



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2021 – 12:10 PM JST

PDB ID : 6K9W
Title : Crystal Structures of Endo-beta-1,4-xylanase II Complexed with Xylotriose
Authors : Li, C.; Wan, Q.
Deposited on : 2019-06-18
Resolution : 1.10 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
Xtriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

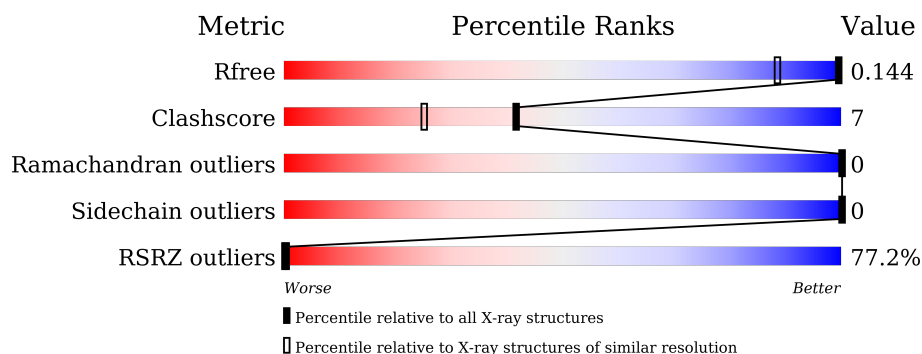
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.10 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	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

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	189	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3387 atoms, of which 1478 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 Endo-1,4-beta-xylanase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	189	Total	C	H	N	O	S	0	35	0
			3067	996	1478	271	321	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ASP	ASN	conflict	UNP P36217
A	177	GLN	GLU	conflict	UNP P36217

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	I	0	0
			3	3		

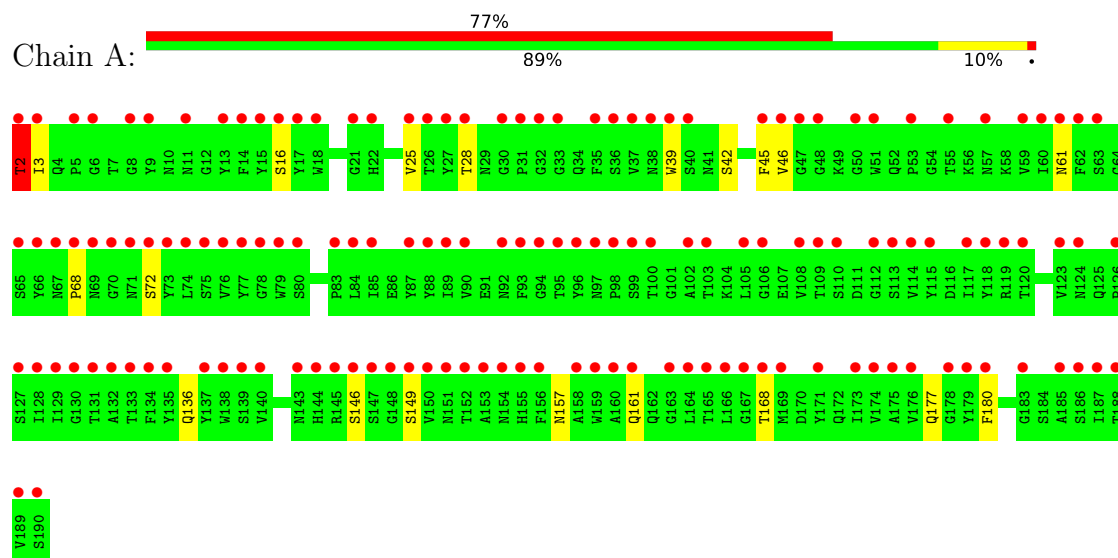
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	317	Total	O	0	0
			317	317		

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: Endo-1,4-beta-xylanase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.19Å 59.53Å 69.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.12 – 1.10 30.12 – 1.02	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.12-1.10) 99.1 (30.12-1.02)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 1.02Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.136 , 0.144 0.135 , 0.144	Depositor DCC
R_{free} test set	5127 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	8.4	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3387	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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: IOD

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	0.71	5/1780 (0.3%)	0.96	3/2428 (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	2	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	ILE	CA-CB	-11.55	1.28	1.54
1	A	2	THR	N-CA	-8.65	1.29	1.46
1	A	146[A]	SER	CB-OG	6.59	1.50	1.42
1	A	146[B]	SER	CB-OG	6.59	1.50	1.42
1	A	2	THR	CA-C	6.03	1.68	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	THR	CA-CB-CG2	-18.06	87.12	112.40
1	A	2	THR	OG1-CB-CG2	-15.50	74.35	110.00
1	A	3	ILE	CA-CB-CG1	7.02	124.34	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2	THR	CB,CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	THR	Mainchain

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	1589	1478	1331	21	0
2	A	3	0	0	0	0
3	A	317	0	0	5	2
All	All	1909	1478	1331	21	2

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 7.

All (21) 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:A:2:THR:N	3:A:303:HOH:O	1.66	1.25
1:A:2:THR:HG21	3:A:307:HOH:O	1.60	1.01
1:A:2:THR:HG22	1:A:28[B]:THR:HG22	1.43	0.98
1:A:2:THR:HG22	1:A:28[B]:THR:CG2	2.03	0.88
1:A:2:THR:CG2	1:A:28[B]:THR:HG22	2.11	0.80
1:A:61:ASN:OD1	1:A:149[B]:SER:OG	2.03	0.77
1:A:25[B]:VAL:CG2	1:A:42:SER:HB2	2.19	0.73
1:A:68:PRO:HB3	1:A:72[B]:SER:OG	2.03	0.59
1:A:46[A]:VAL:HG23	3:A:379:HOH:O	2.06	0.55
1:A:25[B]:VAL:CG2	1:A:42:SER:CB	2.87	0.52
1:A:25[B]:VAL:HG21	1:A:45:PHE:CD2	2.45	0.52
1:A:25[B]:VAL:HG23	1:A:42:SER:HB2	1.91	0.51
1:A:46[B]:VAL:HG13	3:A:316:HOH:O	2.11	0.50
1:A:42:SER:O	1:A:180:PHE:HA	2.11	0.49
1:A:168[C]:THR:HG23	3:A:449:HOH:O	2.15	0.46
1:A:25[B]:VAL:HG22	1:A:39:TRP:HB2	2.00	0.42
1:A:46[A]:VAL:HG22	1:A:177:GLN:HG3	2.00	0.42
1:A:157:ASN:O	1:A:161[B]:GLN:HG3	2.20	0.42
1:A:2:THR:HG22	1:A:28[A]:THR:OG1	2.19	0.41

All (2) 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)
3:A:570:HOH:O	3:A:577:HOH:O[3_644]	1.81	0.39
3:A:462:HOH:O	3:A:590:HOH:O[3_554]	2.08	0.12

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	222/189 (118%)	218 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	187/155 (121%)	187 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	189/189 (100%)	2.78	146 (77%) 0 0	6, 9, 16, 23	2 (1%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	8.9
1	A	9	TYR	6.0
1	A	165[A]	THR	4.9
1	A	76[A]	VAL	4.8
1	A	159	TRP	4.8
1	A	15	TYR	4.7
1	A	89	ILE	4.6
1	A	138	TRP	4.6
1	A	117	ILE	4.6
1	A	46[A]	VAL	4.5
1	A	18	TRP	4.5
1	A	173	ILE	4.4
1	A	74	LEU	4.4
1	A	85[A]	ILE	4.4
1	A	90	VAL	4.2
1	A	17[A]	TYR	4.2
1	A	115	TYR	4.2
1	A	28[A]	THR	4.1
1	A	3	ILE	4.1
1	A	174	VAL	4.0
1	A	93	PHE	3.9
1	A	73[A]	TYR	3.9
1	A	87	TYR	3.9
1	A	175	ALA	3.8
1	A	79	TRP	3.8
1	A	123	VAL	3.8
1	A	84	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	77	TYR	3.7
1	A	108	VAL	3.7
1	A	135	TYR	3.7
1	A	187[A]	ILE	3.7
1	A	39	TRP	3.6
1	A	164	LEU	3.6
1	A	62	PHE	3.6
1	A	143[A]	ASN	3.6
1	A	158	ALA	3.6
1	A	88	TYR	3.6
1	A	114	VAL	3.5
1	A	176	VAL	3.5
1	A	134	PHE	3.5
1	A	45	PHE	3.5
1	A	137	TYR	3.4
1	A	167	GLY	3.4
1	A	37[A]	VAL	3.4
1	A	105[A]	LEU	3.4
1	A	166[A]	LEU	3.4
1	A	102	ALA	3.4
1	A	140	VAL	3.3
1	A	156	PHE	3.3
1	A	33	GLY	3.3
1	A	25[A]	VAL	3.3
1	A	51	TRP	3.3
1	A	27	TYR	3.2
1	A	5	PRO	3.2
1	A	53	PRO	3.2
1	A	22	HIS	3.2
1	A	35	PHE	3.2
1	A	189	VAL	3.2
1	A	31	PRO	3.1
1	A	66[A]	TYR	3.1
1	A	179	TYR	3.1
1	A	126	PRO	3.1
1	A	14	PHE	3.1
1	A	40	SER	3.1
1	A	78	GLY	3.1
1	A	100	THR	3.1
1	A	118	TYR	3.0
1	A	171	TYR	3.0
1	A	60	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	160	ALA	3.0
1	A	98	PRO	3.0
1	A	6	GLY	3.0
1	A	119	ARG	2.9
1	A	11	ASN	2.9
1	A	180	PHE	2.9
1	A	109	THR	2.9
1	A	132	ALA	2.9
1	A	50	GLY	2.9
1	A	38	ASN	2.9
1	A	150[A]	VAL	2.8
1	A	47[A]	GLY	2.8
1	A	106[A]	GLY	2.8
1	A	185	ALA	2.8
1	A	183	GLY	2.8
1	A	48	GLY	2.8
1	A	94	GLY	2.8
1	A	55	THR	2.7
1	A	131	THR	2.7
1	A	103	THR	2.7
1	A	128	ILE	2.7
1	A	129	ILE	2.7
1	A	75[A]	SER	2.7
1	A	72[A]	SER	2.6
1	A	95	THR	2.6
1	A	152	THR	2.6
1	A	96	TYR	2.6
1	A	8	GLY	2.6
1	A	59	VAL	2.6
1	A	83	PRO	2.6
1	A	161[A]	GLN	2.5
1	A	190	SER	2.5
1	A	32	GLY	2.5
1	A	112	GLY	2.5
1	A	113	SER	2.5
1	A	26[A]	THR	2.5
1	A	120	THR	2.5
1	A	97	ASN	2.5
1	A	36[A]	SER	2.5
1	A	133	THR	2.5
1	A	168[B]	THR	2.5
1	A	188	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	21	GLY	2.5
1	A	130	GLY	2.5
1	A	127	SER	2.5
1	A	169[B]	MET	2.4
1	A	178	GLY	2.4
1	A	139	SER	2.4
1	A	151	ASN	2.4
1	A	16[A]	SER	2.4
1	A	147	SER	2.4
1	A	63[A]	SER	2.4
1	A	153	ALA	2.3
1	A	148	GLY	2.3
1	A	71	ASN	2.3
1	A	155	HIS	2.3
1	A	80	SER	2.2
1	A	149[A]	SER	2.2
1	A	13	TYR	2.2
1	A	146[A]	SER	2.2
1	A	67	ASN	2.2
1	A	92	ASN	2.2
1	A	145	ARG	2.2
1	A	65[A]	SER	2.2
1	A	99	SER	2.2
1	A	144[A]	HIS	2.1
1	A	69	ASN	2.1
1	A	70	GLY	2.1
1	A	124	ASN	2.1
1	A	110	SER	2.1
1	A	61	ASN	2.1
1	A	186[A]	SER	2.1
1	A	30	GLY	2.1
1	A	163	GLY	2.1
1	A	68	PRO	2.1
1	A	57	ASN	2.0
1	A	154	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

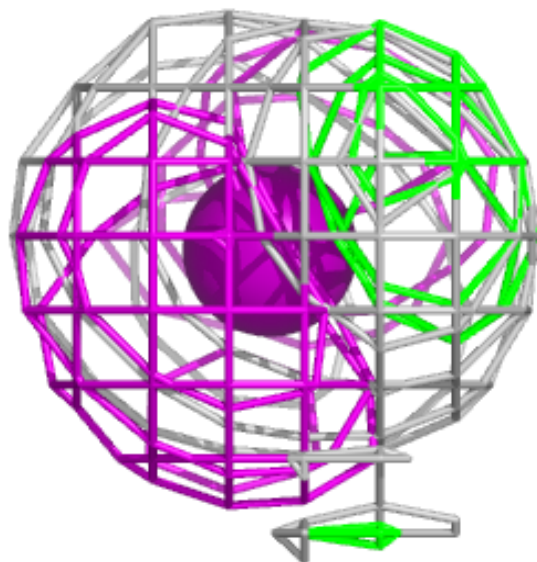
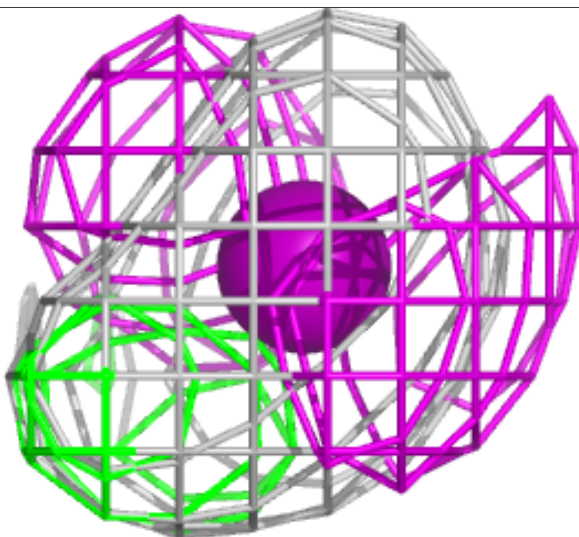
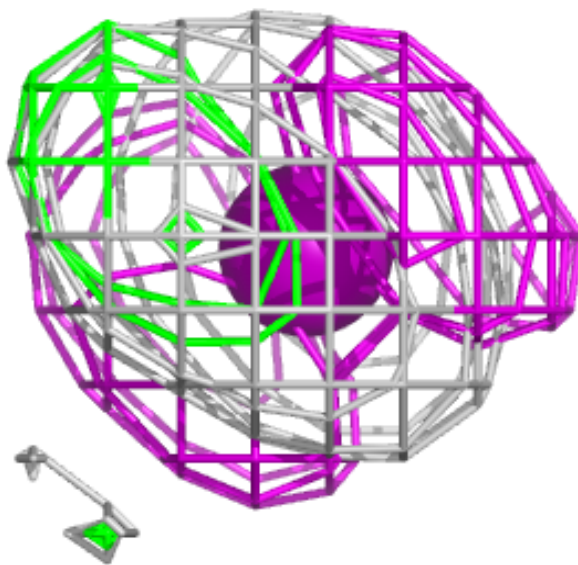
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IOD	A	203	1/1	0.93	0.16	16,16,16,16	1
2	IOD	A	202	1/1	0.96	0.25	22,22,22,22	0
2	IOD	A	201	1/1	1.00	0.16	7,7,7,7	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.

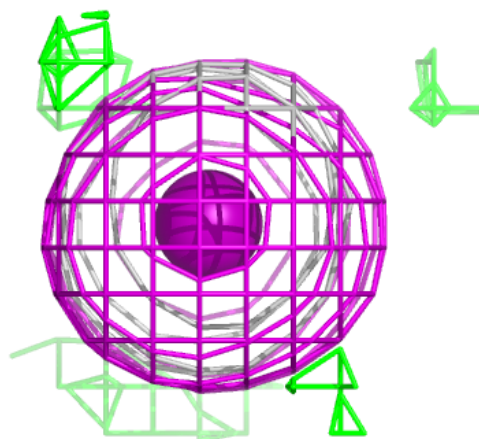
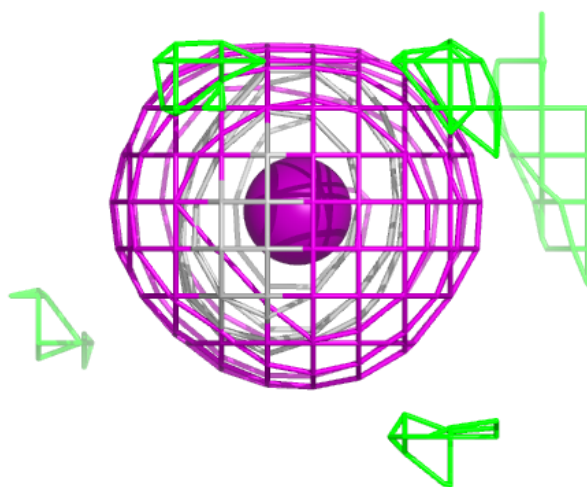
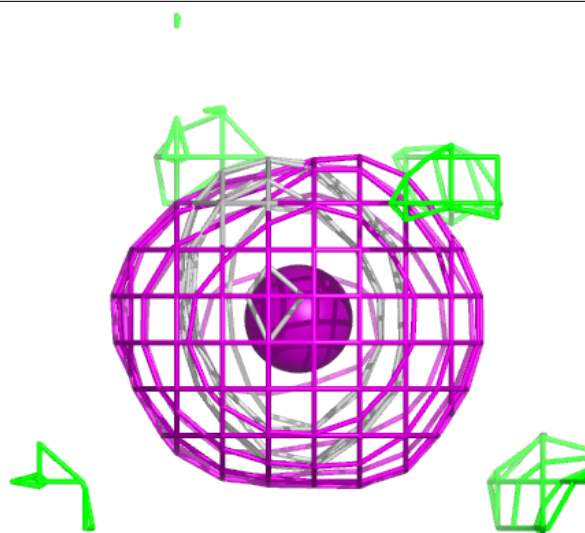
Electron density around IOD A 203:

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



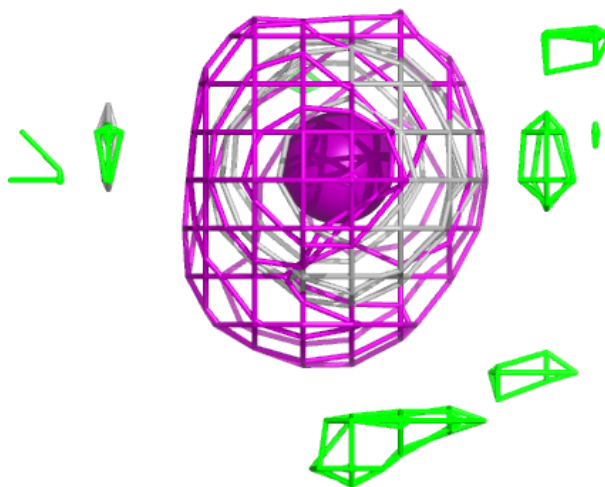
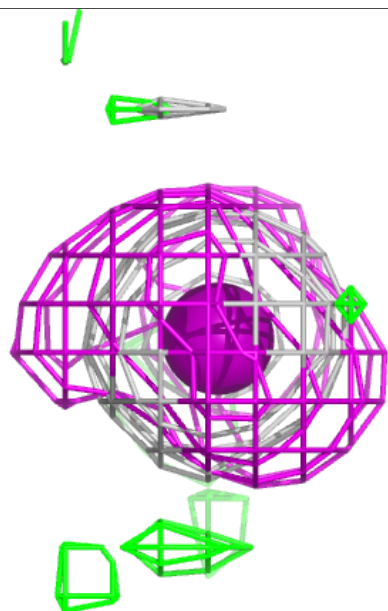
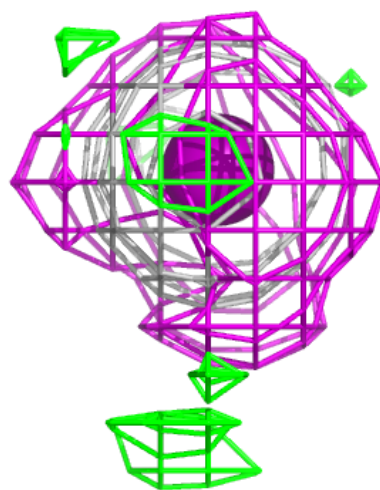
Electron density around IOD A 202:

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



Electron density around IOD A 201:

$2mF_o-DF_c$ (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.