA	508	4/4	0.94	0.08	21,22,24,24	1

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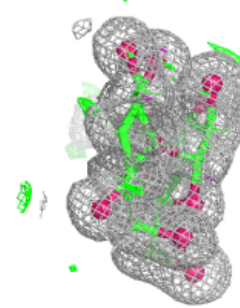
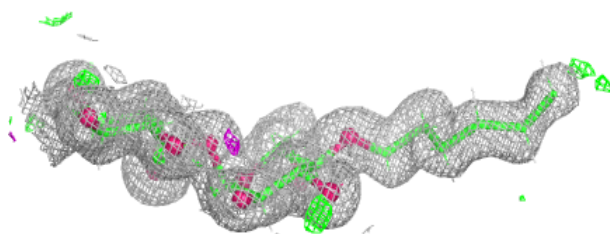
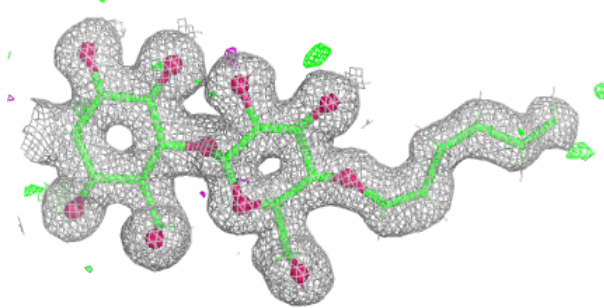
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	AAA	506	4/4	0.94	0.09	21,23,25,25	1
2	EDO	BBB	511	4/4	0.95	0.07	23,25,29,29	1
2	EDO	BBB	505	4/4	0.96	0.07	18,19,25,25	1
2	EDO	BBB	502	4/4	0.96	0.07	17,21,23,23	1
5	CA	AAA	509	1/1	0.96	0.06	14,14,14,14	0
2	EDO	BBB	506	4/4	0.97	0.06	18,20,21,21	1
2	EDO	AAA	501	4/4	0.97	0.06	21,23,24,24	1
4	QJN	AAA	507	29/30	0.97	0.06	11,13,30,30	7
2	EDO	AAA	503	4/4	0.97	0.05	16,17,18,18	1
5	CA	BBB	513	1/1	0.97	0.05	13,13,13,13	0
4	QJN	BBB	512	30/30	0.98	0.06	11,13,35,37	7

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.

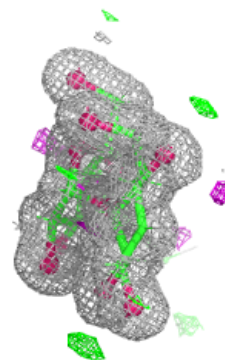
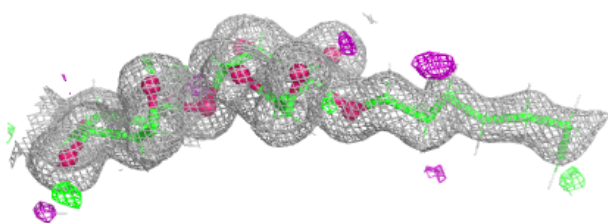
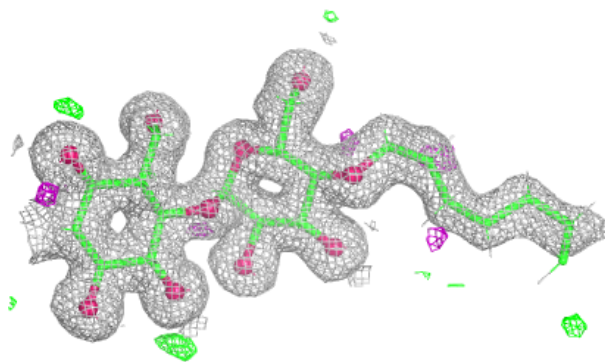
Electron density around QJN AAA 507:

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 QJN BBB 512:

$2mF_o - DF_c$ (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.