

wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 07:39 PM EDT

PDB ID : 2O3S

Title : Structural Basis for Formation and Hydrolysis of Calcium Messenger Cyclic

ADP-ribose by Human CD38

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Deposited on : 2006-12-01

Resolution : 1.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.orgA user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) 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 : 2.35

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

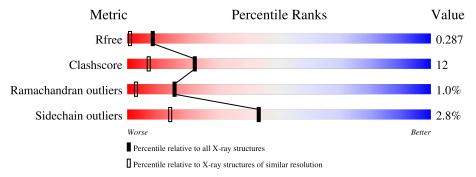
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
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)

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 <=5%

Mol	Chain	Length	Quality of chain		
1	A	262	79%	15%	•
1	В	262	76%	19%	

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	CXR	A	301	X	-	-	-
2	CXR	В	301	X	-	-	-



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4808 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 ADP-ribosyl cyclase 1.

\mathbf{Mol}	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
1	A	252	Total 2038	C 1286	N 352	O 384	S 16	0	0	0
1	В	252	Total 2038	C 1286	N 352	O 384	S 16	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	cloning artifact	UNP P28907
A	40	ARG	_	cloning artifact	UNP P28907
A	41	GLU	-	cloning artifact	UNP P28907
A	42	ALA	-	cloning artifact	UNP P28907
A	43	GLU	-	cloning artifact	UNP P28907
A	44	ALA	-	cloning artifact	UNP P28907
A	45	PHE	ARG	engineered mutation	UNP P28907
A	49	THR	GLN	engineered mutation	UNP P28907
A	100	ASP	ASN	engineered mutation	UNP P28907
A	164	ASP	ASN	engineered mutation	UNP P28907
A	209	ASP	ASN	engineered mutation	UNP P28907
A	219	ASP	ASN	engineered mutation	UNP P28907
A	226	GLY	GLU	engineered mutation	UNP P28907
В	39	LYS	_	cloning artifact	UNP P28907
В	40	ARG	-	cloning artifact	UNP P28907
В	41	GLU	_	cloning artifact	UNP P28907
В	42	ALA	-	cloning artifact	UNP P28907
В	43	GLU	-	cloning artifact	UNP P28907
В	44	ALA	_	cloning artifact	UNP P28907
В	45	PHE	ARG	engineered mutation	UNP P28907
В	49	THR	GLN	engineered mutation	UNP P28907
В	100	ASP	ASN	engineered mutation	UNP P28907
В	164	ASP	ASN	engineered mutation	UNP P28907
В	209	ASP	ASN	engineered mutation	UNP P28907
В	219	ASP	ASN	engineered mutation	UNP P28907

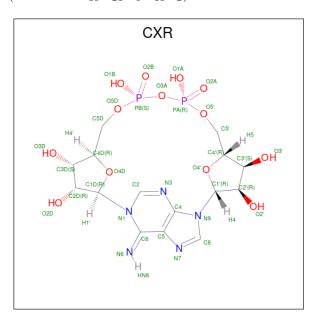
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Chain	Residue	Modelled	Actual	Comment	Reference
В	226	GLY	GLU	engineered mutation	UNP P28907

 \bullet Molecule 2 is CYCLIC ADENOSINE DIPHOSPHATE-RIBOSE (three-letter code: CXR) (formula: $C_{15}H_{21}N_5O_{13}P_2).$



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
9	٨	1	Total	С	N	О	Р	0	0
2	A	1	35	15	5	13	2	0	0
9	D	1	Total	С	N	О	Р	0	0
2	Б	1	35	15	5	13	2	U	U

• Molecule 3 is water.

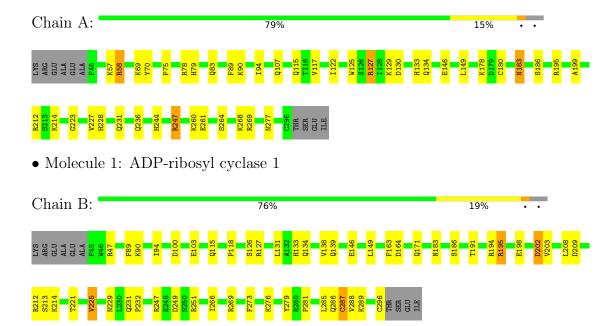
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	386	Total O 386 386	0	0
3	В	276	Total O 276 276	0	0



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. 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. 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: ADP-ribosyl cyclase 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	42.35Å 53.79Å 66.83Å	Donositor
a, b, c, α , β , γ	104.97° 91.71° 95.04°	Depositor
Resolution (Å)	20.00 - 1.50	Depositor
Resolution (A)	36.18 - 1.50	EDS
% Data completeness	86.7 (20.00-1.50)	Depositor
(in resolution range)	86.7 (36.18-1.50)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.16 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.3.0017	Depositor
D D.	0.189 , 0.238	Depositor
R, R_{free}	0.254 , 0.287	DCC
R_{free} test set	3852 reflections $(4.94%)$	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 63.1	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4808	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.41% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: CXR

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				nd angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	1.00	$1/2090 \ (0.0\%)$	0.83	1/2832 (0.0%)
1	В	0.89	$2/2090 \ (0.1\%)$	0.72	0/2832
All	All	0.95	3/4180 (0.1%)	0.78	1/5664 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	В	287	CYS	CB-SG	9.46	1.98	1.82
1	В	202	ASP	C-N	5.41	1.46	1.34
1	A	70	TYR	CD1-CE1	5.30	1.47	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	269	ARG	NE-CZ-NH2	-7.87	116.36	120.30

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	2038	0	1957	47	0
1	В	2038	0	1959	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	35	0	18	0	0
2	В	35	0	19	3	0
3	A	386	0	0	22	0
3	В	276	0	0	8	0
All	All	4808	0	3953	94	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 12.

The worst 5 of 94 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.03	1.18
1:B:195:ARG:HH11	1:B:195:ARG:HG2	0.95	1.11
1:A:268:LYS:HD3	1:B:163:PHE:HE1	1.12	1.05
1:A:268:LYS:HD3	1:B:163:PHE:CE1	1.91	1.05
1:B:195:ARG:HG2	1:B:195:ARG:NH1	1.74	0.93

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	lysed Favoured Allowed		Outliers	Percentiles		
1	A	$250/262 \ (95\%)$	237 (95%)	12 (5%)	1 (0%)	34 13		
1	В	$250/262 \ (95\%)$	229 (92%)	17 (7%)	4 (2%)	9 1		
All	All	500/524 (95%)	466 (93%)	29 (6%)	5 (1%)	15 3		

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	247	ARG
1	В	225	VAL
1	В	213	SER
1	В	247	ARG
1	В	249	ASP

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	231/240 (96%)	224 (97%)	7 (3%)	41	12	
1	В	231/240 (96%)	225 (97%)	6 (3%)	46	16	
All	All	462/480 (96%)	449 (97%)	13 (3%)	43	14	

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	89	PHE
1	В	127	ARG
1	В	276	LYS
1	В	195	ARG
1	В	251	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	183	ASN
1	В	171	GLN
1	В	48	GLN
1	В	139	GLN
1	A	244	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	Trme	Chain	Res	Link	Bond lengths			Bond angles		
IVIOI	Туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CXR	В	301	-	31,39,39	2.63	10 (32%)	37,62,62	1.54	5 (13%)
2	CXR	A	301	-	31,39,39	2.08	10 (32%)	37,62,62	1.42	7 (18%)

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	ype Chain Res		Cype Chain Res Link Chirals		Chirals	Torsions	Rings	
2	CXR	В	301	-	1/1/10/10	7/22/58/58	0/3/5/5		
2	CXR	A	301	-	1/1/10/10	2/22/58/58	0/3/5/5		

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(\mathring{A})$	Ideal(Å)
2	В	301	CXR	O4'-C1'	6.92	1.50	1.41
2	В	301	CXR	C2-N3	6.38	1.36	1.29
2	A	301	CXR	C2-N3	6.07	1.36	1.29
2	В	301	CXR	C2-N1	6.00	1.50	1.36
2	В	301	CXR	C6-N6	5.46	1.41	1.27



The worst	5	of	12	bond	angle	outliers	are	listed	below:
TITO HOLDO	$\overline{}$	O.		OIIG	WII SIC	Cathere	COL C	IID CCL	CIC III.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	301	CXR	C3'-C2'-C1'	4.03	107.04	100.98
2	В	301	CXR	N1-C6-N6	3.78	125.68	119.21
2	В	301	CXR	PA-O3A-PB	-3.62	120.41	132.83
2	A	301	CXR	O3'-C3'-C4'	2.93	119.52	111.05
2	A	301	CXR	O2'-C2'-C3'	-2.85	102.60	111.82

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	CXR	C3'
2	В	301	CXR	C3'

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	301	CXR	C5D-O5D-PB-O2B
2	В	301	CXR	C5D-O5D-PB-O1B
2	В	301	CXR	C3D-C4D-C5D-O5D
2	В	301	CXR	O4D-C4D-C5D-O5D
2	A	301	CXR	C3'-C4'-C5'-O5'

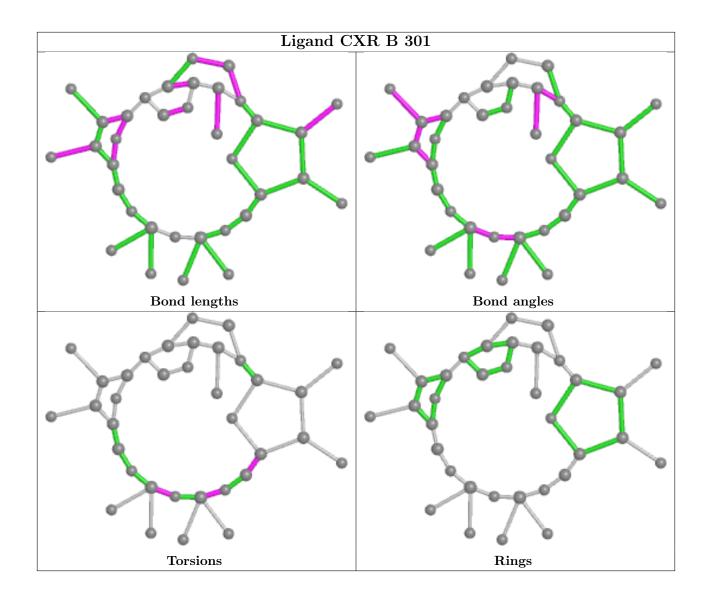
There are no ring outliers.

1 monomer is involved in 3 short contacts:

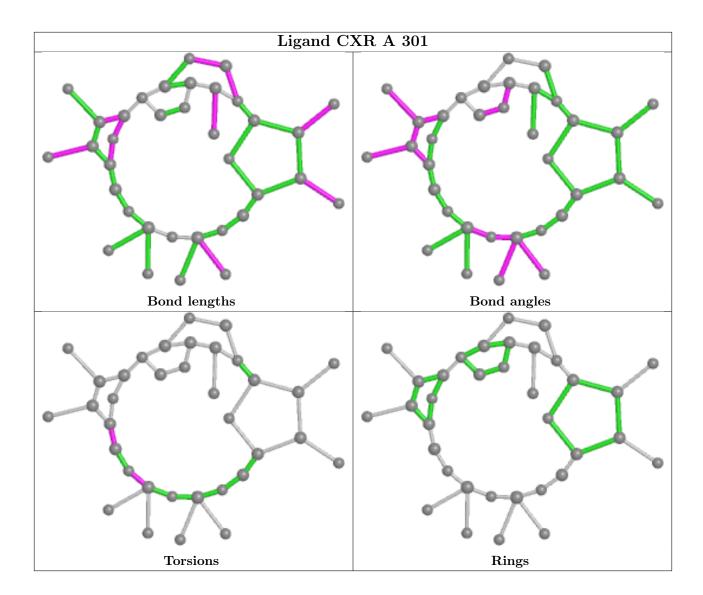
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	301	CXR	3	0

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 then 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

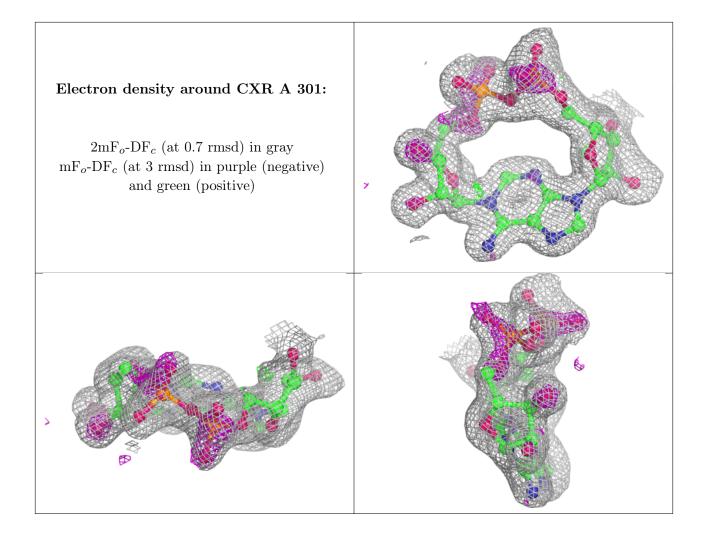
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6.4 Ligands (i)

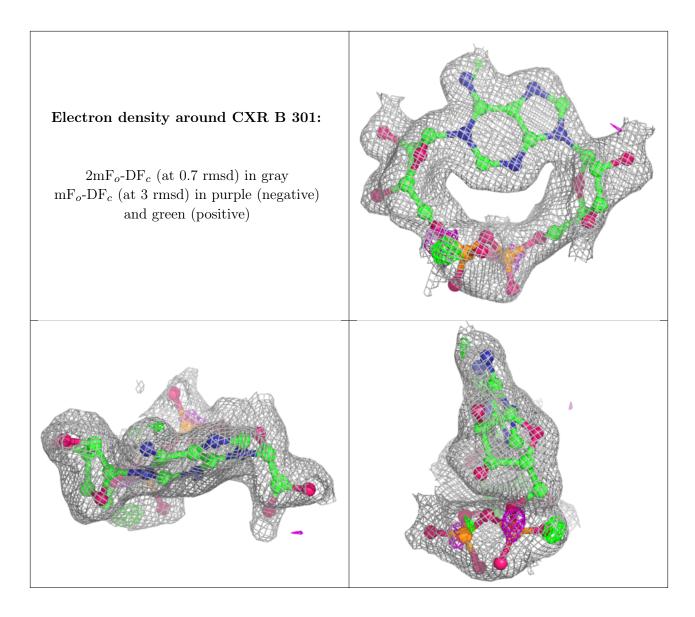
Unable to reproduce the depositors R factor - this section is therefore empty.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

