



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5ABE / pdb_00005abe
Title : Structure of GH84 with ligand
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Deposited on : 2015-08-05
Resolution : 2.00 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

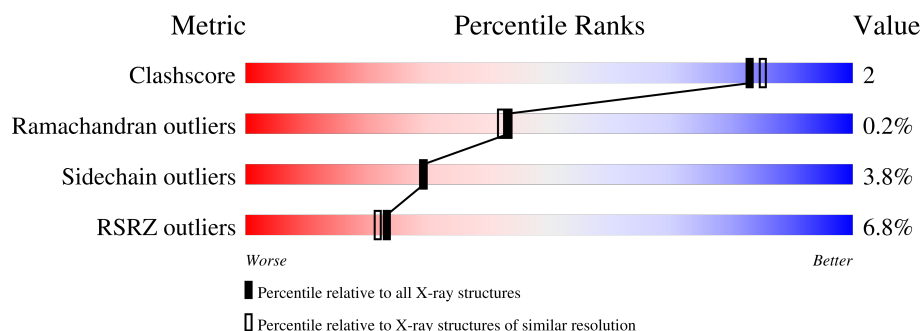
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	726	5% 84% 9% • 6%
1	B	726	7% 82% 10% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11263 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.

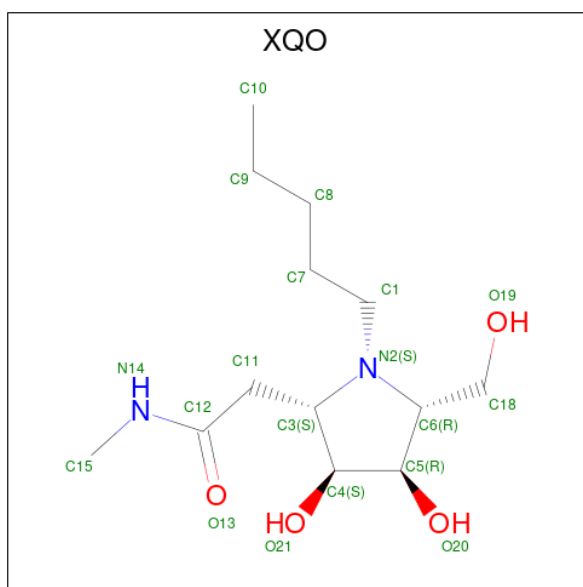
- Molecule 1 is a protein called O-GLCNACASE BT_4395.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	681	Total	C	N	O	S	0	1	0
			5527	3541	934	1033	19			
1	B	670	Total	C	N	O	S	0	1	0
			5456	3497	924	1017	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP Q89ZI2
A	-8	GLY	-	expression tag	UNP Q89ZI2
A	-7	SER	-	expression tag	UNP Q89ZI2
A	-6	SER	-	expression tag	UNP Q89ZI2
A	-5	HIS	-	expression tag	UNP Q89ZI2
A	-4	HIS	-	expression tag	UNP Q89ZI2
A	-3	HIS	-	expression tag	UNP Q89ZI2
A	-2	HIS	-	expression tag	UNP Q89ZI2
A	-1	HIS	-	expression tag	UNP Q89ZI2
A	0	HIS	-	expression tag	UNP Q89ZI2
B	-9	MET	-	expression tag	UNP Q89ZI2
B	-8	GLY	-	expression tag	UNP Q89ZI2
B	-7	SER	-	expression tag	UNP Q89ZI2
B	-6	SER	-	expression tag	UNP Q89ZI2
B	-5	HIS	-	expression tag	UNP Q89ZI2
B	-4	HIS	-	expression tag	UNP Q89ZI2
B	-3	HIS	-	expression tag	UNP Q89ZI2
B	-2	HIS	-	expression tag	UNP Q89ZI2
B	-1	HIS	-	expression tag	UNP Q89ZI2
B	0	HIS	-	expression tag	UNP Q89ZI2

- Molecule 2 is 2-[(2S,3S,4R,5R)-5-(hydroxymethyl)-3,4-bis(oxidanyl)-1-pentyl-pyrrolidin-2-yl]-N-methyl-ethanamide (CCD ID: XQO) (formula: C₁₃H₂₆N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	13	2	4		
2	B	1	Total	C	N	O	0	0
			19	13	2	4		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total	O	0	0
			125	125		
4	B	116	Total	O	0	0
			116	116		

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	51.57Å 159.60Å 223.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	129.81 – 2.00 129.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (129.81-2.00) 89.1 (129.81-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.207 , 0.244 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11263	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7042e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CA, XQO

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	1.01	0/5662	0.96	5/7669 (0.1%)
1	B	1.04	4/5589 (0.1%)	1.00	3/7566 (0.0%)
All	All	1.02	4/11251 (0.0%)	0.98	8/15235 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	316	SER	CA-C	-5.86	1.45	1.52
1	B	489	LYS	C-O	-5.62	1.19	1.24
1	B	74	ILE	C-O	-5.52	1.17	1.24
1	B	495	ILE	C-O	-5.11	1.18	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	693	ARG	N-CA-C	5.56	117.52	109.07
1	B	399	THR	CB-CA-C	-5.30	102.50	110.92
1	A	496	THR	CA-C-N	-5.25	113.50	119.28
1	A	496	THR	C-N-CA	-5.25	113.50	119.28
1	A	630	SER	N-CA-C	5.24	117.15	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	558	THR	N-CA-C	5.17	117.81	111.82
1	A	399	THR	CB-CA-C	-5.13	102.77	110.92
1	B	408	ARG	CG-CD-NE	5.12	123.26	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	628	GLY	Peptide
1	B	457	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5527	0	5446	28	1
1	B	5456	0	5389	26	0
2	A	19	0	26	2	0
2	B	19	0	26	0	0
3	B	1	0	0	0	0
4	A	125	0	0	0	0
4	B	116	0	0	0	0
All	All	11263	0	10887	53	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 (53) 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:B:355:VAL:O	1:B:399:THR:HG23	1.90	0.71
1:A:355:VAL:O	1:A:399:THR:HG23	1.94	0.67
1:A:438:GLU:OE1	1:A:441:MET:HG3	1.96	0.65
1:A:452:LYS:N	1:A:452:LYS:HD3	2.18	0.58
1:B:591:MET:HE1	1:B:609:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LEU:HD13	1:A:229:MET:HE1	1.87	0.56
1:A:673:LEU:HD22	1:A:680:LEU:HB3	1.88	0.56
1:B:263:GLU:HA	1:B:267:GLN:HG2	1.90	0.54
1:A:557:ALA:HB1	1:A:561:ILE:HB	1.89	0.54
1:A:537:GLN:HG2	1:B:484:MET:HE3	1.93	0.50
1:B:70:TYR:OH	1:B:89:GLU:OE2	2.26	0.50
1:A:661:ILE:HD13	1:A:671:VAL:HG21	1.94	0.49
1:A:591:MET:HG3	1:A:593:HIS:O	2.13	0.48
1:A:644:ILE:HD11	1:A:661:ILE:HD11	1.95	0.48
1:B:354:PRO:HB2	1:B:399:THR:HG22	1.95	0.48
1:B:62[A]:LYS:NZ	1:B:71:SER:O	2.45	0.48
1:A:137:TYR:CE2	2:A:1716:XQO:H4	2.49	0.48
1:A:137:TYR:HE2	2:A:1716:XQO:H4	1.78	0.48
1:A:252:GLN:HE22	1:A:300:LYS:HE2	1.79	0.47
1:A:354:PRO:HB2	1:A:399:THR:HG22	1.96	0.47
1:B:676:LYS:HE3	1:B:676:LYS:C	2.39	0.47
1:B:310:THR:HA	1:B:337:TRP:O	2.14	0.47
1:B:536:GLN:HG2	1:B:590:TYR:CD1	2.50	0.47
1:B:616:ILE:HD12	1:B:709:PHE:CG	2.50	0.47
1:A:125:PRO:HB3	1:A:392:TRP:CE3	2.50	0.46
1:A:310:THR:HA	1:A:337:TRP:O	2.16	0.46
1:A:308:MET:HA	1:A:335:TYR:O	2.17	0.45
1:B:562:LYS:HB3	1:B:563:PRO:HD3	1.99	0.45
1:A:131:GLY:O	1:A:370:VAL:HA	2.17	0.45
1:B:356:TYR:HB3	1:B:399:THR:HG21	1.98	0.45
1:B:708:GLN:HG2	1:B:710:VAL:HG23	1.99	0.45
1:B:86:ASN:HA	1:B:118:GLU:HG3	1.98	0.45
1:A:423[A]:MET:HE3	1:A:423[A]:MET:HB2	1.64	0.44
1:B:443:ILE:C	1:B:443:ILE:HD12	2.42	0.44
1:B:557:ALA:HB1	1:B:561:ILE:HB	1.99	0.44
1:A:443:ILE:C	1:A:443:ILE:HD12	2.43	0.44
1:A:562:LYS:HB3	1:A:563:PRO:HD3	2.00	0.43
1:A:625:TRP:CZ2	1:A:706:LEU:N	2.87	0.43
1:B:468:LEU:HD23	1:B:468:LEU:HA	1.88	0.43
1:A:238:ALA:HA	1:A:276:VAL:O	2.19	0.42
1:B:354:PRO:HB2	1:B:399:THR:CG2	2.50	0.41
1:B:33:ALA:HB2	1:B:60:GLY:HA2	2.02	0.41
1:B:131:GLY:HA3	1:B:160:THR:O	2.21	0.41
1:A:644:ILE:CD1	1:A:661:ILE:HD11	2.51	0.41
1:A:283:ASN:HB3	1:A:310:THR:OG1	2.20	0.41
1:A:515:MET:HE1	1:A:569:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:TYR:HB2	1:A:180:TYR:CE2	2.55	0.41
1:B:362:ILE:HD12	1:B:366:MET:HE3	2.03	0.40
1:B:134:GLU:O	1:B:164:GLY:C	2.64	0.40
1:A:72:ARG:HG2	1:A:72:ARG:HH11	1.87	0.40
1:B:308:MET:HA	1:B:335:TYR:O	2.21	0.40
1:B:483:LEU:HG	1:B:499:VAL:HG11	2.04	0.40
1:B:81:TYR:CZ	1:B:123:ASP:HB3	2.56	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:A:170:TYR:OH	1:A:442:ASP:OD1[1_655]	2.19	0.01

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	A	670/726 (92%)	644 (96%)	25 (4%)	1 (0%)	48	46
1	B	659/726 (91%)	635 (96%)	23 (4%)	1 (0%)	43	42
All	All	1329/1452 (92%)	1279 (96%)	48 (4%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	629	ASN
1	B	291	GLY

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	599/639 (94%)	574 (96%)	25 (4%)	26	25
1	B	592/639 (93%)	571 (96%)	21 (4%)	32	32
All	All	1191/1278 (93%)	1145 (96%)	46 (4%)	29	28

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	49	GLN
1	A	52	LYS
1	A	53	LYS
1	A	65	LYS
1	A	72	ARG
1	A	183	LYS
1	A	371	THR
1	A	423[A]	MET
1	A	423[B]	MET
1	A	444	GLN
1	A	452	LYS
1	A	476	LYS
1	A	519	ARG
1	A	532	LYS
1	A	594	LYS
1	A	615	LEU
1	A	660	GLU
1	A	666	LYS
1	A	671	VAL
1	A	689	VAL
1	A	695	THR
1	A	707	ARG
1	A	713	ILE
1	A	715	LYS
1	B	15	GLN
1	B	48	LYS

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Mol	Chain	Res	Type
1	B	112	LYS
1	B	113	ASP
1	B	258	LEU
1	B	299	ASP
1	B	371	THR
1	B	423	MET
1	B	451	LEU
1	B	496	THR
1	B	574	LYS
1	B	594	LYS
1	B	608	GLN
1	B	615	LEU
1	B	632	GLU
1	B	644	ILE
1	B	661	ILE
1	B	666	LYS
1	B	670	THR
1	B	676	LYS
1	B	694	PHE

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	16	ASN
1	A	144	GLN
1	A	156	ASN
1	A	252	GLN
1	A	349	HIS
1	A	578	GLN
1	A	604	ASN
1	A	696	ASN
1	B	2	ASN
1	B	73	GLN

5.3.3 RNA ⓘ

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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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$
2	XQO	A	1716	-	19,19,19	1.02	3 (15%)	22,25,25	2.36	6 (27%)
2	XQO	B	1717	-	19,19,19	1.02	2 (10%)	22,25,25	1.99	5 (22%)

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	XQO	A	1716	-	-	1/13/33/33	0/1/1/1
2	XQO	B	1717	-	-	1/13/33/33	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1716	XQO	C4-C3	-2.88	1.49	1.53
2	B	1717	XQO	C1-N2	2.83	1.51	1.46
2	A	1716	XQO	C1-N2	2.32	1.50	1.46
2	B	1717	XQO	C4-C3	-2.23	1.50	1.53
2	A	1716	XQO	C3-N2	2.00	1.50	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1716	XQO	C3-C11-C12	-6.64	100.04	112.84
2	B	1717	XQO	C3-C11-C12	-5.76	101.73	112.84
2	A	1716	XQO	C7-C1-N2	4.41	123.56	113.10
2	A	1716	XQO	C4-C5-C6	4.14	108.79	102.46
2	B	1717	XQO	C4-C5-C6	3.76	108.21	102.46
2	A	1716	XQO	O19-C18-C6	-3.63	103.53	111.55
2	B	1717	XQO	C7-C1-N2	3.42	121.21	113.10
2	A	1716	XQO	C1-N2-C3	2.82	119.84	114.05
2	B	1717	XQO	O13-C12-C11	-2.52	117.86	121.54
2	A	1716	XQO	O13-C12-C11	-2.33	118.12	121.54
2	B	1717	XQO	C1-N2-C6	2.10	118.36	114.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

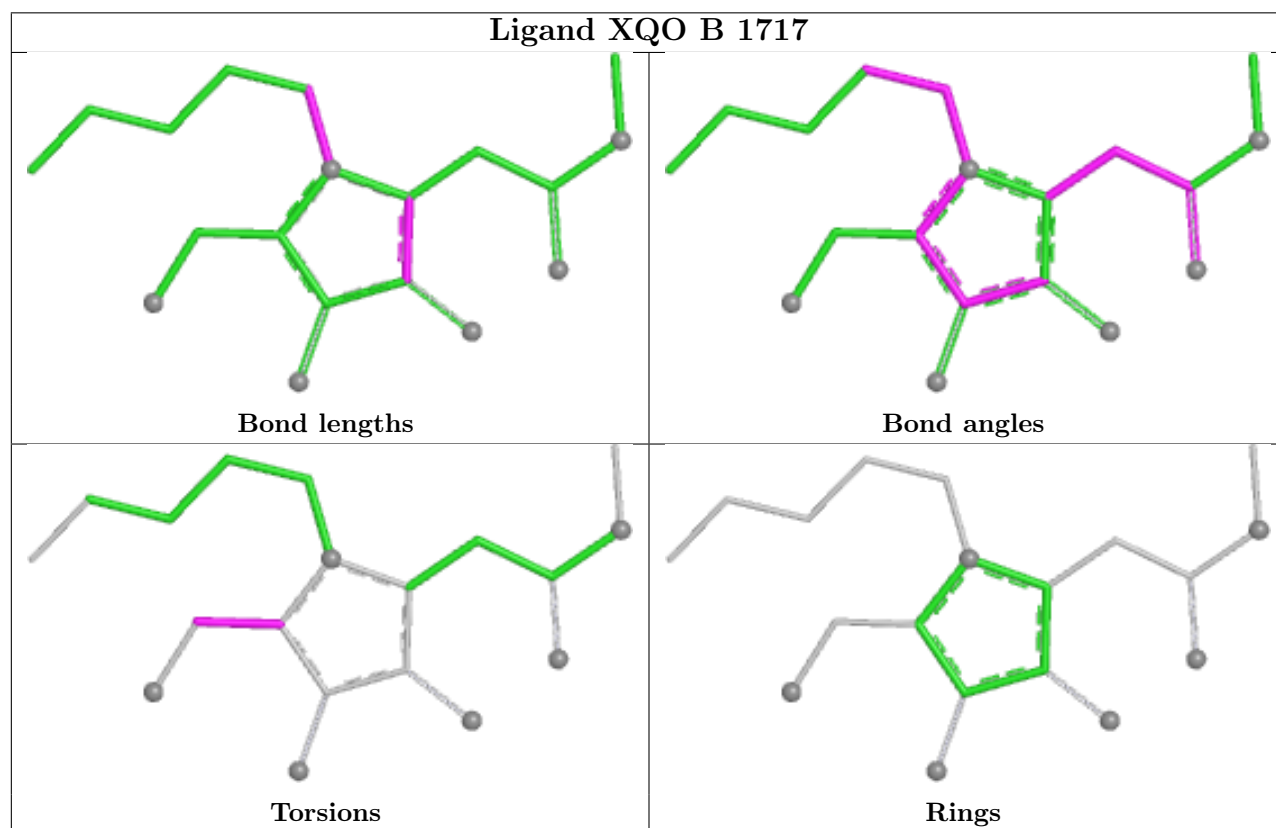
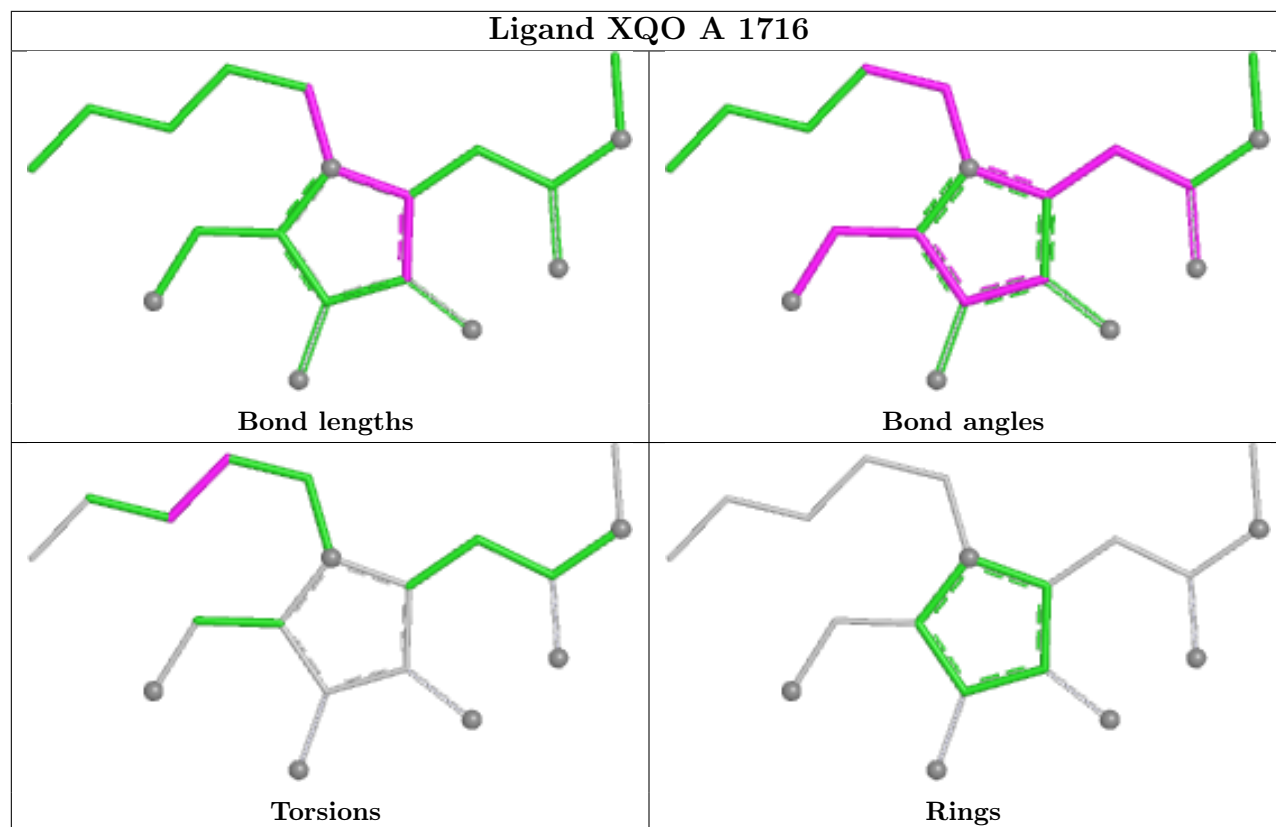
Mol	Chain	Res	Type	Atoms
2	B	1717	XQO	O19-C18-C6-C5
2	A	1716	XQO	C1-C7-C8-C9

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1716	XQO	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

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, 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	681/726 (93%)	0.39	38 (5%) 30 29	21, 48, 92, 116	1 (0%)
1	B	670/726 (92%)	0.55	54 (8%) 18 17	21, 50, 95, 122	1 (0%)
All	All	1351/1452 (93%)	0.47	92 (6%) 23 22	21, 49, 94, 122	2 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	680	LEU	6.4
1	B	648	PHE	6.3
1	A	625	TRP	5.4
1	B	694	PHE	5.1
1	A	627	ALA	4.8
1	B	676	LYS	4.7
1	A	626	ALA	4.5
1	A	680	LEU	4.5
1	A	628	GLY	3.8
1	B	244	ILE	3.8
1	B	286	TRP	3.6
1	A	706	LEU	3.6
1	B	673	LEU	3.6
1	B	715	LYS	3.4
1	A	624	LYS	3.3
1	B	605	LEU	3.3
1	B	454	PHE	3.3
1	A	3	VAL	3.2
1	A	661	ILE	3.2
1	B	646	ILE	3.2
1	A	715	LYS	3.2
1	A	648	PHE	3.1
1	A	682	ALA	3.1
1	A	695	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	631	VAL	3.0
1	A	694	PHE	3.0
1	B	706	LEU	2.9
1	A	24	VAL	2.9
1	A	602	ILE	2.9
1	B	671	VAL	2.9
1	B	709	PHE	2.9
1	A	23	ALA	2.9
1	B	595	MET	2.8
1	B	258	LEU	2.8
1	B	689	VAL	2.8
1	A	618	PRO	2.7
1	B	291	GLY	2.7
1	B	665	GLY	2.7
1	B	51	SER	2.7
1	B	245	SER	2.7
1	A	19	ILE	2.7
1	B	212	ILE	2.7
1	B	243	ASP	2.7
1	B	52	LYS	2.7
1	A	696	ASN	2.6
1	B	223	LEU	2.6
1	A	671	VAL	2.5
1	B	46	SER	2.5
1	B	685	GLN	2.5
1	A	659	LEU	2.5
1	B	214	TRP	2.5
1	B	290	ASN	2.5
1	A	673	LEU	2.4
1	A	441	MET	2.4
1	B	441	MET	2.4
1	B	249	THR	2.4
1	B	455	LYS	2.4
1	B	457	GLY	2.3
1	B	232	LEU	2.3
1	B	659	LEU	2.3
1	A	709	PHE	2.3
1	B	248	GLY	2.3
1	B	610	LYS	2.3
1	A	522	SER	2.2
1	A	598	ASN	2.2
1	A	4	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	674	LYS	2.2
1	B	442	ASP	2.2
1	B	297	LEU	2.2
1	B	670	THR	2.2
1	B	688	PRO	2.1
1	B	644	ILE	2.1
1	B	661	ILE	2.1
1	B	692	VAL	2.1
1	B	687	ALA	2.1
1	A	584	LEU	2.1
1	A	540	TYR	2.1
1	A	519	ARG	2.1
1	A	644	ILE	2.1
1	B	216	LYS	2.1
1	A	605	LEU	2.1
1	A	470	TYR	2.1
1	A	452	LYS	2.1
1	B	253	LYS	2.1
1	B	666	LYS	2.1
1	A	681	SER	2.1
1	B	222	LEU	2.0
1	B	18	THR	2.0
1	B	606	PRO	2.0
1	B	62[A]	LYS	2.0
1	B	518	GLY	2.0
1	A	53	LYS	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](#)

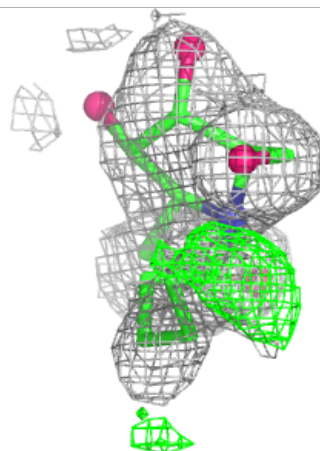
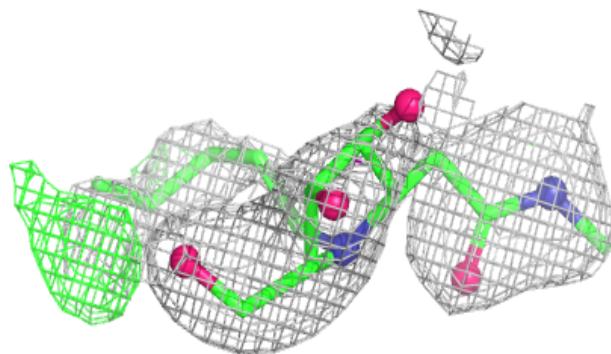
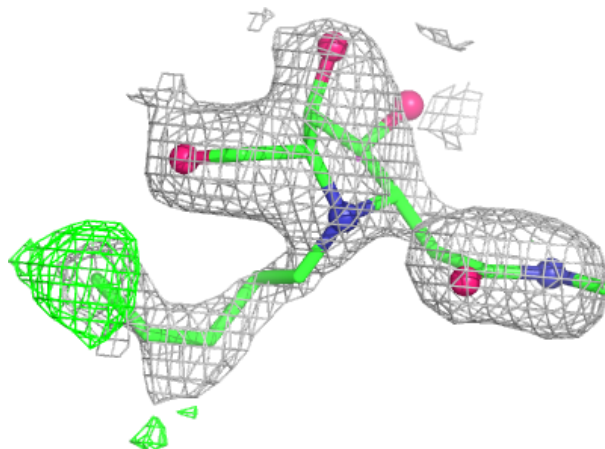
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XQO	B	1717	19/19	0.83	0.23	46,56,66,66	19
2	XQO	A	1716	19/19	0.88	0.18	42,59,67,69	0
3	CA	B	1716	1/1	0.98	0.04	42,42,42,42	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.

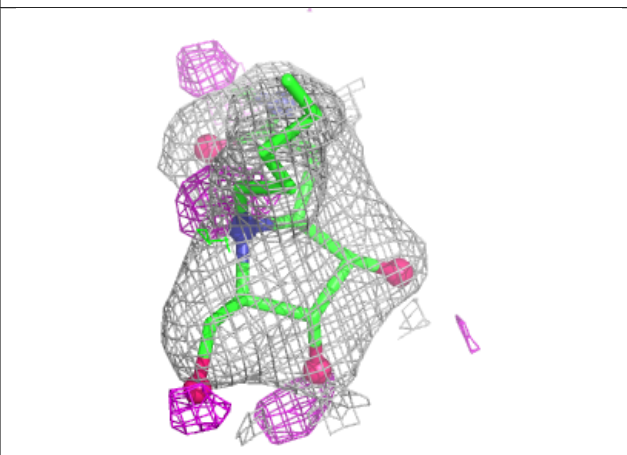
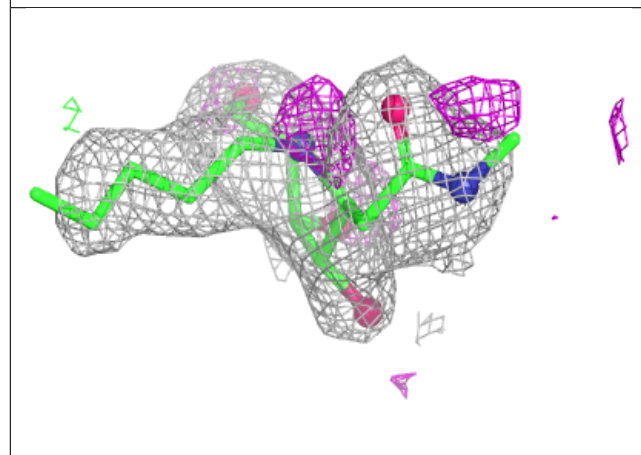
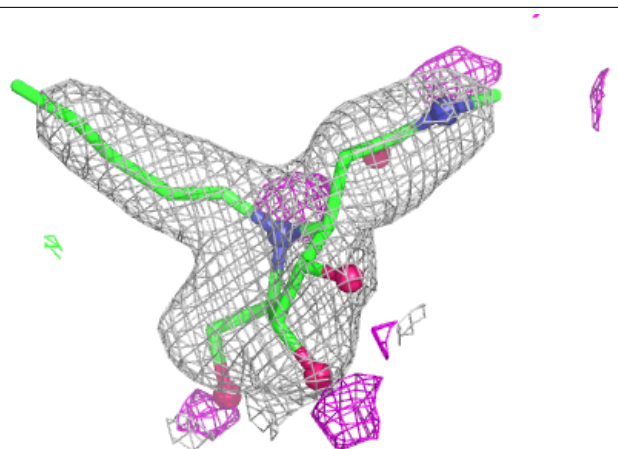
Electron density around XQO B 1717:

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 XQO A 1716:

$2mF_o-DF_c$ (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.