



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:21 pm BST

PDB ID : 3ARW
Title : Crystal Structure Analysis of Chitinase A from *Vibrio harveyi* with novel inhibitors - complex structure with chelerythrine
Authors : Pantoom, S.; Vetter, I.R.; Prinz, H.; Suginta, W.
Deposited on : 2010-12-09
Resolution : 1.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

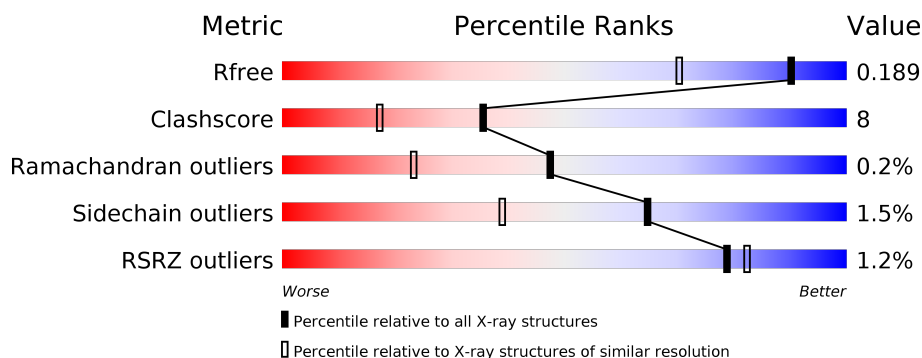
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	584	<div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div>

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
2	CTI	A	606	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5531 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.

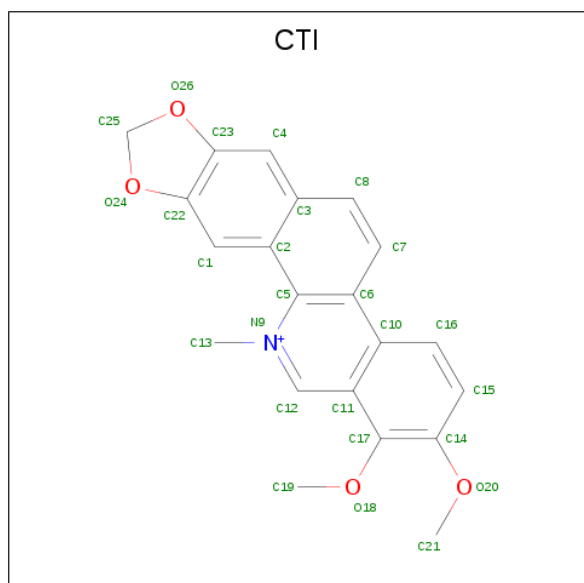
- Molecule 1 is a protein called Chitinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	575	4561	2911	725	897	28	0	28	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ARG	-	EXPRESSION TAG	UNP Q9AMP1
A	599	SER	-	EXPRESSION TAG	UNP Q9AMP1
A	600	HIS	-	EXPRESSION TAG	UNP Q9AMP1
A	601	HIS	-	EXPRESSION TAG	UNP Q9AMP1
A	602	HIS	-	EXPRESSION TAG	UNP Q9AMP1
A	603	HIS	-	EXPRESSION TAG	UNP Q9AMP1
A	604	HIS	-	EXPRESSION TAG	UNP Q9AMP1
A	605	HIS	-	EXPRESSION TAG	UNP Q9AMP1

- Molecule 2 is 1,2-dimethoxy-12-methyl[1,3]benzodioxolo[5,6-c]phenanthridin-12-ium (three-letter code: CTI) (formula: C₂₁H₁₈NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	21	1	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

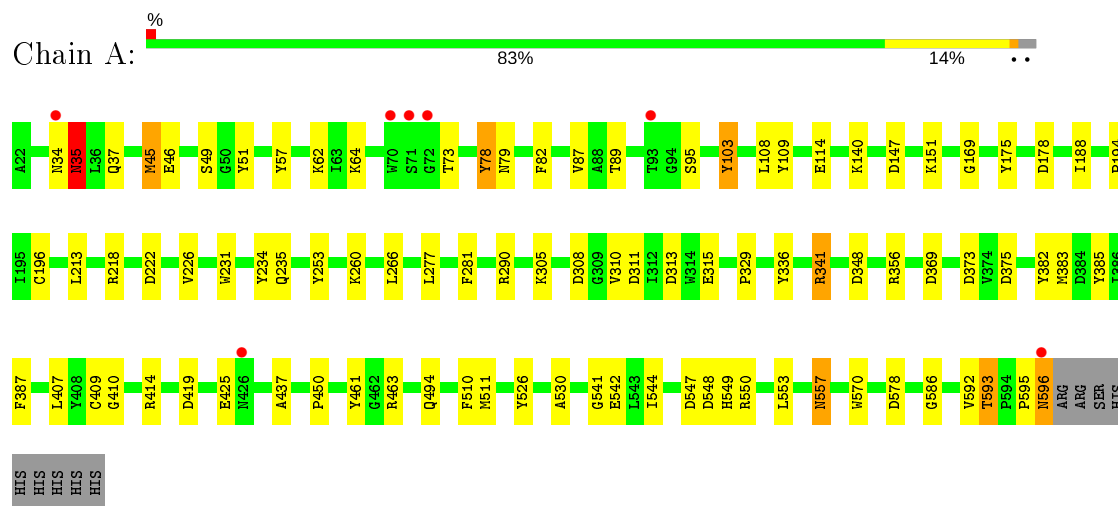


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	926	Total	O	0	0
			926	926		

- Molecule 1: Chitinase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.01Å 50.78Å 93.29Å 90.00° 99.59° 90.00°	Depositor
Resolution (Å)	44.45 – 1.50 44.46 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.0 (44.45-1.50) 96.0 (44.46-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.6.0093	Depositor
R, R_{free}	0.153 , 0.190 0.151 , 0.189	Depositor DCC
R_{free} test set	4641 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5531	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: GOL, CTI

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	1.37	16/4750 (0.3%)	1.32	33/6462 (0.5%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	593	THR	CB-OG1	6.72	1.56	1.43
1	A	51	TYR	CD2-CE2	6.18	1.48	1.39
1	A	557	ASN	CB-CG	6.00	1.64	1.51
1	A	387	PHE	CG-CD2	5.99	1.47	1.38
1	A	78	TYR	CD2-CE2	5.96	1.48	1.39
1	A	542	GLU	CD-OE1	5.74	1.31	1.25
1	A	175	TYR	CD1-CE1	5.34	1.47	1.39
1	A	310	VAL	CB-CG1	-5.26	1.41	1.52
1	A	461	TYR	CE1-CZ	-5.18	1.31	1.38
1	A	103	TYR	CB-CG	-5.12	1.44	1.51
1	A	425	GLU	CG-CD	5.09	1.59	1.51
1	A	51	TYR	CE1-CZ	-5.07	1.31	1.38
1	A	253	TYR	CD2-CE2	5.06	1.47	1.39
1	A	541	GLY	C-O	5.04	1.31	1.23
1	A	315	GLU	CD-OE1	-5.03	1.20	1.25
1	A	109	TYR	CE2-CZ	5.03	1.45	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	ASP	CB-CG-OD2	11.42	128.57	118.30
1	A	290	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	A	419	ASP	CB-CG-OD1	-8.67	110.50	118.30
1	A	550	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	A	45	MET	N-CA-C	7.67	131.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	336	TYR	CB-CG-CD2	-7.18	116.69	121.00
1	A	578	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	385	TYR	CB-CG-CD1	-6.76	116.94	121.00
1	A	461	TYR	CZ-CE2-CD2	-6.74	113.73	119.80
1	A	213	LEU	CB-CG-CD2	-6.62	99.74	111.00
1	A	108	LEU	CB-CG-CD1	-6.28	100.32	111.00
1	A	356	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	348	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	375	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	234	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	A	178	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	281	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	A	82	PHE	CB-CG-CD1	5.73	124.81	120.80
1	A	341[A]	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	341[B]	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	463	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	234	TYR	CB-CG-CD1	5.67	124.40	121.00
1	A	383	MET	CG-SD-CE	-5.66	91.14	100.20
1	A	369	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	308	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	526	TYR	CZ-CE2-CD2	-5.36	114.98	119.80
1	A	373	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	548	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	253	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	222	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	147	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	461	TYR	CE1-CZ-CE2	5.15	128.05	119.80

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	4561	0	4365	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	26	0	18	10	0
3	A	18	0	24	0	0
4	A	926	0	0	22	0
All	All	5531	0	4407	73	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 8.

All (73) 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)
2:A:606:CTI:H1	2:A:606:CTI:C13	1.54	1.36
1:A:409:CYS:HB2	4:A:890:HOH:O	1.04	1.20
2:A:606:CTI:H13B	2:A:606:CTI:H1	1.29	1.08
2:A:606:CTI:H13A	2:A:606:CTI:H1	1.34	1.04
2:A:606:CTI:C1	2:A:606:CTI:C13	2.37	1.00
1:A:196:CYS:HB3	4:A:1488:HOH:O	0.81	0.99
1:A:511[B]:MET:SD	1:A:544:ILE:CD1	2.52	0.98
1:A:511[B]:MET:SD	1:A:544:ILE:HD12	2.10	0.91
1:A:34:ASN:O	1:A:34:ASN:ND2	2.04	0.89
1:A:305:LYS:NZ	4:A:636:HOH:O	2.07	0.88
1:A:34:ASN:O	1:A:34:ASN:CG	2.15	0.80
1:A:79:ASN:OD1	1:A:89[B]:THR:HG22	1.81	0.79
1:A:57:TYR:OH	1:A:305:LYS:HE2	1.84	0.78
1:A:87[A]:VAL:CG2	1:A:103:TYR:CE1	2.67	0.78
2:A:606:CTI:H21A	2:A:606:CTI:H19B	1.68	0.75
2:A:606:CTI:H13B	2:A:606:CTI:C1	2.09	0.74
1:A:57:TYR:OH	1:A:305:LYS:CE	2.38	0.72
1:A:87[A]:VAL:HG21	1:A:103:TYR:CE1	2.26	0.71
2:A:606:CTI:H13A	2:A:606:CTI:C1	2.14	0.70
2:A:606:CTI:H21A	2:A:606:CTI:C19	2.20	0.70
1:A:557:ASN:ND2	4:A:841:HOH:O	2.27	0.67
1:A:87[A]:VAL:CG2	1:A:103:TYR:HE1	2.09	0.65
1:A:151:LYS:HE3	4:A:727:HOH:O	1.96	0.65
1:A:87[B]:VAL:HG13	4:A:1192:HOH:O	1.98	0.63
1:A:46:GLU:N	4:A:674:HOH:O	1.63	0.62
1:A:511[B]:MET:SD	1:A:544:ILE:HD13	2.38	0.62
1:A:596:ASN:H	1:A:596:ASN:HD22	1.48	0.61
1:A:511[B]:MET:CE	1:A:544:ILE:HD11	2.32	0.59
1:A:35:ASN:OD1	1:A:37:GLN:HG2	2.03	0.59
1:A:511[B]:MET:CE	1:A:544:ILE:CD1	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592[B]:VAL:HG12	1:A:593:THR:N	2.20	0.57
1:A:592[A]:VAL:HG23	4:A:881:HOH:O	2.04	0.56
1:A:570[B]:TRP:HZ2	4:A:1477:HOH:O	1.89	0.55
1:A:188:ILE:HD12	1:A:266:LEU:HD21	1.88	0.55
1:A:34:ASN:HB2	4:A:1435:HOH:O	2.06	0.55
1:A:341[A]:ARG:NH2	4:A:1321:HOH:O	2.42	0.52
1:A:34:ASN:ND2	1:A:37:GLN:O	2.43	0.51
1:A:595:PRO:HB2	4:A:1440:HOH:O	2.10	0.51
1:A:35:ASN:O	1:A:37:GLN:OE1	2.29	0.51
1:A:596:ASN:HD22	1:A:596:ASN:N	2.08	0.50
1:A:35:ASN:O	1:A:35:ASN:CG	2.51	0.48
1:A:35:ASN:ND2	4:A:1493:HOH:O	2.05	0.48
1:A:586:GLY:HA3	4:A:1253:HOH:O	2.13	0.48
1:A:592[B]:VAL:CG1	1:A:593:THR:N	2.76	0.48
2:A:606:CTI:O18	2:A:606:CTI:H21A	2.14	0.47
1:A:87[B]:VAL:HG11	1:A:103:TYR:CE1	2.50	0.47
1:A:407[A]:LEU:HA	1:A:437:ALA:HB3	1.98	0.46
1:A:341[A]:ARG:HD3	1:A:382:TYR:OH	2.16	0.45
1:A:592[B]:VAL:HG13	4:A:881:HOH:O	2.16	0.45
1:A:169:GLY:HA3	4:A:1094:HOH:O	2.16	0.45
1:A:194:PRO:HD2	1:A:226:VAL:O	2.16	0.45
1:A:511[B]:MET:HE1	1:A:544:ILE:HD11	2.00	0.44
1:A:494:GLN:HA	1:A:510:PHE:CE2	2.53	0.43
1:A:414:ARG:NH1	4:A:1087:HOH:O	2.19	0.43
1:A:73[B]:THR:HA	4:A:1267:HOH:O	2.18	0.43
1:A:341[B]:ARG:HB2	1:A:382:TYR:CZ	2.54	0.43
1:A:34:ASN:CA	4:A:1435:HOH:O	2.66	0.43
1:A:410:GLY:HA2	1:A:530:ALA:HB2	2.01	0.43
1:A:311:ASP:OD2	1:A:313:ASP:OD1	2.37	0.42
1:A:49[B]:SER:HB2	1:A:218:ARG:NH1	2.34	0.42
1:A:45:MET:CA	4:A:674:HOH:O	2.65	0.42
1:A:87[B]:VAL:HG11	1:A:103:TYR:CD1	2.55	0.41
1:A:140:LYS:HD2	1:A:140:LYS:HA	1.77	0.41
1:A:341[B]:ARG:HB2	1:A:382:TYR:CE1	2.56	0.41
1:A:78:TYR:HA	1:A:114:GLU:O	2.21	0.41
1:A:570[B]:TRP:NE1	4:A:1154:HOH:O	2.30	0.41
2:A:606:CTI:H21	4:A:614:HOH:O	2.21	0.41
1:A:260:LYS:HB3	1:A:260:LYS:HE2	1.83	0.41
1:A:231:TRP:HA	1:A:235:GLN:HB2	2.02	0.41
1:A:549:HIS:CE1	1:A:553:LEU:HD11	2.55	0.40
1:A:194:PRO:HB3	1:A:277:LEU:HD22	2.02	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	601/584 (103%)	583 (97%)	17 (3%)	1 (0%)	47 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ASN

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	488/469 (104%)	480 (98%)	8 (2%)	62 36

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

Mol	Chain	Res	Type
1	A	35	ASN
1	A	62	LYS
1	A	64	LYS
1	A	95	SER
1	A	329[A]	PRO
1	A	329[B]	PRO
1	A	450	PRO
1	A	596	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	37	GLN
1	A	52	ASN
1	A	447	GLN
1	A	557	ASN
1	A	596	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
3	GOL	A	3501	-	5,5,5	0.40	0	5,5,5	0.77	0
3	GOL	A	3500[B]	-	5,5,5	0.52	0	5,5,5	1.26	0
3	GOL	A	3500[A]	-	5,5,5	0.72	0	5,5,5	1.21	0
2	CTI	A	606	-	28,30,30	1.29	4 (14%)	41,45,45	2.33	13 (31%)

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	GOL	A	3501	-	-	0/4/4/4	-
3	GOL	A	3500[B]	-	-	0/4/4/4	-
3	GOL	A	3500[A]	-	-	0/4/4/4	-
2	CTI	A	606	-	-	2/4/10/10	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	606	CTI	C8-C7	2.62	1.42	1.35
2	A	606	CTI	O24-C25	2.28	1.47	1.43
2	A	606	CTI	C2-C3	-2.11	1.38	1.42
2	A	606	CTI	C16-C15	2.03	1.40	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	606	CTI	C12-C11-C17	-6.26	117.13	121.62
2	A	606	CTI	O26-C23-C4	5.64	132.62	128.11
2	A	606	CTI	O24-C22-C1	5.36	132.40	128.11
2	A	606	CTI	C19-O18-C17	5.23	128.36	114.88
2	A	606	CTI	C12-N9-C5	-3.13	118.81	121.69
2	A	606	CTI	C1-C22-C23	-2.92	118.06	121.78
2	A	606	CTI	C21-O20-C14	-2.89	113.17	117.53
2	A	606	CTI	O26-C25-O24	-2.88	103.48	108.08
2	A	606	CTI	C15-C14-C17	2.76	121.71	119.76
2	A	606	CTI	O18-C17-C11	2.62	122.48	117.27
2	A	606	CTI	C1-C2-C5	-2.43	119.68	124.00
2	A	606	CTI	C4-C23-C22	-2.23	118.93	121.78
2	A	606	CTI	O20-C14-C15	-2.07	120.82	124.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

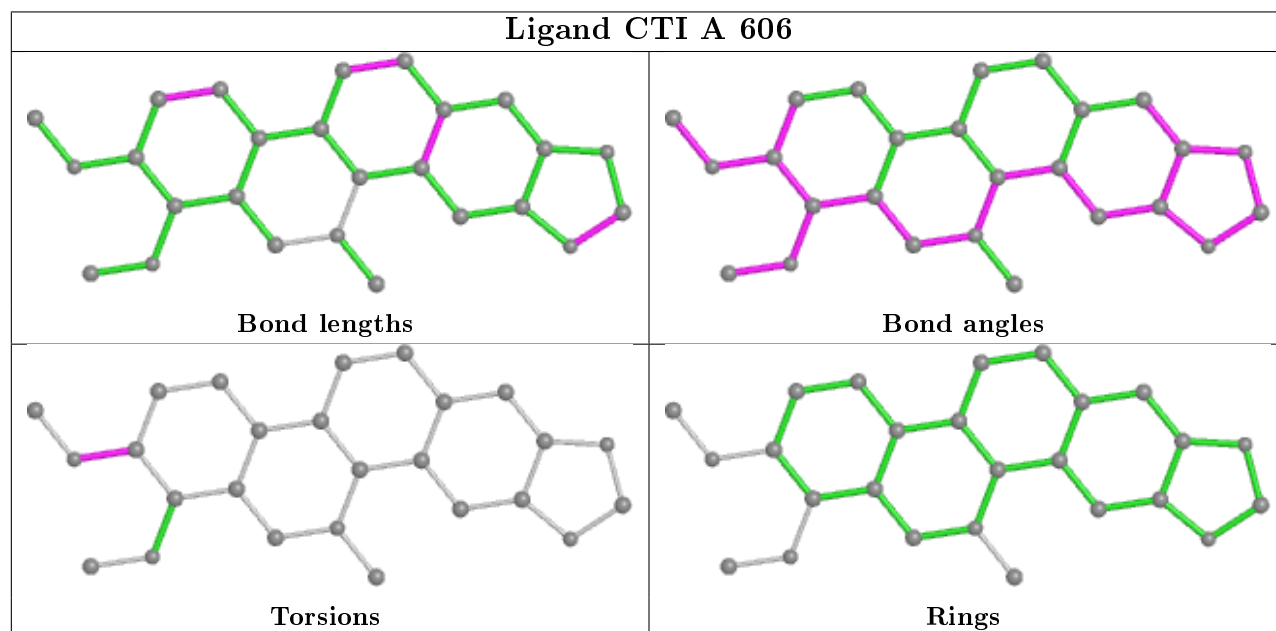
Mol	Chain	Res	Type	Atoms
2	A	606	CTI	C15-C14-O20-C21
2	A	606	CTI	C17-C14-O20-C21

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	606	CTI	10	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	575/584 (98%)	-0.31	7 (1%) 79 82	6, 12, 28, 59	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	TRP	3.2
1	A	596	ASN	2.7
1	A	71	SER	2.7
1	A	72	GLY	2.5
1	A	93	THR	2.4
1	A	426	ASN	2.4
1	A	34	ASN	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

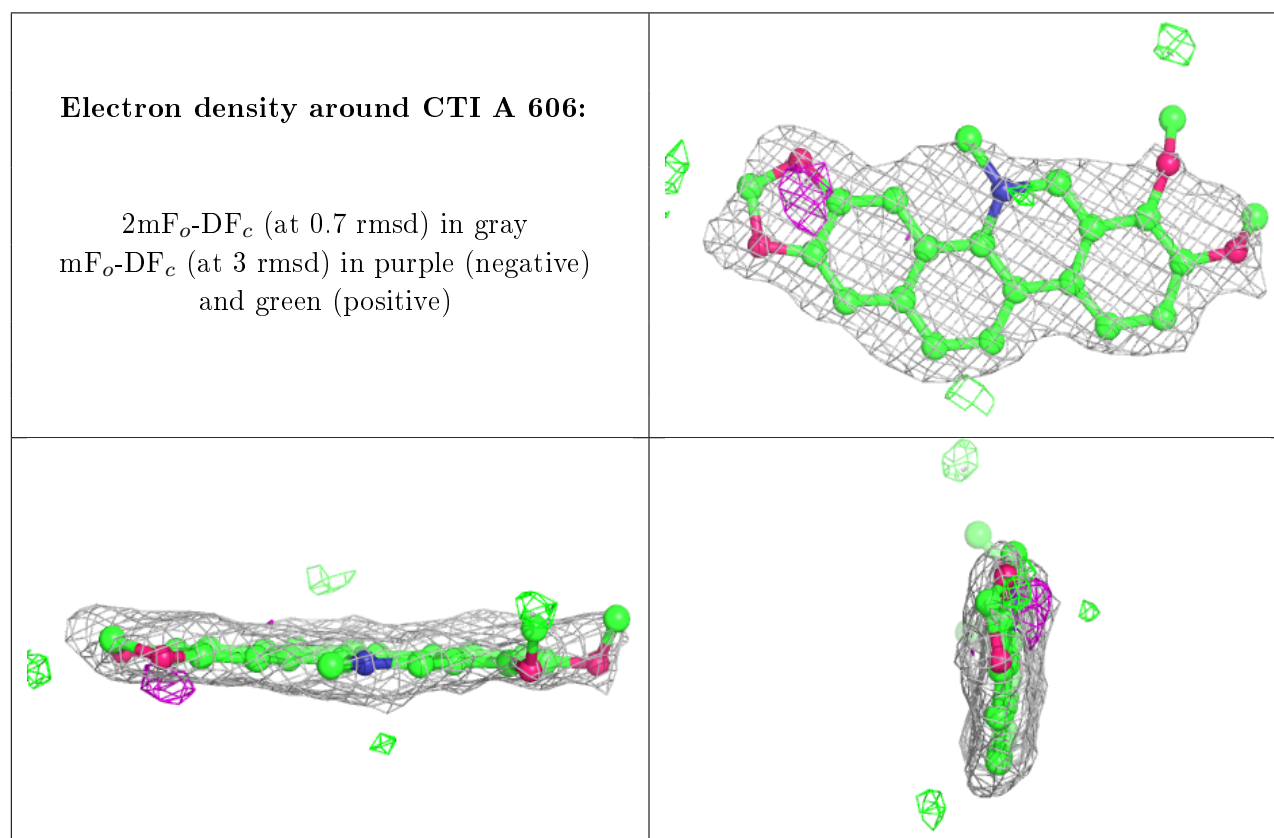
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CTI	A	606	26/26	0.88	0.14	26,37,56,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	3501	6/6	0.93	0.10	19,22,25,27	0
3	GOL	A	3500[A]	6/6	0.97	0.09	8,10,10,13	6
3	GOL	A	3500[B]	6/6	0.97	0.09	9,12,15,18	6

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.



6.5 Other polymers [i](#)

There are no such residues in this entry.