



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:11 PM UTC

PDB ID : 5MZA / pdb_00005mza
Title : The DBLb domain of PF11_0521 PfEMP1 bound to human ICAM-1
Authors : Lennartz, F.; Higgins, M.K.
Deposited on : 2017-01-31
Resolution : 2.78 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

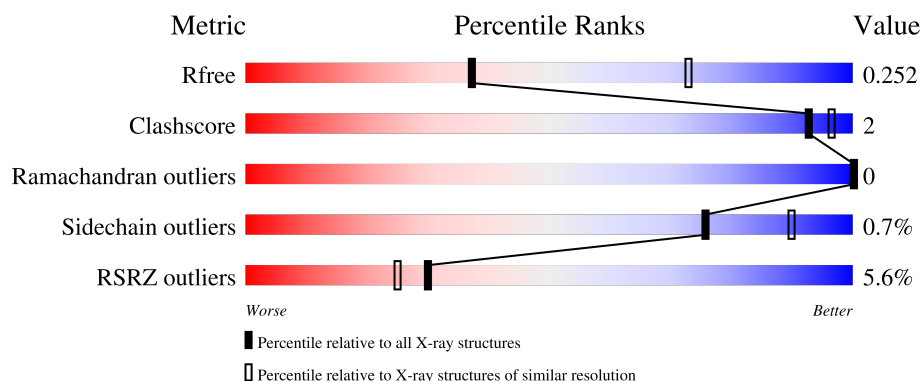
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	488	5% 85% 5% 10%
2	B	186	5% 95% 5%
3	C	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5092 atoms, of which 6 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 Erythrocyte membrane protein 1 (PfEMP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3534	2210	634	670	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	727	SER	-	expression tag	UNP Q8IHM0

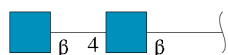
- Molecule 2 is a protein called Intercellular adhesion molecule 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	186	Total	C	N	O	S	0	0	0
			1436	900	252	277	7			

There is a discrepancy between the modelled and reference sequences:

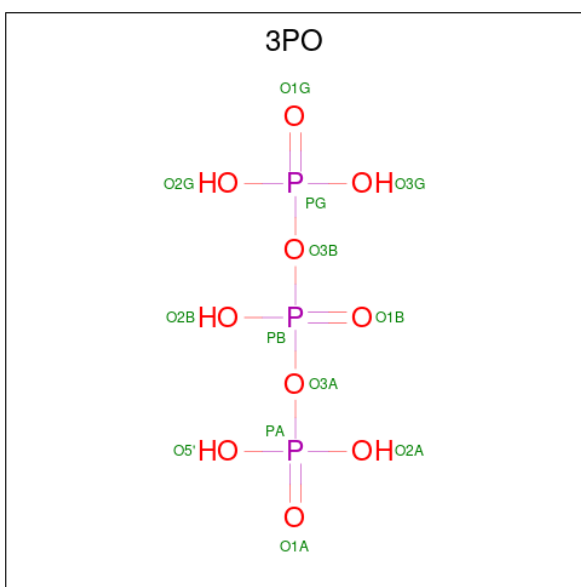
Chain	Residue	Modelled	Actual	Comment	Reference
B	186	GLY	-	expression tag	UNP P05362

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is TRIPHOSPHATE (CCD ID: 3PO) (formula: H₅O₁₀P₃).



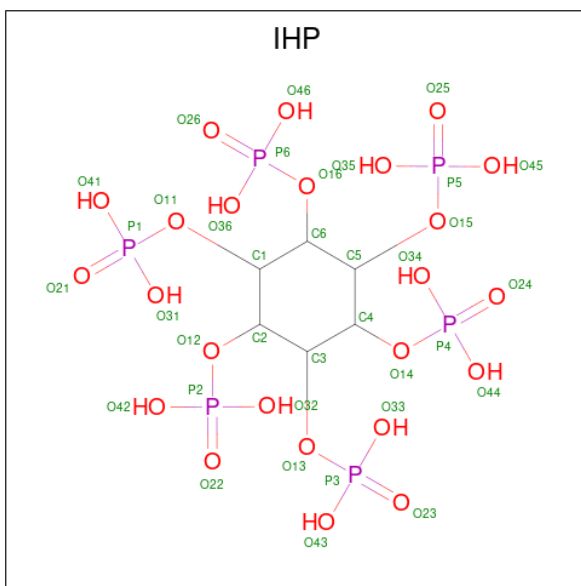
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			13	10	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).

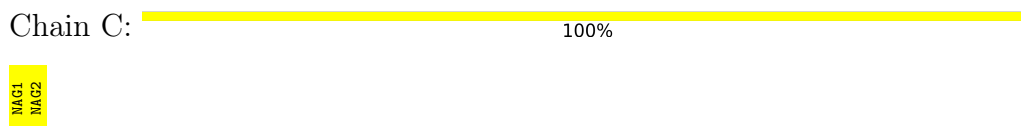
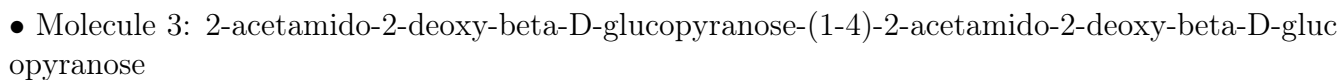


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	O	P	0	0
			42	6	6	24	6		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	7	Total O	0	0
			7 7		
7	B	4	Total O	0	0
			4 4		

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.64Å 109.83Å 112.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.19 – 2.78 30.19 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.19-2.78) 99.6 (30.19-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.76Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.205 , 0.236 0.214 , 0.252	Depositor DCC
R_{free} test set	1103 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5092	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: IHP, 3PO, NAG

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	0/3616	1.34	1/4873 (0.0%)
2	B	0.66	0/1466	1.03	1/1998 (0.1%)
All	All	0.70	0/5082	1.26	2/6871 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1203	ASP	CA-CB-CG	5.19	117.79	112.60
2	B	14	GLY	N-CA-C	-5.08	108.31	115.32

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	3534	0	3399	12	0
2	B	1436	0	1441	4	0
3	C	28	0	25	0	0
4	A	13	0	0	0	0
5	B	28	0	26	1	0
6	B	36	6	6	0	0
7	A	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	4	0	0	0	0
All	All	5086	6	4897	15	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 2.

All (15) 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:1114:LYS:HG2	1:A:1115:GLY:H	1.68	0.58
2:B:121:VAL:HG12	2:B:161:THR:HG22	1.88	0.56
1:A:736:LYS:HE3	1:A:1111:GLY:HA3	1.98	0.46
1:A:997:PRO:HD2	1:A:1000:LEU:HD12	1.97	0.46
2:B:122:VAL:HG22	2:B:132:ARG:HG3	1.98	0.46
1:A:750:ARG:HA	1:A:753:TYR:CE2	2.51	0.45
1:A:1078:ILE:HD11	2:B:53:GLU:HG3	1.99	0.44
1:A:809:ASP:HB2	1:A:841:HIS:HB3	2.01	0.43
1:A:1123:VAL:HG12	5:B:203:NAG:H83	2.00	0.43
1:A:728:ASN:ND2	1:A:1168:GLN:HG2	2.33	0.42
1:A:1114:LYS:CG	1:A:1115:GLY:H	2.32	0.42
1:A:839:ARG:HG2	1:A:1002:TRP:CZ2	2.56	0.41
1:A:998:GLN:HG3	1:A:1001:ARG:NH2	2.36	0.41
2:B:38:PRO:HD2	2:B:55:SER:O	2.21	0.40
1:A:787:LEU:O	1:A:790:ILE:HG12	2.20	0.40

There are no symmetry-related clashes.

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	432/488 (88%)	414 (96%)	18 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	184/186 (99%)	182 (99%)	2 (1%)	0	100	100
All	All	616/674 (91%)	596 (97%)	20 (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	A	374/414 (90%)	372 (100%)	2 (0%)	81	92
2	B	165/165 (100%)	163 (99%)	2 (1%)	63	84
All	All	539/579 (93%)	535 (99%)	4 (1%)	76	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	866	ILE
1	A	1090	THR
2	B	82	VAL
2	B	172	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	728	ASN
1	A	757	ASN
1	A	771	GLN
1	A	803	ASN
1	A	856	GLN
1	A	860	ASN
1	A	1105	ASN
1	A	1109	GLN
1	A	1206	HIS

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Mol	Chain	Res	Type
1	A	1208	HIS
2	B	58	GLN
2	B	168	GLN

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 ⓘ

2 monosaccharides 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	NAG	C	1	3,2	14,14,15	0.30	0	17,19,21	0.73	1 (5%)
3	NAG	C	2	3	14,14,15	0.32	0	17,19,21	0.74	1 (5%)

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	C	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-O5-C5	2.65	115.74	112.19
3	C	1	NAG	C1-O5-C5	2.59	115.66	112.19

There are no chirality outliers.

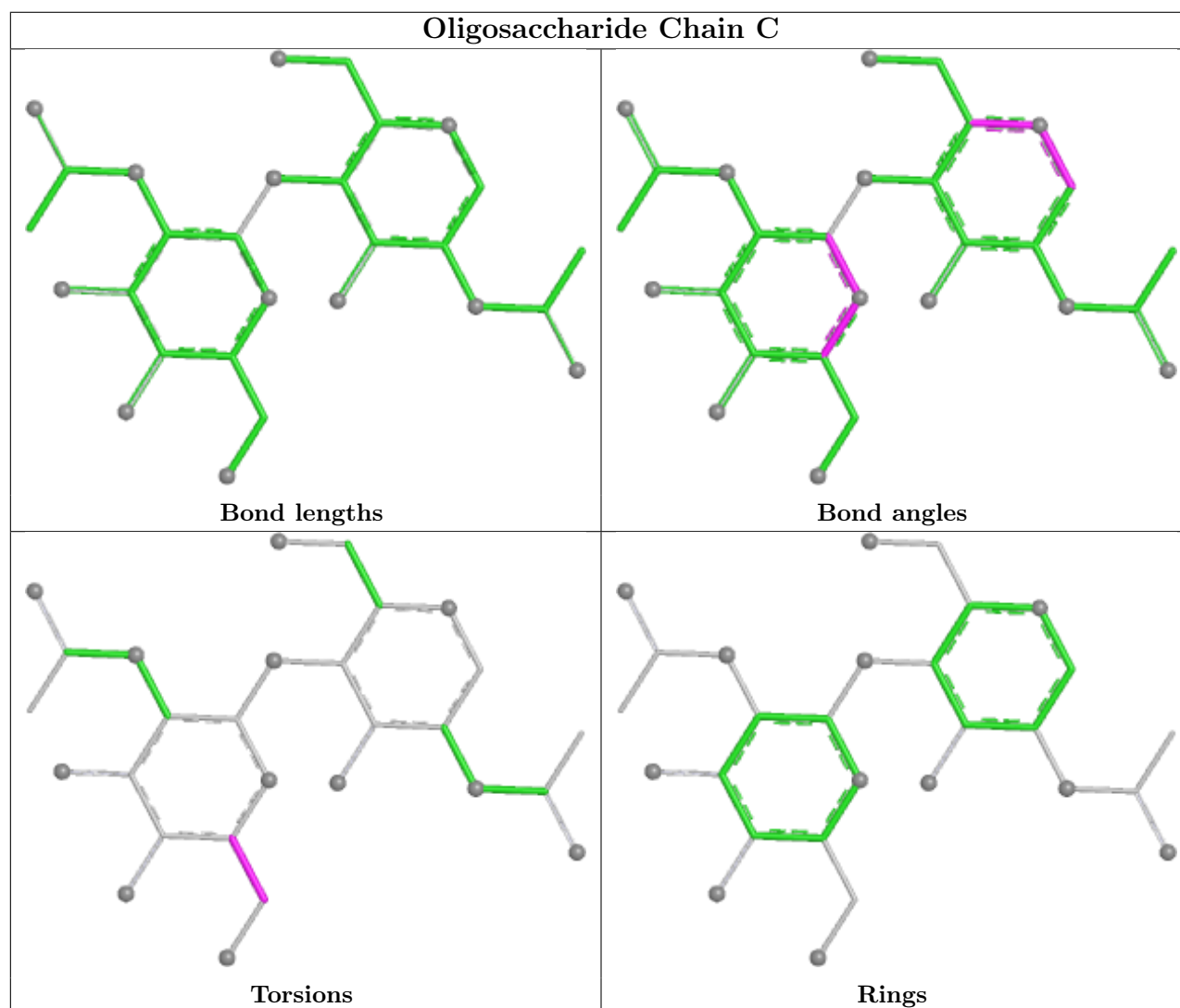
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



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	$\# Z > 2$
6	IHP	B	205	-	36,36,36	1.30	5 (13%)	60,60,60	0.79	1 (1%)
4	3PO	A	1301	-	10,12,12	0.82	0	17,20,20	0.91	0
5	NAG	B	204	2	14,14,15	0.29	0	17,19,21	0.53	0
5	NAG	B	203	2	14,14,15	0.33	0	17,19,21	0.68	1 (5%)

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
6	IHP	B	205	-	-	5/30/54/54	0/1/1/1
4	3PO	A	1301	-	-	3/12/12/12	-
5	NAG	B	204	2	-	0/6/23/26	0/1/1/1
5	NAG	B	203	2	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	205	IHP	P4-O14	4.02	1.66	1.59
6	B	205	IHP	P6-O16	3.42	1.65	1.59
6	B	205	IHP	P3-O13	3.31	1.65	1.59
6	B	205	IHP	P5-O15	3.28	1.65	1.59
6	B	205	IHP	P2-O12	2.75	1.64	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	205	IHP	C6-C1-C2	2.80	116.57	110.43
5	B	203	NAG	C1-O5-C5	2.34	115.33	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	3PO	PB-O3A-PA-O5'
6	B	205	IHP	C3-C4-O14-P4
4	A	1301	3PO	PB-O3B-PG-O3G
5	B	203	NAG	C4-C5-C6-O6
6	B	205	IHP	C2-C3-O13-P3
6	B	205	IHP	C4-C3-O13-P3
6	B	205	IHP	C5-C4-O14-P4
4	A	1301	3PO	PB-O3A-PA-O2A
5	B	203	NAG	O5-C5-C6-O6
6	B	205	IHP	C1-O11-P1-O21

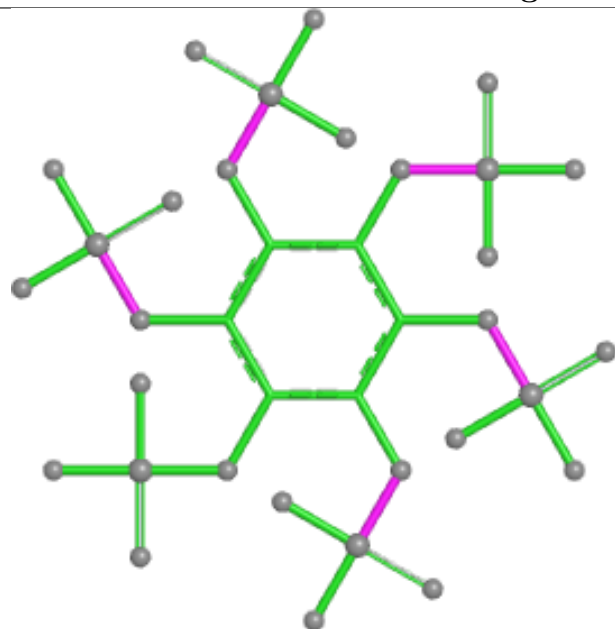
There are no ring outliers.

1 monomer is involved in 1 short contact:

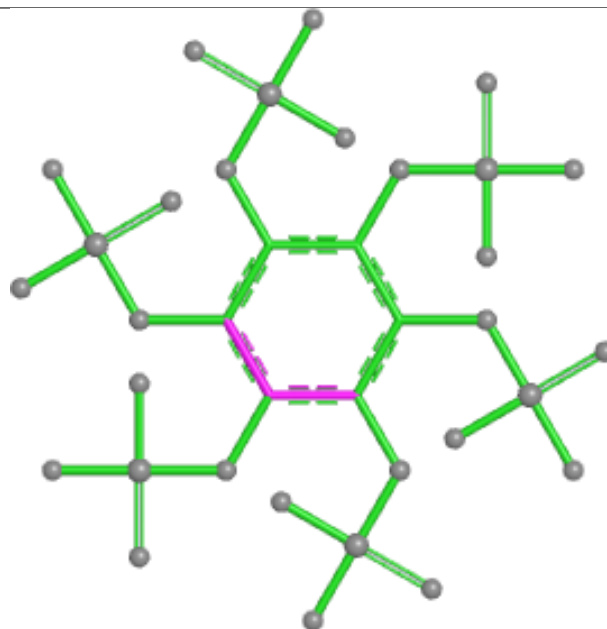
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	203	NAG	1	0

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.

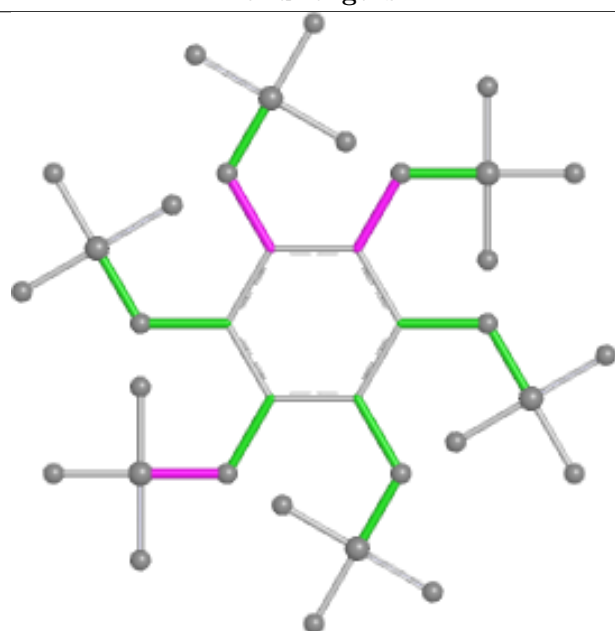
Ligand IHP B 205



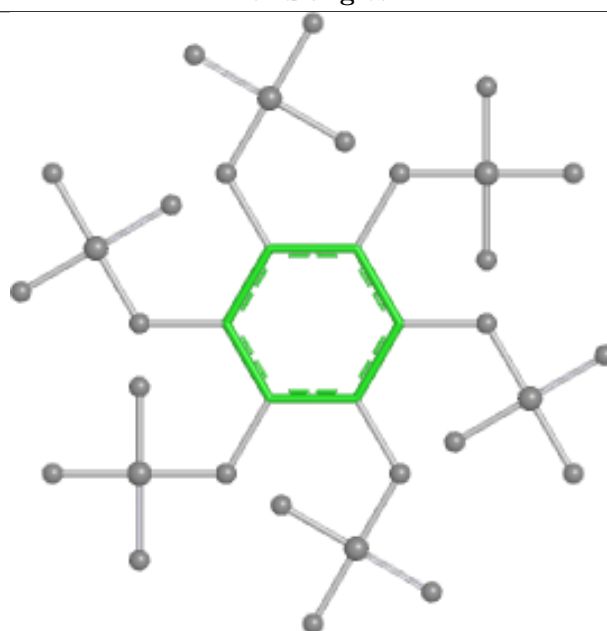
Bond lengths



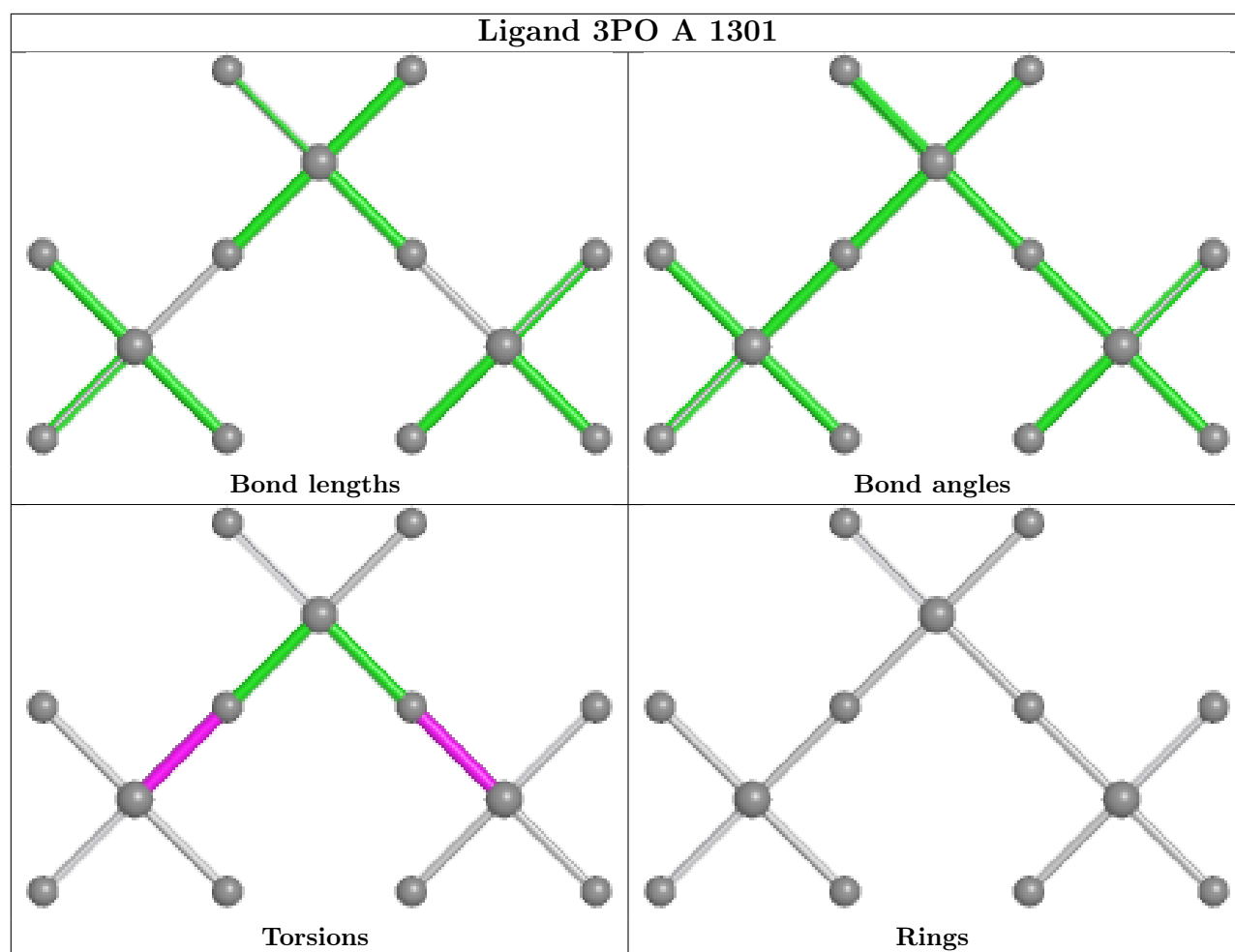
Bond angles



Torsions



Rings



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	440/488 (90%)	0.17	26 (5%) 28 23	19, 40, 80, 127	0
2	B	186/186 (100%)	0.36	9 (4%) 35 30	29, 46, 88, 109	0
All	All	626/674 (92%)	0.23	35 (5%) 30 25	19, 42, 87, 127	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1125	ALA	6.9
1	A	1187	GLY	4.0
1	A	1026	GLU	3.7
1	A	893	ASN	3.7
1	A	1041	CYS	3.5
1	A	1042	ALA	3.4
1	A	1157	THR	3.4
1	A	863	ASN	3.2
1	A	890	LYS	3.1
1	A	1214	CYS	3.1
1	A	1023	VAL	3.0
1	A	1213	LYS	2.9
2	B	1	GLN	2.9
1	A	735	GLY	2.9
2	B	70	PRO	2.8
1	A	1045	LYS	2.8
2	B	3	SER	2.8
1	A	892	LYS	2.7
2	B	46	GLY	2.7
1	A	894	ASP	2.5
2	B	186	GLY	2.5
1	A	1210	THR	2.4
2	B	74	SER	2.4
1	A	817	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	45	PRO	2.3
2	B	73	GLN	2.3
1	A	1211	ALA	2.3
1	A	1067	TYR	2.2
1	A	1024	CYS	2.2
2	B	29	LYS	2.2
1	A	1209	ASP	2.1
1	A	733	PRO	2.1
1	A	1038	SER	2.1
1	A	895	LYS	2.0
1	A	1022	LYS	2.0

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

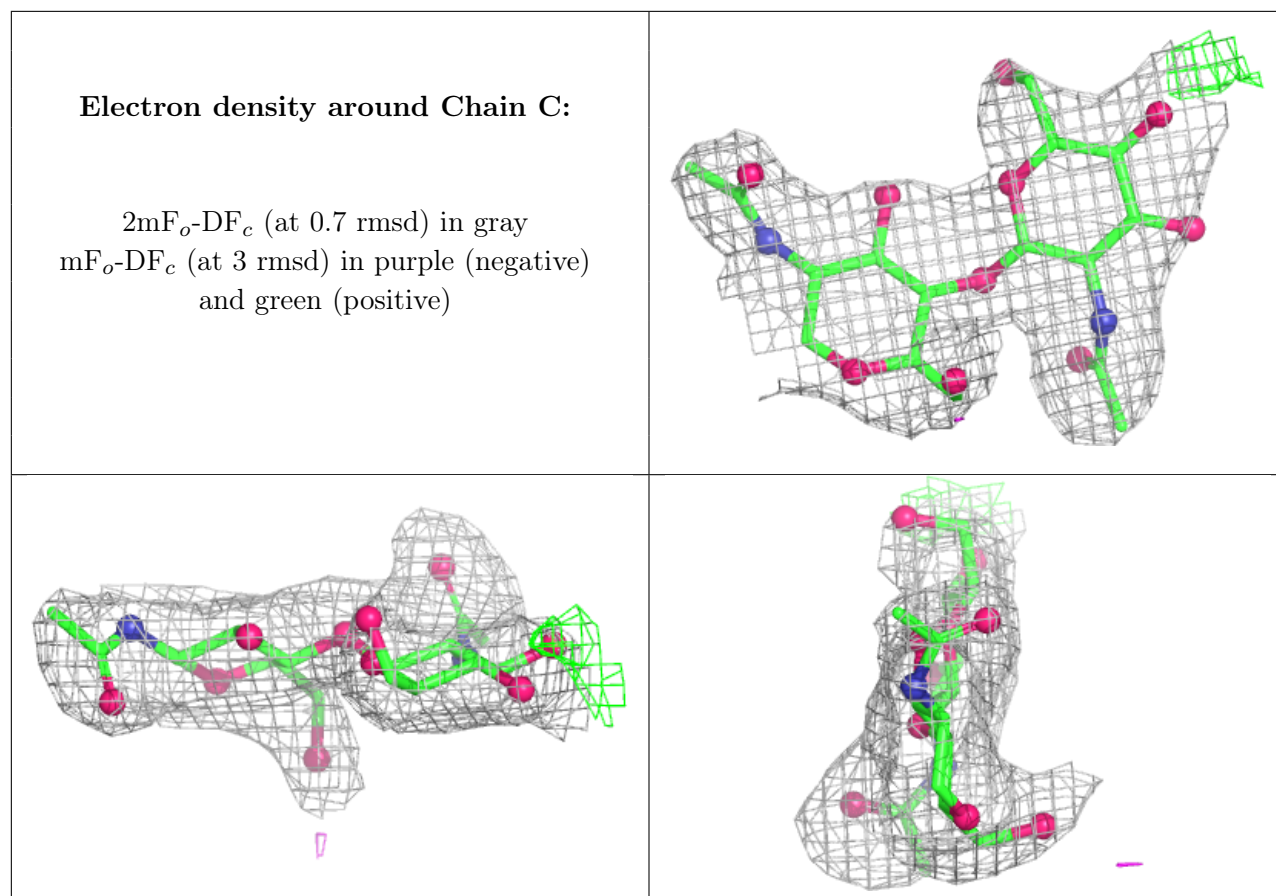
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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
3	NAG	C	2	14/15	0.76	0.13	72,76,82,83	0
3	NAG	C	1	14/15	0.90	0.09	51,59,63,68	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

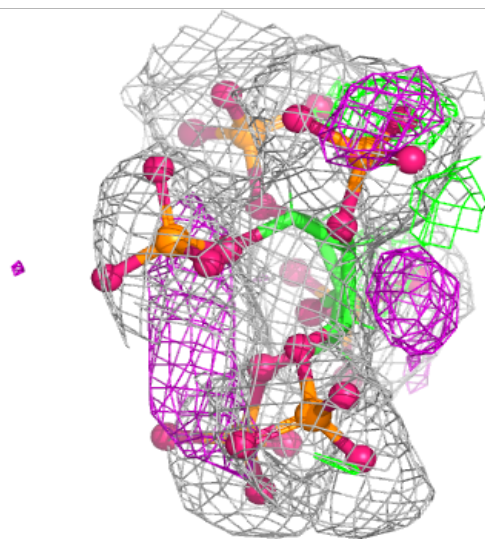
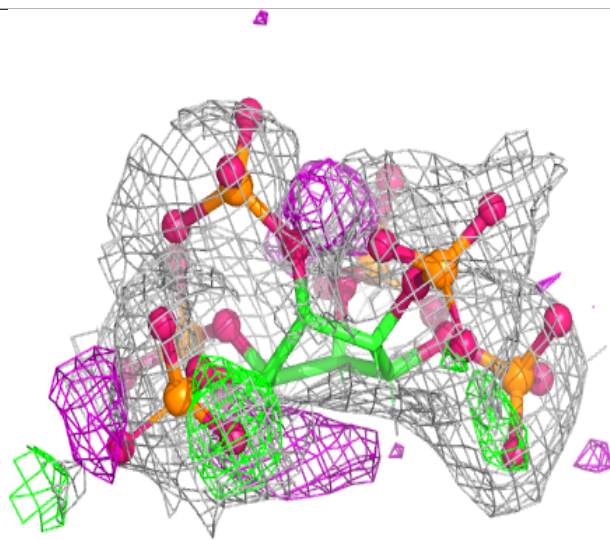
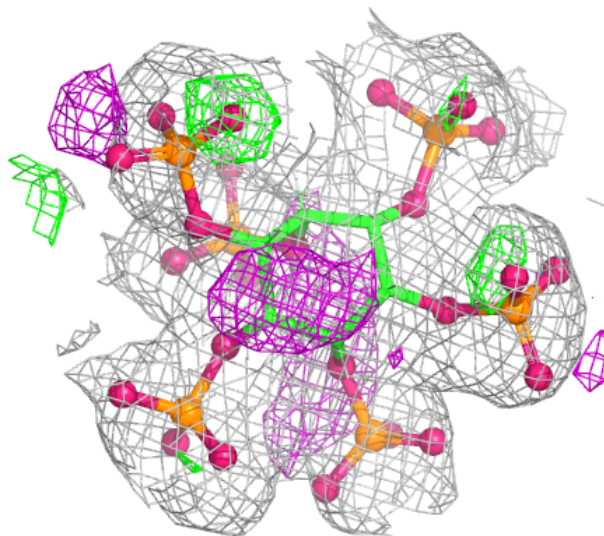
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	IHP	B	205	36/36	0.73	0.16	83,92,103,107	0
5	NAG	B	204	14/15	0.77	0.12	67,70,76,78	0
4	3PO	A	1301	13/13	0.77	0.21	153,156,157,157	0
5	NAG	B	203	14/15	0.88	0.12	41,45,50,51	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.

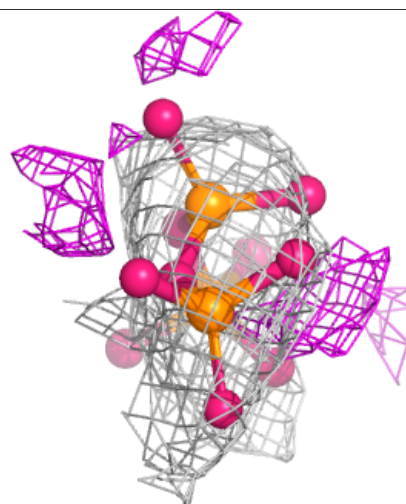
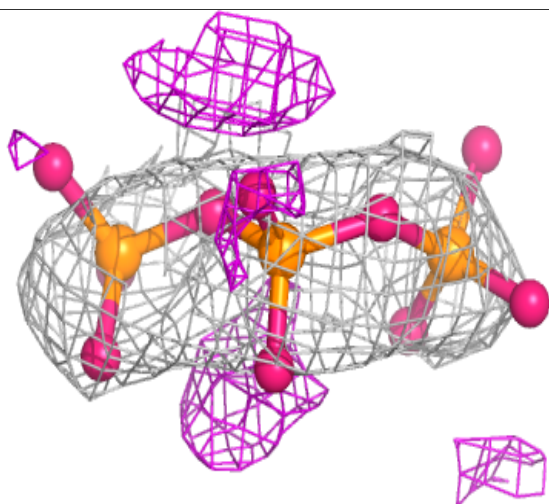
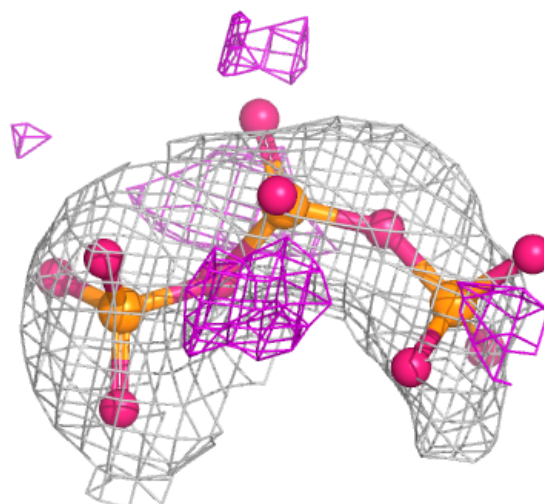
Electron density around IHP B 205:

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



Electron density around 3PO A 1301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.