Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 08:13 AM EST

PDB ID	:	3PE4
Title	:	Structure of human O-GlcNAc transferase and its complex with a peptide substrate
Authors	:	Lazarus, M.B.; Nam, Y.; Jiang, J.; Sliz, P.; Walker, S.
Deposited on	:	2010-10-25
Resolution	:	1.95 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

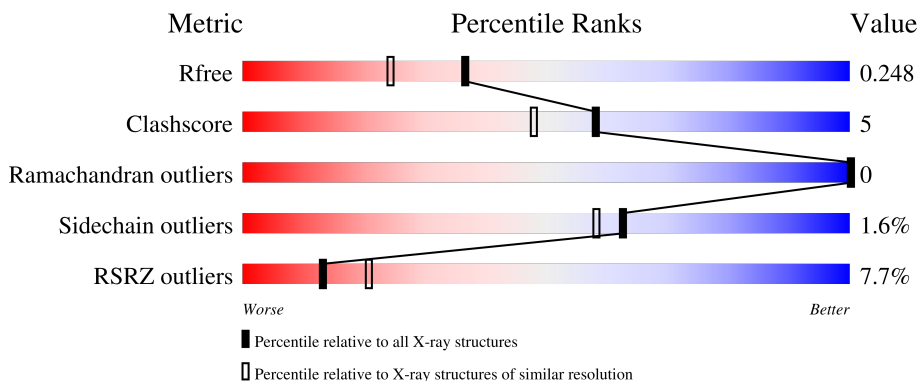|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.95 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	Percentile Ranks	Value
Rfree		0.248
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		1.6%
RSRZ outliers		7.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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% 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	723	7% / 86% / 9% · ·
1	C	723	8% / 84% / 9% / 7%
2	B	14	79% / 21%
2	D	14	79% / 21%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12036 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 UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total 5549	C 3527	N 966	O 1019	S 37	0	9	0
1	C	674	Total 5378	C 3427	N 933	O 981	S 37	0	8	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	GLY	-	expression tag	UNP O15294
A	310	PRO	-	expression tag	UNP O15294
A	311	GLY	-	expression tag	UNP O15294
A	312	SER	-	expression tag	UNP O15294
C	309	GLY	-	expression tag	UNP O15294
C	310	PRO	-	expression tag	UNP O15294
C	311	GLY	-	expression tag	UNP O15294
C	312	SER	-	expression tag	UNP O15294

- Molecule 2 is a protein called Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total 95	C 58	N 15	O 20	S 2	0	0	0
2	D	14	Total 95	C 58	N 15	O 20	S 2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	TYR	-	expression tag	UNP P68400
D	13	TYR	-	expression tag	UNP P68400

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).
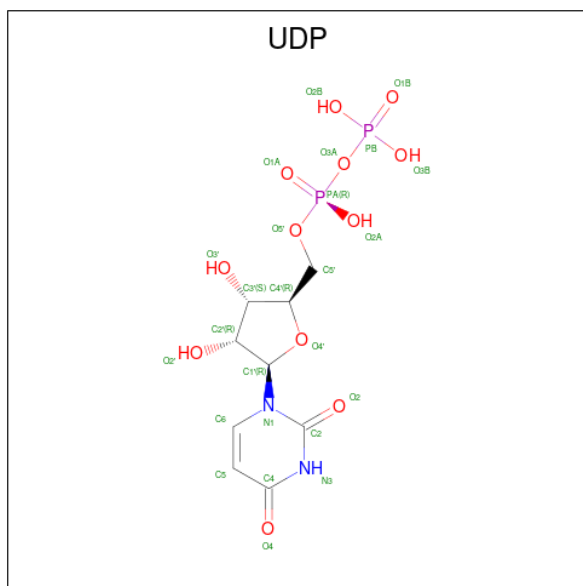
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
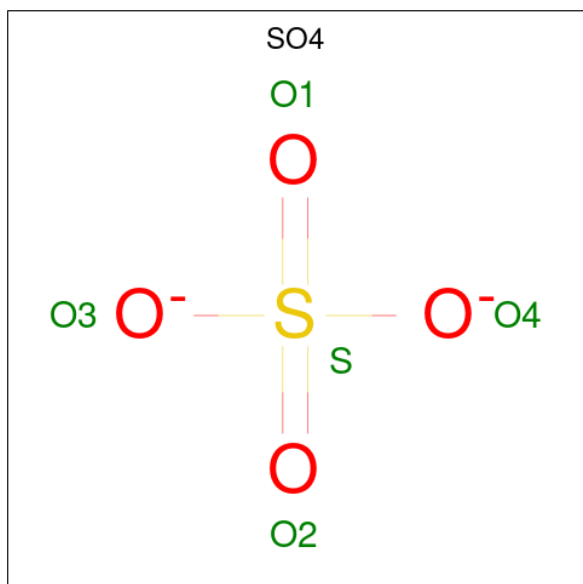
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	412	Total 412	O 412	0	0
5	B	12	Total 12	O 12	0	0
5	C	415	Total 415	O 415	0	0
5	D	15	Total 15	O 15	0	0

3 Residue-property plots ⓘ

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.

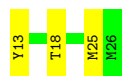• Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit
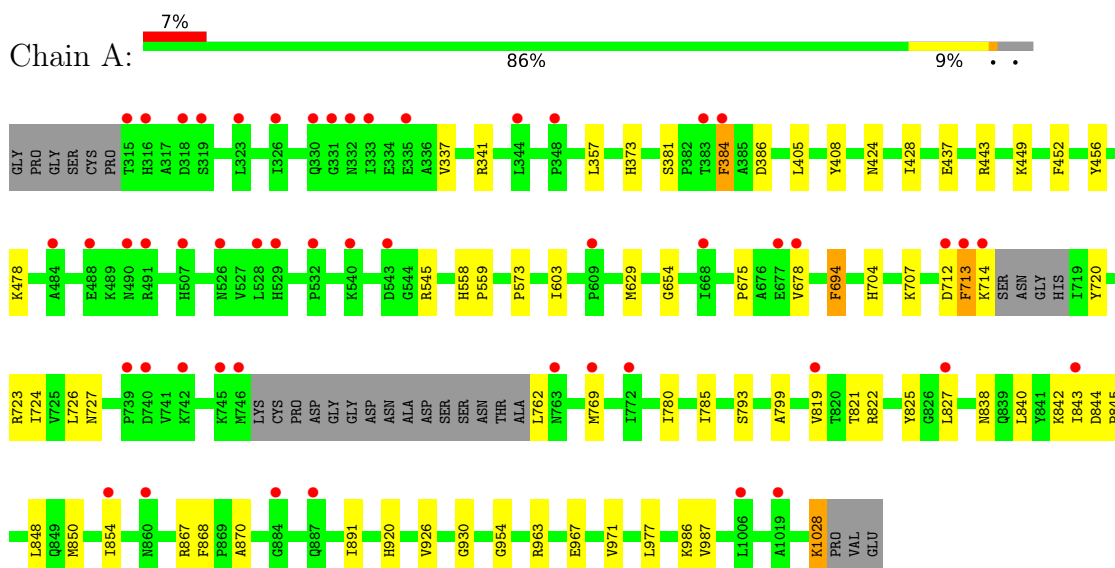
• Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit
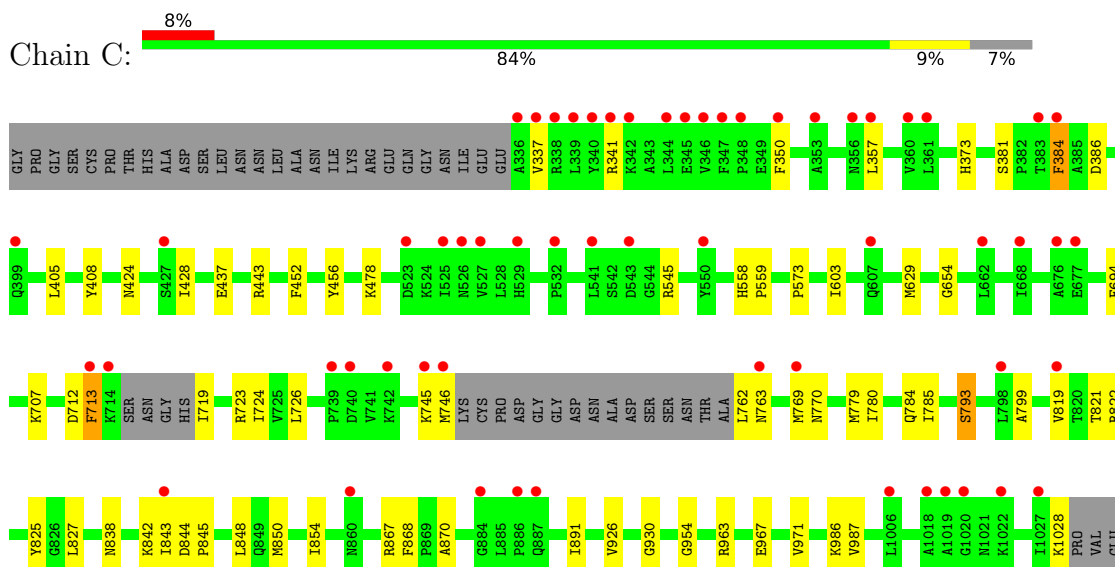
• Molecule 2: Casein kinase II subunit alpha

Chain B:

79%　　　　　　21%

Y13 T18 M25 M26

• Molecule 2: Casein kinase II subunit alpha

Chain D:

79%　　　　　　21%

Y13 T18 M25 M26

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	98.60Å 136.70Å 153.50Å 90.00° 102.90° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 29.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-1.95) 98.3 (29.99-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.72 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.224 , 0.252 0.219 , 0.248	Depositor DCC
R_{free} test set	7099 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 56.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12036	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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 28.64 % 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 1.7790e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, UDP

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	0.37	0/5687	0.51	0/7714
1	C	0.37	0/5515	0.52	0/7482
2	B	0.34	0/97	0.53	0/131
2	D	0.36	0/97	0.52	0/131
All	All	0.37	0/11396	0.51	0/15458

There are no bond length outliers.

There are no bond angle outliers.

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	5549	0	5542	55	0
1	C	5378	0	5382	48	0
2	B	95	0	88	2	0
2	D	95	0	88	2	0
3	A	25	0	11	0	0
3	C	25	0	11	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	412	0	0	6	0
5	B	12	0	0	0	0
5	C	415	0	0	9	0
5	D	15	0	0	0	0
All	All	12036	0	11122	107	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 5.

All (107) 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:C:763:ASN:HA	5:C:1249:HOH:O	1.50	1.11
1:C:854[B]:ILE:HD11	1:C:967:GLU:HA	1.49	0.92
1:A:854[B]:ILE:HD11	1:A:967:GLU:HA	1.51	0.91
1:A:723:ARG:O	1:A:724[B]:ILE:HD13	1.84	0.78
1:C:723:ARG:O	1:C:724[B]:ILE:HD13	1.85	0.77
1:A:545:ARG:HD3	1:A:573:PRO:O	1.90	0.72
1:C:854[B]:ILE:HD11	1:C:967:GLU:CA	2.20	0.71
1:C:545:ARG:HD3	1:C:573:PRO:O	1.92	0.70
1:A:1028:LYS:HE2	5:A:1143:HOH:O	1.92	0.67
1:A:854[B]:ILE:HD11	1:A:967:GLU:CA	2.22	0.65
2:D:13:TYR:N	2:D:18:THR:HG1	1.95	0.65
2:B:13:TYR:N	2:B:18:THR:HG1	1.98	0.60
1:C:746:MET:N	5:C:1249:HOH:O	2.37	0.57
1:A:456:TYR:CZ	1:A:478:LYS:HD3	2.40	0.57
1:C:456:TYR:CZ	1:C:478:LYS:HD3	2.40	0.56
1:A:726:LEU:HD23	1:A:819[A]:VAL:HG22	1.87	0.56
1:C:707:LYS:HE2	1:C:762:LEU:HD22	1.88	0.56
1:A:954:GLY:O	1:A:986:LYS:HE2	2.06	0.55
1:C:726:LEU:CD2	1:C:819[A]:VAL:HG22	2.37	0.55
1:A:726:LEU:CD2	1:A:819[A]:VAL:HG22	2.37	0.55
1:C:726:LEU:HD23	1:C:819[A]:VAL:HG22	1.88	0.54
1:A:707:LYS:HE2	1:A:762:LEU:HD22	1.89	0.54
1:A:843[B]:ILE:HD11	1:A:848:LEU:HB2	1.90	0.54
1:C:770:ASN:HB2	5:C:1170:HOH:O	2.08	0.54
1:C:954:GLY:O	1:C:986:LYS:HE2	2.07	0.54
1:A:381[B]:SER:HB2	1:A:384:PHE:HB2	1.91	0.53
1:C:827[A]:LEU:HD23	1:C:891:ILE:HD12	1.91	0.53
1:C:443:ARG:NE	5:C:1260:HOH:O	2.42	0.52
1:C:843[B]:ILE:HD11	1:C:848:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:LEU:HD23	1:A:819[B]:VAL:HG12	1.92	0.52
1:A:726:LEU:CD2	1:A:819[B]:VAL:HG12	2.40	0.52
1:A:443:ARG:NH1	5:A:1257:HOH:O	2.39	0.52
1:A:854[B]:ILE:HD12	1:A:971:VAL:HG23	1.91	0.51
1:C:381[B]:SER:HB2	1:C:384:PHE:HB2	1.92	0.51
1:A:780:ILE:HD11	1:A:819[B]:VAL:CG2	2.41	0.51
1:C:780:ILE:HD11	1:C:819[B]:VAL:CG2	2.40	0.51
1:A:408:TYR:CZ	1:A:424:ASN:HB3	2.46	0.51
1:C:854[B]:ILE:HD12	1:C:971:VAL:HG23	1.92	0.51
1:C:408:TYR:CZ	1:C:424:ASN:HB3	2.47	0.50
1:C:780:ILE:HD11	1:C:819[B]:VAL:HG21	1.93	0.50
1:C:726:LEU:CD2	1:C:819[B]:VAL:HG12	2.41	0.50
1:C:762:LEU:HD23	5:C:1201:HOH:O	2.11	0.49
1:A:780:ILE:HD11	1:A:819[B]:VAL:HG21	1.94	0.49
1:A:827[A]:LEU:HD23	1:A:891:ILE:HD12	1.95	0.49
1:C:357:LEU:HD23	1:C:373:HIS:CE1	2.47	0.49
1:A:558:HIS:CG	1:A:559:PRO:HD2	2.47	0.48
1:C:825:TYR:HB2	1:C:827[B]:LEU:HD13	1.95	0.48
1:C:726:LEU:HD23	1:C:819[B]:VAL:HG12	1.94	0.48
1:A:825:TYR:HB2	1:A:827[B]:LEU:HD13	1.96	0.48
1:A:867:ARG:HB3	1:A:870:ALA:HA	1.95	0.48
1:C:558:HIS:CG	1:C:559:PRO:HD2	2.49	0.48
1:A:850:MET:SD	1:A:963:ARG:HG2	2.54	0.47
1:C:930:GLY:HA2	1:C:987:VAL:HG12	1.95	0.47
1:C:712:ASP:O	1:C:769:MET:HB2	2.14	0.47
1:A:762:LEU:HD23	5:A:1135:HOH:O	2.15	0.47
1:A:712:ASP:O	1:A:769:MET:HB2	2.15	0.47
1:A:930:GLY:HA2	1:A:987:VAL:HG12	1.97	0.47
1:A:844:ASP:HB2	1:A:845:PRO:HD2	1.97	0.46
1:C:713:PHE:H	1:C:713:PHE:HD1	1.64	0.46
1:C:850:MET:SD	1:C:963:ARG:HG2	2.55	0.46
1:C:629:MET:O	1:C:654:GLY:HA3	2.16	0.46
1:A:713:PHE:H	1:A:713:PHE:HD1	1.64	0.46
1:C:745:LYS:HA	5:C:1249:HOH:O	2.15	0.46
1:C:456:TYR:CE1	1:C:478:LYS:HD3	2.51	0.46
1:A:822:ARG:HG2	1:A:827[B]:LEU:HD23	1.96	0.46
1:A:629:MET:O	1:A:654:GLY:HA3	2.16	0.45
1:C:822:ARG:HG2	1:C:827[B]:LEU:HD23	1.99	0.45
1:A:449:LYS:HD2	5:A:1261:HOH:O	2.16	0.45
1:C:724[B]:ILE:CD1	1:C:821:THR:HB	2.46	0.44
1:C:867:ARG:HB3	1:C:870:ALA:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:838:ASN:HB3	1:C:842:LYS:HD2	1.99	0.44
1:C:844:ASP:HB2	1:C:845:PRO:HD2	2.00	0.44
1:A:838:ASN:HB3	1:A:842:LYS:HD2	2.00	0.44
1:C:719:ILE:N	5:C:1243:HOH:O	2.51	0.44
1:A:977:LEU:HD22	5:A:1242:HOH:O	2.17	0.44
1:A:724[B]:ILE:CD1	1:A:821:THR:HB	2.48	0.44
1:C:785:ILE:HD12	1:C:799:ALA:HB1	2.00	0.43
1:A:854[B]:ILE:CD1	1:A:971:VAL:HG23	2.48	0.43
1:A:769:MET:O	1:A:769:MET:HG3	2.19	0.43
1:A:456:TYR:CE1	1:A:478:LYS:HD3	2.52	0.43
1:A:357:LEU:HD23	1:A:373:HIS:CE1	2.54	0.43
1:C:603:ILE:HD12	1:C:603:ILE:N	2.34	0.43
1:A:603:ILE:N	1:A:603:ILE:HD12	2.34	0.43
1:C:437:GLU:HG3	5:C:307:HOH:O	2.18	0.43
1:C:337:VAL:O	1:C:341:ARG:HG3	2.19	0.42
1:A:437:GLU:HG3	5:A:1061:HOH:O	2.19	0.42
1:A:785:ILE:HD12	1:A:799:ALA:HB1	2.01	0.42
1:A:840:LEU:O	1:A:843[B]:ILE:HG23	2.20	0.42
1:A:405:LEU:HD12	1:A:428:ILE:HG21	2.01	0.42
1:C:405:LEU:HD12	1:C:428:ILE:HG21	2.01	0.42
1:C:822:ARG:HB3	1:C:827[B]:LEU:HB2	2.02	0.42
1:C:793:SER:HB3	5:C:1244:HOH:O	2.20	0.41
1:A:675:PRO:O	1:A:678:VAL:HG22	2.20	0.41
1:A:822:ARG:HB3	1:A:827[B]:LEU:HB2	2.02	0.41
1:A:723:ARG:C	1:A:724[B]:ILE:HD13	2.38	0.41
2:D:25:MET:HA	2:D:25:MET:CE	2.51	0.41
1:A:694:PHE:CZ	1:A:920:HIS:HB3	2.55	0.41
1:A:714:LYS:HE2	1:A:714:LYS:HB2	1.86	0.41
1:A:720:TYR:HB3	1:A:723:ARG:HD3	2.03	0.41
1:A:724[B]:ILE:HD12	1:A:821:THR:HB	2.03	0.41
1:A:844:ASP:HB2	1:A:845:PRO:CD	2.51	0.41
2:B:25:MET:HA	2:B:25:MET:CE	2.51	0.40
1:A:337:VAL:O	1:A:341:ARG:HG3	2.20	0.40
1:A:704:HIS:O	1:A:727:ASN:HB3	2.22	0.40
1:C:779:MET:HA	1:C:784:GLN:HE21	1.86	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	698/723 (96%)	682 (98%)	16 (2%)	0	100	100
1	C	676/723 (94%)	661 (98%)	15 (2%)	0	100	100
2	B	12/14 (86%)	12 (100%)	0	0	100	100
2	D	12/14 (86%)	12 (100%)	0	0	100	100
All	All	1398/1474 (95%)	1367 (98%)	31 (2%)	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	606/618 (98%)	597 (98%)	9 (2%)	65	60
1	C	587/618 (95%)	577 (98%)	10 (2%)	60	55
2	B	11/11 (100%)	11 (100%)	0	100	100
2	D	11/11 (100%)	11 (100%)	0	100	100
All	All	1215/1258 (97%)	1196 (98%)	19 (2%)	62	58

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	PHE
1	A	386	ASP

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Mol	Chain	Res	Type
1	A	452	PHE
1	A	694	PHE
1	A	713	PHE
1	A	793	SER
1	A	868	PHE
1	A	926	VAL
1	A	1028	LYS
1	C	350	PHE
1	C	384	PHE
1	C	386	ASP
1	C	452	PHE
1	C	694	PHE
1	C	713	PHE
1	C	793	SER
1	C	868	PHE
1	C	926	VAL
1	C	1028	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	GLN
1	A	364	GLN
1	A	406	GLN
1	A	681	GLN
1	C	363	GLN
1	C	406	GLN
1	C	498	HIS
1	C	681	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	UDP	C	1212	-	24,26,26	1.00	1 (4%)	37,40,40	1.55	4 (10%)
4	SO4	B	1	-	4,4,4	0.18	0	6,6,6	0.12	0
3	UDP	A	1212	-	24,26,26	1.03	2 (8%)	37,40,40	1.49	4 (10%)
4	SO4	A	5	-	4,4,4	0.16	0	6,6,6	0.07	0
4	SO4	D	3	-	4,4,4	0.20	0	6,6,6	0.16	0

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	UDP	C	1212	-	-	3/16/32/32	0/2/2/2
3	UDP	A	1212	-	-	3/16/32/32	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1212	UDP	C6-C5	2.14	1.40	1.35
3	C	1212	UDP	C5-C4	-2.10	1.39	1.43
3	A	1212	UDP	C5-C4	-2.02	1.39	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1212	UDP	C4-N3-C2	-4.88	120.14	126.58
3	A	1212	UDP	C4-N3-C2	-4.56	120.57	126.58
3	C	1212	UDP	C5-C4-N3	4.27	121.23	114.84
3	A	1212	UDP	C5-C4-N3	4.13	121.02	114.84
3	C	1212	UDP	O4-C4-C5	-3.38	119.22	125.16
3	A	1212	UDP	N3-C2-N1	2.96	118.82	114.89
3	C	1212	UDP	N3-C2-N1	2.82	118.64	114.89
3	A	1212	UDP	O4-C4-C5	-2.75	120.32	125.16

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1212	UDP	O4'-C4'-C5'-O5'
3	C	1212	UDP	O4'-C4'-C5'-O5'
3	A	1212	UDP	C3'-C4'-C5'-O5'
3	C	1212	UDP	C3'-C4'-C5'-O5'
3	A	1212	UDP	PA-O3A-PB-O1B
3	C	1212	UDP	PA-O3A-PB-O1B

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 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.

Ligand UDP C 1212

Bond lengths

Bond angles

Torsions

Rings

Ligand UDP A 1212

Bond lengths

Bond angles

Torsions

Rings
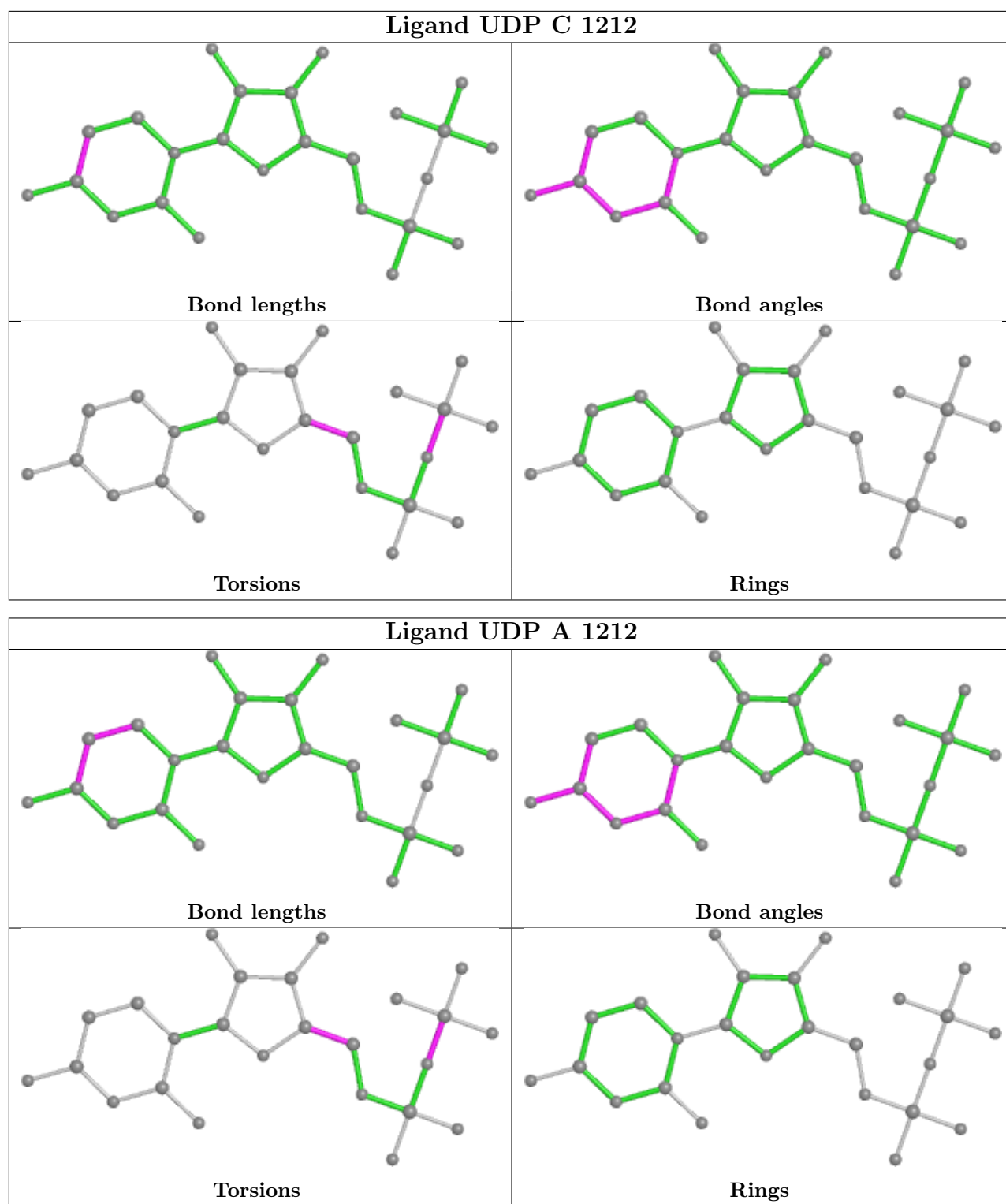
5.7　Other polymers ⓘ

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	695/723 (96%)	0.41	50 (7%)	15	23	7, 18, 46, 73	0
1	C	674/723 (93%)	0.44	58 (8%)	10	16	7, 17, 44, 73	0
2	B	14/14 (100%)	-0.04	0	100	100	10, 17, 36, 46	0
2	D	14/14 (100%)	-0.18	0	100	100	9, 17, 36, 46	0
All	All	1397/1474 (94%)	0.41	108 (7%)	13	21	7, 18, 46, 73	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	347	PHE	6.8
1	C	339	LEU	6.6
1	C	348	PRO	6.6
1	C	337	VAL	6.3
1	C	338	ARG	6.1
1	C	344	LEU	5.6
1	A	713	PHE	5.4
1	C	346	VAL	5.4
1	A	315	THR	5.1
1	A	335	GLU	4.8
1	C	526	ASN	4.6
1	C	342	LYS	4.6
1	C	527	VAL	4.5
1	A	526	ASN	4.4
1	A	332	ASN	4.4
1	C	340	TYR	4.3
1	C	713	PHE	4.1
1	C	714	LYS	4.0
1	A	769	MET	3.9
1	A	746	MET	3.8
1	C	860	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	714	LYS	3.6
1	C	357	LEU	3.6
1	C	350	PHE	3.5
1	C	819[A]	VAL	3.5
1	C	529	HIS	3.5
1	C	345	GLU	3.4
1	C	746	MET	3.4
1	A	384	PHE	3.4
1	A	488	GLU	3.3
1	C	1027	ILE	3.2
1	C	383	THR	3.2
1	A	316	HIS	3.2
1	A	772	ILE	3.1
1	C	884	GLY	3.0
1	A	331	GLY	3.0
1	C	1019	ALA	3.0
1	A	490	ASN	3.0
1	C	360	VAL	3.0
1	A	529	HIS	3.0
1	C	353	ALA	2.9
1	A	739	PRO	2.9
1	A	330	GLN	2.9
1	A	742	LYS	2.9
1	C	843[A]	ILE	2.9
1	A	860	ASN	2.8
1	C	745	LYS	2.8
1	A	745	LYS	2.8
1	C	541	LEU	2.8
1	A	318	ASP	2.6
1	C	543	ASP	2.6
1	C	676	ALA	2.6
1	C	384	PHE	2.6
1	A	491	ARG	2.6
1	A	712	ASP	2.6
1	C	677	GLU	2.5
1	A	827[A]	LEU	2.5
1	A	383	THR	2.5
1	A	333	ILE	2.5
1	C	740	ASP	2.5
1	A	843[A]	ILE	2.4
1	C	1006	LEU	2.4
1	A	484	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	739	PRO	2.4
1	A	887	GLN	2.4
1	C	769	MET	2.3
1	A	540	LYS	2.3
1	A	668	ILE	2.3
1	A	1019	ALA	2.3
1	A	532	PRO	2.3
1	C	886	PRO	2.3
1	C	550	TYR	2.3
1	A	543	ASP	2.3
1	A	819[A]	VAL	2.3
1	C	336	ALA	2.3
1	C	532	PRO	2.3
1	A	884	GLY	2.2
1	C	356	ASN	2.2
1	A	319[A]	SER	2.2
1	C	341	ARG	2.2
1	A	609	PRO	2.2
1	A	740	ASP	2.2
1	A	323	LEU	2.2
1	C	1022	LYS	2.2
1	C	668	ILE	2.2
1	C	523	ASP	2.2
1	A	677	GLU	2.1
1	C	1020	GLY	2.1
1	C	361	LEU	2.1
1	C	399	GLN	2.1
1	C	887	GLN	2.1
1	C	525	ILE	2.1
1	C	607	GLN	2.1
1	A	344	LEU	2.1
1	A	528	LEU	2.1
1	C	427	SER	2.1
1	A	507	HIS	2.1
1	C	763	ASN	2.1
1	A	326	ILE	2.1
1	A	854[A]	ILE	2.1
1	C	662	LEU	2.1
1	A	763	ASN	2.0
1	C	1018	ALA	2.0
1	A	348	PRO	2.0
1	C	798	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	678	VAL	2.0
1	A	1006	LEU	2.0
1	C	742	LYS	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
4	SO4	A	5	5/5	0.95	0.31	48,55,60,65	0
3	UDP	C	1212	25/25	0.98	0.08	5,9,11,15	0
3	UDP	A	1212	25/25	0.98	0.08	3,9,12,13	0
4	SO4	B	1	5/5	0.98	0.18	20,25,37,38	0
4	SO4	D	3	5/5	0.98	0.13	25,26,41,41	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 UDP C 1212:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
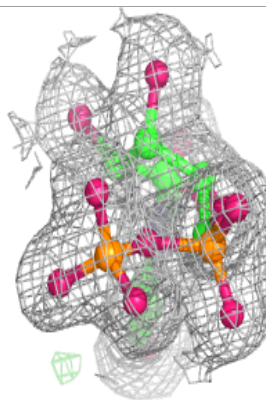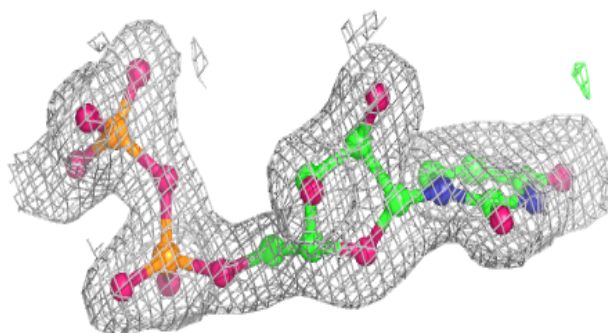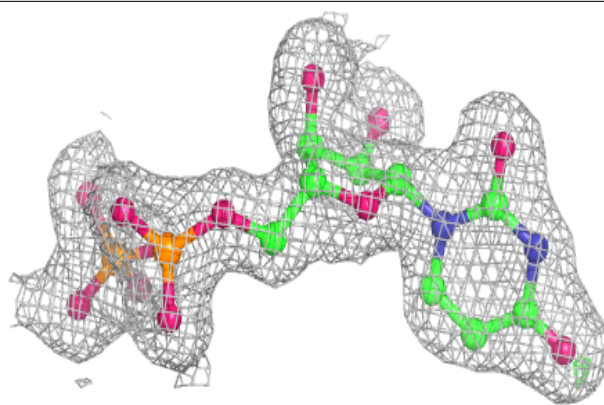
Electron density around UDP A 1212:

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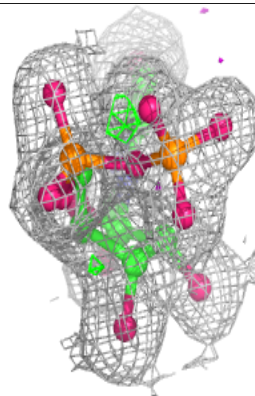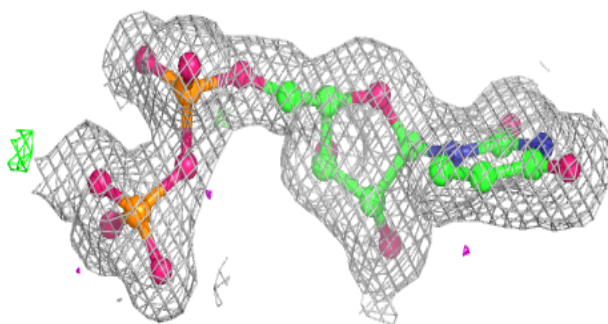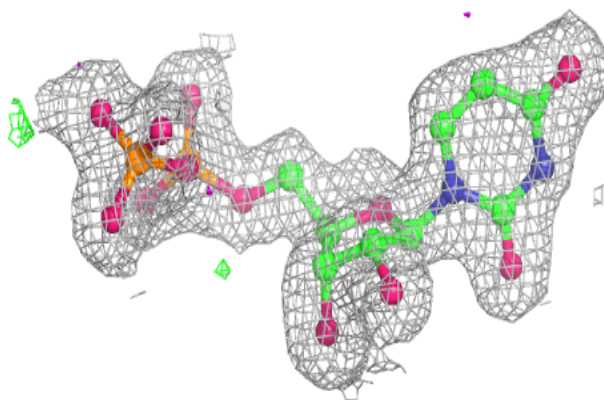
6.5 Other polymers (i)

There are no such residues in this entry.