Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 11:27 AM EST

PDB ID	:	1O23
Title	:	CRYSTAL STRUCTURE OF LACTOSE SYNTHASE IN THE PRESENCE OF UDP-GLUCOSE
Authors	:	Ramakrishnan, B.; Shah, P.S.; Qasba, P.K.
Deposited on	:	2003-01-29
Resolution	:	2.32 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 (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 (i)) were used in the production of this report:

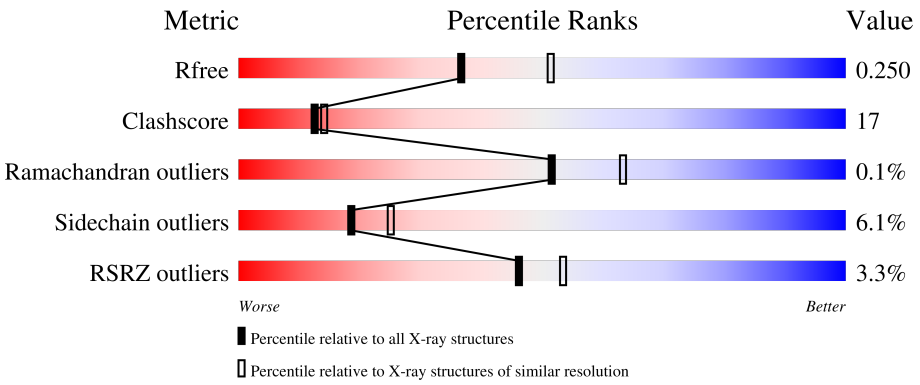
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	123	7% 76% 22% •
1	C	123	4% 70% 28% •
2	B	286	2% 66% 27% • 5%
2	D	286	2% 64% 27% • 5%

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
5	MES	A	815	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6972 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 ALPHA-LACTALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	123	980	620	156	195	9	0	0	0
1	C	123	980	620	156	195	9	0	0	0

- Molecule 2 is a protein called BETA-1,4-GALACTOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	272	2218	1424	382	398	14	0	0	0
2	D	272	2218	1424	382	398	14	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	117	ALA	-	SEE REMARK 999	UNP P08037
B	118	SER	-	SEE REMARK 999	UNP P08037
B	119	MET	-	SEE REMARK 999	UNP P08037
B	120	THR	-	SEE REMARK 999	UNP P08037
B	121	GLY	-	SEE REMARK 999	UNP P08037
B	122	GLY	-	SEE REMARK 999	UNP P08037
B	123	GLN	-	SEE REMARK 999	UNP P08037
B	124	GLN	-	SEE REMARK 999	UNP P08037
B	125	MET	-	SEE REMARK 999	UNP P08037
B	126	GLY	-	SEE REMARK 999	UNP P08037
B	127	ARG	-	SEE REMARK 999	UNP P08037
B	128	GLY	-	SEE REMARK 999	UNP P08037
B	129	SER	-	SEE REMARK 999	UNP P08037
D	519	ALA	-	SEE REMARK 999	UNP P08037
D	520	SER	-	SEE REMARK 999	UNP P08037
D	521	MET	-	SEE REMARK 999	UNP P08037

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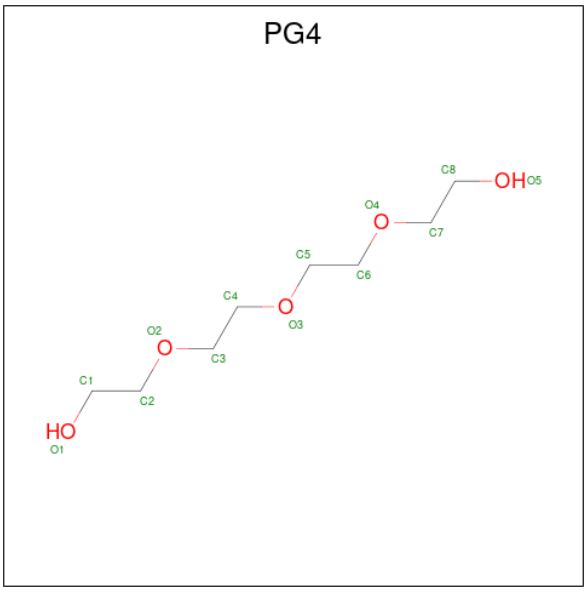
Chain	Residue	Modelled	Actual	Comment	Reference
D	522	THR	-	SEE REMARK 999	UNP P08037
D	523	GLY	-	SEE REMARK 999	UNP P08037
D	524	GLY	-	SEE REMARK 999	UNP P08037
D	525	GLN	-	SEE REMARK 999	UNP P08037
D	526	GLN	-	SEE REMARK 999	UNP P08037
D	527	MET	-	SEE REMARK 999	UNP P08037
D	528	GLY	-	SEE REMARK 999	UNP P08037
D	529	ARG	-	SEE REMARK 999	UNP P08037
D	530	GLY	-	SEE REMARK 999	UNP P08037
D	531	SER	-	SEE REMARK 999	UNP P08037

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

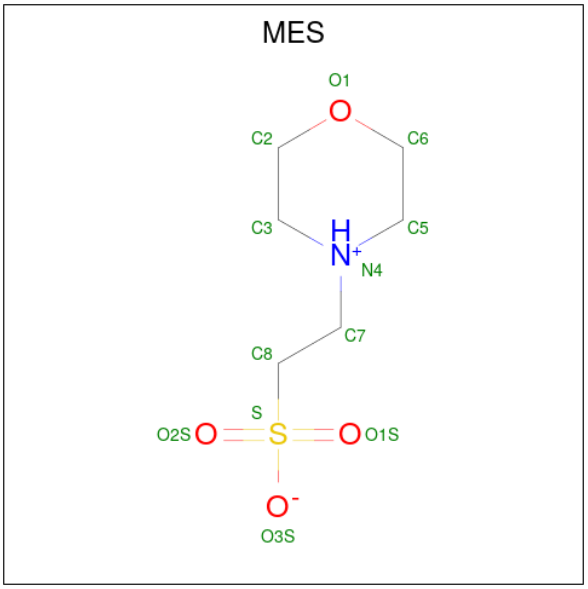
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	1	1	0	0
			Total	Ca		
3	C	1	1	1	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	13	8	5	0	0
			Total	C	O		
4	C	1	13	8	5	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

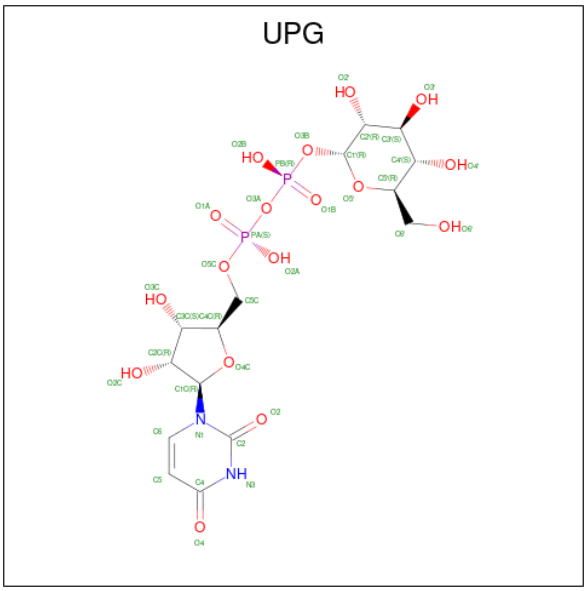


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	12	6	1	4	1	0	0

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

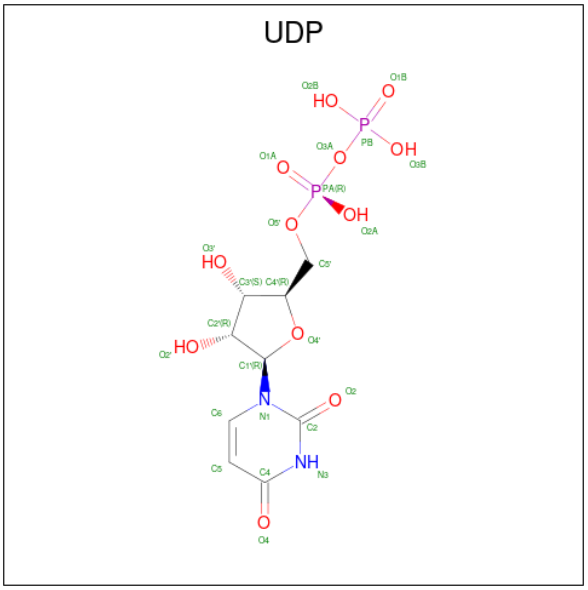
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
6	B	1	1	1	0	0
6	D	1	1	1	0	0

- Molecule 7 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	36	15	2	17	2	0	0
			Total	C	N	O	P		
7	D	1	36	15	2	17	2	0	0

- Molecule 8 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	25	9	2	12	2	0	0
			Total	C	N	O	P		
8	D	1	25	9	2	12	2	0	0

- Molecule 9 is water.

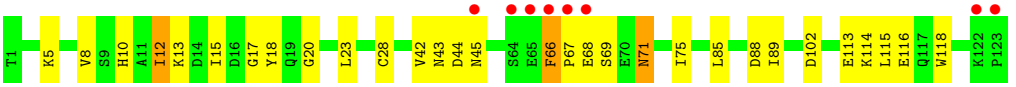
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	63	63	63	0	0
			Total	O		
9	B	138	138	138	0	0
			Total	O		
9	C	87	87	87	0	0
			Total	O		
9	D	124	124	124	0	0

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 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.

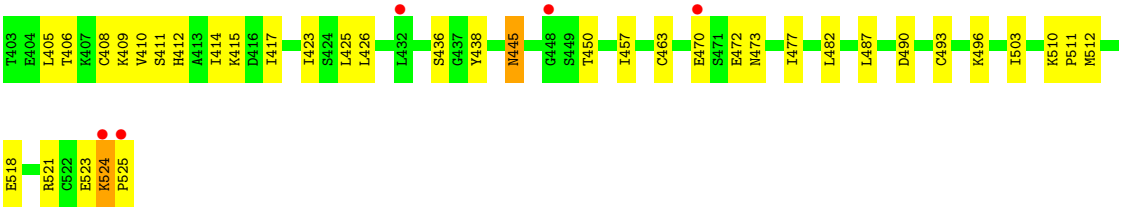
• Molecule 1: ALPHA-LACTALBUMIN

Chain A:



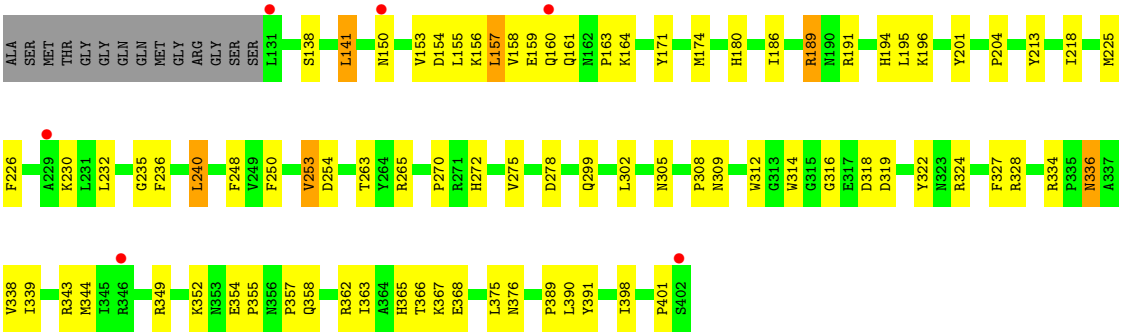
• Molecule 1: ALPHA-LACTALBUMIN

Chain C:



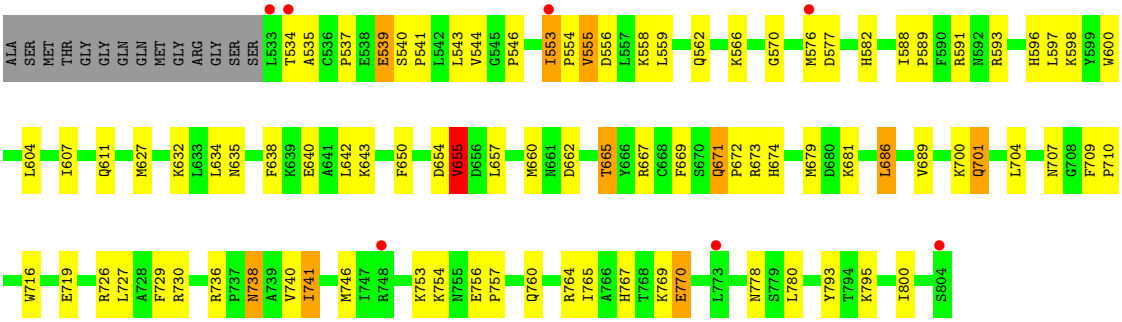
• Molecule 2: BETA-1,4-GALACTOSYLTRANSFERASE

Chain B:



• Molecule 2: BETA-1,4-GALACTOSYLTRANSFERASE

Chain D:


ALA SER MET THR GLY GLY GLN GLN MET GLY ARG GLY SER SER L533 T534 A535 C536 P537 E538 E539 S540 P541 L542 L543 V544 G545 P546 I553 P554 V555 D556 L557 K558 L559 Q562 K566 G570 M576 D577 H582 I588 P589 F590 R591 N592 R593 H596 L597 K598 Y599 W600
L604 I607 Q611 M627 K632 L633 L634 N635 F638 K639 E640 A641 L642 K643 F650 D654 V655 D656 L657 M660 N661 D662 T665 Y666 R667 C668 F669 S670 Q671 P672 R673 H674 M679 D680 K681 L686 V689 K700 Q701 L704 N707 G708 F709 P710
W716 E719 R726 L727 A728 F729 R730 R736 P737 N738 A739 V740 I741 M746 I747 R748 K753 K754 N755 E756 P757 Q760 R764 I765 A766 H767 T768 K769 E770 L773 N778 S779 L780 Y793 T794 K795 I800 S804

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.55Å 99.38Å 102.57Å 90.00° 104.09° 90.00°	Depositor
Resolution (Å)	19.96 – 2.32 19.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.96-2.32) 98.5 (19.96-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.30Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.201 , 0.265 0.190 , 0.250	Depositor DCC
R_{free} test set	4762 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6972	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 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UPG, MN, MES, CA, UDP, PG4

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	0.50	0/1001	0.71	0/1350
1	C	0.59	0/1001	0.77	0/1350
2	B	0.52	0/2278	0.74	1/3085 (0.0%)
2	D	0.51	0/2278	0.73	2/3085 (0.1%)
All	All	0.52	0/6558	0.74	3/8870 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	655	VAL	CB-CA-C	-6.28	99.46	111.40
2	B	253	VAL	CB-CA-C	-5.37	101.19	111.40
2	D	686	LEU	CA-CB-CG	5.19	127.24	115.30

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	980	0	936	33	0
1	C	980	0	933	32	0
2	B	2218	0	2185	62	0
2	D	2218	0	2185	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	13	0	18	0	0
4	C	13	0	18	3	0
5	A	12	0	13	11	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	36	0	21	2	0
7	D	36	0	21	6	0
8	B	25	0	11	1	0
8	D	25	0	11	1	0
9	A	63	0	0	2	0
9	B	138	0	0	3	0
9	C	87	0	0	1	0
9	D	124	0	0	5	0
All	All	6972	0	6352	217	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 17.

All (217) 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:D:553:ILE:HD12	2:D:554:PRO:HD2	1.39	1.04
2:D:738:ASN:C	2:D:738:ASN:HD22	1.69	0.94
2:D:738:ASN:HD21	2:D:741:ILE:H	1.12	0.91
2:D:701:GLN:H	2:D:701:GLN:NE2	1.71	0.88
1:C:523:GLU:O	1:C:524:LYS:HG2	1.75	0.85
2:D:669:PHE:CE1	2:D:673:ARG:HD2	2.14	0.83
2:D:738:ASN:ND2	2:D:741:ILE:H	1.77	0.83
2:D:553:ILE:HD12	2:D:554:PRO:CD	2.09	0.81
2:B:336:ASN:HD22	2:B:338:VAL:H	1.28	0.80
1:A:114:LYS:HG2	5:A:815:MES:H82	1.63	0.80
2:D:707:ASN:HD21	2:D:778:ASN:H	1.30	0.80
2:B:225:MET:HE1	2:B:352:LYS:HA	1.66	0.77
2:D:544:VAL:HG12	2:D:662:ASP:OD1	1.87	0.75
1:A:10:HIS:HA	1:A:13:LYS:HE2	1.70	0.74
2:D:738:ASN:C	2:D:738:ASN:ND2	2.43	0.73
1:C:473:ASN:HD21	1:C:477:ILE:H	1.37	0.73
2:B:305:ASN:HD21	2:B:376:ASN:H	1.36	0.72
1:A:71:ASN:HD21	1:A:75:ILE:H	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:ASN:ND2	2:B:338:VAL:H	1.88	0.71
1:C:405:LEU:HD22	1:C:409:LYS:HE2	1.72	0.70
2:B:225:MET:HE2	2:B:352:LYS:HE3	1.73	0.69
2:D:588:ILE:HG21	2:D:655:VAL:HG13	1.73	0.69
2:D:638:PHE:O	2:D:642:LEU:HD23	1.92	0.69
2:D:700:LYS:HB3	2:D:701:GLN:NE2	2.08	0.69
2:D:671:GLN:HE21	2:D:671:GLN:HA	1.59	0.68
1:C:412:HIS:NE2	1:C:525:PRO:HG2	2.10	0.67
1:A:116:GLU:H	5:A:815:MES:H61	1.58	0.67
2:D:701:GLN:NE2	2:D:701:GLN:N	2.41	0.67
1:A:116:GLU:H	5:A:815:MES:C6	2.08	0.66
2:D:611:GLN:NE2	2:D:665:THR:HA	2.10	0.66
1:C:518:GLU:OE2	1:C:521:ARG:HD2	1.96	0.65
2:D:589:PRO:HD3	2:D:634:LEU:HD21	1.79	0.65
2:B:254:ASP:O	2:B:344:MET:HA	1.97	0.65
2:B:154:ASP:OD1	2:B:156:LYS:HB2	1.97	0.65
2:B:191:ARG:HD2	2:B:194:HIS:CD2	2.31	0.64
2:D:555:VAL:HG22	2:D:598:LYS:HB3	1.80	0.64
1:A:115:LEU:N	5:A:815:MES:H62	2.13	0.63
2:B:349:ARG:HG2	2:B:349:ARG:HH11	1.63	0.63
2:D:588:ILE:CG2	2:D:655:VAL:HG13	2.29	0.63
2:D:593:ARG:HH11	2:D:596:HIS:HD2	1.45	0.62
2:D:760:GLN:O	2:D:764:ARG:HG3	2.00	0.62
2:D:558:LYS:HE3	8:D:812:UDP:O2	2.00	0.61
2:D:555:VAL:CG2	2:D:598:LYS:HB3	2.30	0.61
1:C:412:HIS:NE2	1:C:525:PRO:CG	2.64	0.60
2:D:701:GLN:H	2:D:701:GLN:CD	2.05	0.60
2:D:669:PHE:CD1	2:D:673:ARG:HD2	2.37	0.60
1:A:102:ASP:HB2	9:A:1103:HOH:O	2.01	0.60
2:D:632:LYS:HD3	2:D:800:ILE:HD12	1.82	0.59
1:C:408:CYS:HB3	1:C:525:PRO:HG3	1.84	0.59
2:D:593:ARG:NH1	2:D:596:HIS:HD2	2.00	0.59
2:D:738:ASN:HD21	2:D:741:ILE:N	1.92	0.59
2:B:365:HIS:O	2:B:368:GLU:HG2	2.02	0.59
1:C:523:GLU:O	1:C:524:LYS:CG	2.50	0.59
2:B:390:LEU:O	2:B:391:TYR:HB3	2.04	0.58
2:B:316:GLY:HA2	2:B:363:ILE:HD11	1.85	0.58
2:B:336:ASN:HD22	2:B:336:ASN:C	2.07	0.58
2:D:719:GLU:OE1	7:D:810:UPG:O4'	2.21	0.58
1:A:12:ILE:HD13	1:A:89:ILE:CD1	2.33	0.58
2:D:657:LEU:HD21	2:D:679:MET:HE3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:815:MES:H31	9:A:948:HOH:O	2.04	0.57
2:B:158:VAL:HA	2:B:161:GLN:HE21	1.70	0.56
1:A:66:PHE:N	1:A:67:PRO:HD3	2.20	0.56
2:D:534:THR:HG22	2:D:535:ALA:N	2.21	0.56
2:B:138:SER:HB3	2:B:141:LEU:HD13	1.88	0.56
2:D:738:ASN:HD21	2:D:740:VAL:HG13	1.71	0.56
1:A:66:PHE:HD2	1:A:69:SER:HB2	1.70	0.55
1:C:457:ILE:HB	1:C:482:LEU:HD13	1.87	0.55
2:B:389:PRO:HG2	8:B:811:UDP:O4	2.06	0.55
2:D:738:ASN:HD21	2:D:740:VAL:CG1	2.19	0.55
2:B:157:LEU:O	2:B:160:GLN:HB3	2.07	0.55
2:D:746:MET:HE1	9:D:907:HOH:O	2.07	0.55
2:B:155:LEU:O	2:B:159:GLU:HG3	2.06	0.54
2:B:344:MET:HE2	9:B:919:HOH:O	2.06	0.54
2:B:180:HIS:CE1	2:B:265:ARG:HD2	2.43	0.54
2:B:191:ARG:HH11	2:B:194:HIS:HD2	1.53	0.54
2:D:710:PRO:HB3	2:D:726:ARG:NH2	2.23	0.54
2:D:539:GLU:CD	2:D:539:GLU:N	2.62	0.53
2:D:686:LEU:HD21	2:D:736:ARG:CZ	2.39	0.53
1:C:415:LYS:HD3	1:C:425:LEU:HD11	1.90	0.53
1:C:411:SER:O	1:C:415:LYS:HE2	2.08	0.53
2:D:729:PHE:CE2	2:D:769:LYS:HD3	2.43	0.53
1:A:12:ILE:HG22	1:A:23:LEU:HD21	1.91	0.53
2:B:272:HIS:HB3	2:B:334:ARG:HG2	1.91	0.52
2:B:196:LYS:HE3	9:B:1179:HOH:O	2.10	0.52
2:D:570:GLY:HA3	9:D:1296:HOH:O	2.08	0.52
2:D:537:PRO:HG3	2:D:541:PRO:HD3	1.92	0.52
2:B:230:LYS:HE2	2:B:398:ILE:HB	1.92	0.52
2:D:582:HIS:CE1	2:D:667:ARG:HD2	2.45	0.52
1:A:115:LEU:H	5:A:815:MES:H62	1.74	0.52
2:B:278:ASP:OD2	2:B:343:ARG:HG2	2.09	0.52
2:B:336:ASN:HD22	2:B:338:VAL:N	2.02	0.52
1:C:426:LEU:HD11	1:C:521:ARG:NH2	2.25	0.52
1:A:12:ILE:HD13	1:A:89:ILE:HD11	1.93	0.51
2:D:654:ASP:HB3	7:D:810:UPG:O3C	2.09	0.51
2:B:157:LEU:HA	2:B:160:GLN:HE21	1.75	0.51
2:B:157:LEU:HD22	2:B:160:GLN:HE22	1.75	0.51
1:A:8:VAL:O	1:A:12:ILE:HB	2.11	0.51
2:B:318:ASP:OD1	2:B:318:ASP:N	2.44	0.51
1:A:28:CYS:HB2	1:A:118:TRP:CD1	2.46	0.51
2:D:539:GLU:CD	2:D:539:GLU:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:TRP:CD2	2:B:401:PRO:HG3	2.47	0.50
2:D:710:PRO:HB3	2:D:726:ARG:HH21	1.77	0.50
2:D:679:MET:HE1	2:D:746:MET:HE3	1.93	0.50
2:B:308:PRO:HB3	2:B:324:ARG:NH2	2.27	0.50
2:D:674:HIS:HB3	2:D:736:ARG:HG2	1.93	0.50
2:D:716:TRP:NE1	7:D:810:UPG:H6'1	2.26	0.50
2:B:230:LYS:HD2	2:B:309:ASN:HB3	1.94	0.49
2:D:767:HIS:HD2	2:D:770:GLU:OE2	1.96	0.49
1:C:423:ILE:HG13	1:C:503:ILE:HD13	1.95	0.48
2:D:701:GLN:N	2:D:701:GLN:HE21	2.11	0.48
1:C:512:MET:SD	2:D:765:ILE:HD12	2.54	0.48
2:B:154:ASP:OD1	2:B:157:LEU:N	2.46	0.48
2:B:174:MET:HG2	9:B:1227:HOH:O	2.13	0.48
2:B:316:GLY:CA	2:B:363:ILE:HD11	2.44	0.48
2:B:225:MET:HE1	2:B:354:GLU:OE2	2.14	0.47
2:D:709:PHE:HB3	2:D:710:PRO:HD2	1.96	0.47
2:D:672:PRO:HG2	2:D:727:LEU:HD22	1.96	0.47
2:D:716:TRP:CD1	7:D:810:UPG:H6'1	2.49	0.47
2:B:253:VAL:HG22	7:B:809:UPG:H2C	1.95	0.47
2:D:638:PHE:O	2:D:642:LEU:CD2	2.60	0.47
2:D:611:GLN:HE22	2:D:665:THR:HA	1.78	0.47
2:B:336:ASN:ND2	2:B:336:ASN:C	2.68	0.46
2:D:627:MET:HA	2:D:754:LYS:O	2.15	0.46
1:A:114:LYS:H	5:A:815:MES:H21	1.81	0.46
2:B:236:PHE:CE2	2:B:375:LEU:HD11	2.51	0.46
2:D:607:ILE:O	2:D:611:GLN:HG3	2.16	0.46
2:B:327:PHE:CD2	2:B:367:LYS:HD3	2.51	0.46
2:B:201:TYR:O	2:B:204:PRO:HD2	2.16	0.46
2:B:225:MET:CE	2:B:352:LYS:HA	2.38	0.46
1:C:436:SER:HA	4:C:814:PG4:H32	1.97	0.46
2:D:655:VAL:HG22	7:D:810:UPG:O2C	2.16	0.46
2:D:679:MET:HE1	2:D:746:MET:CE	2.45	0.46
2:D:738:ASN:ND2	2:D:740:VAL:CG1	2.79	0.46
2:D:738:ASN:ND2	2:D:740:VAL:HG12	2.30	0.46
2:B:191:ARG:NH1	2:B:194:HIS:HD2	2.14	0.46
1:A:66:PHE:CD2	1:A:69:SER:HB2	2.50	0.45
1:A:12:ILE:CD1	1:A:89:ILE:HG12	2.47	0.45
2:B:232:LEU:HD22	2:B:250:PHE:HD2	1.81	0.45
2:B:186:ILE:CG2	2:B:253:VAL:HG13	2.47	0.45
2:D:738:ASN:ND2	2:D:740:VAL:N	2.65	0.45
1:A:12:ILE:HG22	1:A:23:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:760:GLN:OE1	2:D:764:ARG:NH1	2.50	0.45
1:A:12:ILE:O	1:A:12:ILE:CG2	2.64	0.45
1:A:42:VAL:HG12	1:A:43:ASN:O	2.16	0.45
1:A:116:GLU:HB2	5:A:815:MES:H61	1.97	0.45
2:B:171:TYR:HB3	2:B:213:TYR:CE2	2.51	0.45
1:C:405:LEU:CD2	1:C:409:LYS:HE2	2.43	0.45
1:A:13:LYS:HD3	1:A:23:LEU:HD11	1.98	0.45
1:C:445:ASN:ND2	1:C:450:THR:OG1	2.50	0.45
2:D:729:PHE:CD2	2:D:769:LYS:HD3	2.51	0.45
2:D:756:GLU:O	2:D:757:PRO:C	2.55	0.45
1:A:12:ILE:O	1:A:12:ILE:HG23	2.17	0.44
4:C:814:PG4:H51	2:D:716:TRP:HH2	1.82	0.44
2:D:729:PHE:CZ	2:D:769:LYS:HB2	2.52	0.44
2:B:157:LEU:HD22	2:B:160:GLN:NE2	2.32	0.44
2:B:240:LEU:HD12	2:B:240:LEU:HA	1.79	0.44
1:A:116:GLU:H	5:A:815:MES:H62	1.82	0.44
2:B:159:GLU:HA	2:B:390:LEU:HD21	1.99	0.44
2:B:355:PRO:O	2:B:357:PRO:HD3	2.18	0.44
2:D:753:LYS:NZ	2:D:753:LYS:HB3	2.33	0.44
1:A:17:GLY:O	1:A:18:TYR:C	2.56	0.44
2:B:327:PHE:CZ	2:B:367:LYS:HB2	2.52	0.44
2:D:600:TRP:CZ2	2:D:604:LEU:HG	2.52	0.44
2:D:700:LYS:HB3	2:D:701:GLN:HE22	1.82	0.44
2:D:753:LYS:O	2:D:754:LYS:HB2	2.18	0.44
1:C:406:THR:HG23	1:C:409:LYS:HD3	1.98	0.44
2:D:767:HIS:CD2	2:D:770:GLU:OE2	2.71	0.44
1:C:412:HIS:CD2	1:C:525:PRO:HG2	2.52	0.43
1:C:457:ILE:HD13	1:C:493:CYS:SG	2.58	0.43
1:C:472:GLU:O	1:C:473:ASN:C	2.55	0.43
2:D:738:ASN:ND2	2:D:740:VAL:H	2.16	0.43
2:B:240:LEU:HD11	2:B:248:PHE:HZ	1.83	0.43
4:C:814:PG4:H41	2:D:716:TRP:CZ3	2.54	0.43
1:A:114:LYS:HA	5:A:815:MES:HN4	1.84	0.43
2:D:593:ARG:HH11	2:D:596:HIS:CD2	2.32	0.43
2:D:596:HIS:HE1	9:D:1288:HOH:O	2.02	0.43
2:D:640:GLU:O	2:D:643:LYS:HB2	2.18	0.43
1:C:408:CYS:O	1:C:412:HIS:CD2	2.72	0.42
2:B:327:PHE:CE1	2:B:367:LYS:HB2	2.54	0.42
2:D:540:SER:HB3	2:D:543:LEU:HD13	2.01	0.42
1:C:406:THR:OG1	1:C:409:LYS:HD3	2.20	0.42
2:B:189:ARG:HB2	2:B:226:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HG23	1:A:15:ILE:HG22	2.02	0.42
1:A:17:GLY:O	1:A:20:GLY:N	2.48	0.42
2:B:157:LEU:HA	2:B:160:GLN:NE2	2.35	0.42
2:D:546:PRO:HA	2:D:660:MET:O	2.19	0.42
2:D:700:LYS:HB3	2:D:701:GLN:HE21	1.81	0.42
1:C:410:VAL:HG21	1:C:438:TYR:CD1	2.55	0.42
2:D:593:ARG:NH1	2:D:596:HIS:CD2	2.84	0.42
2:D:635:ASN:HB3	2:D:780:LEU:HD22	2.02	0.42
2:D:793:TYR:HE1	2:D:795:LYS:HB2	1.85	0.42
1:A:114:LYS:N	5:A:815:MES:H21	2.34	0.41
7:D:810:UPG:H1'	9:D:1203:HOH:O	2.19	0.41
2:D:576:MET:HG2	9:D:1115:HOH:O	2.20	0.41
2:B:275:VAL:HG22	2:B:334:ARG:HD3	2.02	0.41
2:D:642:LEU:HD21	2:D:650:PHE:CZ	2.55	0.41
1:C:463:CYS:HA	1:C:473:ASN:ND2	2.35	0.41
2:D:556:ASP:OD2	2:D:558:LYS:HB2	2.20	0.41
1:A:5:LYS:HD2	1:A:118:TRP:O	2.20	0.41
2:B:218:ILE:HD11	2:B:235:GLY:HA2	2.01	0.41
2:B:314:TRP:CZ2	7:B:809:UPG:H6'2	2.55	0.41
2:B:365:HIS:O	2:B:366:THR:C	2.59	0.41
1:A:44:ASP:HB3	1:A:45:ASN:H	1.73	0.41
1:A:85:LEU:O	1:A:89:ILE:HG13	2.21	0.41
2:B:358:GLN:O	2:B:362:ARG:HG3	2.21	0.41
1:C:523:GLU:O	1:C:524:LYS:CE	2.68	0.41
1:C:412:HIS:HA	1:C:415:LYS:HE2	2.02	0.41
2:D:559:LEU:O	2:D:562:GLN:HB3	2.21	0.41
2:D:604:LEU:HD13	2:D:604:LEU:HA	1.92	0.41
2:D:635:ASN:O	2:D:638:PHE:HB3	2.21	0.41
2:B:319:ASP:O	2:B:322:TYR:HB3	2.22	0.40
1:C:417:ILE:HG12	1:C:417:ILE:O	2.21	0.40
1:C:445:ASN:HD22	1:C:445:ASN:HA	1.63	0.40
1:C:496:LYS:HE3	9:C:1281:HOH:O	2.21	0.40
2:B:160:GLN:O	2:B:163:PRO:HD3	2.21	0.40
1:C:414:ILE:O	1:C:417:ILE:HG22	2.22	0.40
1:C:510:LYS:N	1:C:511:PRO:HD2	2.37	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	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
1	C	121/123 (98%)	115 (95%)	5 (4%)	1 (1%)	19	23
2	B	270/286 (94%)	264 (98%)	6 (2%)	0	100	100
2	D	270/286 (94%)	256 (95%)	14 (5%)	0	100	100
All	All	782/818 (96%)	748 (96%)	33 (4%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	524	LYS

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	109/109 (100%)	103 (94%)	6 (6%)	21	29
1	C	109/109 (100%)	105 (96%)	4 (4%)	34	47
2	B	245/254 (96%)	230 (94%)	15 (6%)	18	25
2	D	245/254 (96%)	227 (93%)	18 (7%)	14	17
All	All	708/726 (98%)	665 (94%)	43 (6%)	18	25

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	66	PHE
1	A	68	GLU
1	A	71	ASN
1	A	88	ASP
1	A	113	GLU
2	B	141	LEU
2	B	150	ASN
2	B	153	VAL
2	B	157	LEU
2	B	164	LYS
2	B	189	ARG
2	B	195	LEU
2	B	240	LEU
2	B	263	THR
2	B	270	PRO
2	B	299	GLN
2	B	302	LEU
2	B	328	ARG
2	B	336	ASN
2	B	339	ILE
1	C	445	ASN
1	C	470	GLU
1	C	487	LEU
1	C	490	ASP
2	D	539	GLU
2	D	553	ILE
2	D	555	VAL
2	D	566	LYS
2	D	577	ASP
2	D	591	ARG
2	D	597	LEU
2	D	655	VAL
2	D	665	THR
2	D	671	GLN
2	D	681	LYS
2	D	689	VAL
2	D	701	GLN
2	D	704	LEU
2	D	730	ARG
2	D	738	ASN
2	D	741	ILE
2	D	770	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	71	ASN
2	B	160	GLN
2	B	161	GLN
2	B	194	HIS
2	B	210	GLN
2	B	305	ASN
2	B	310	ASN
2	B	336	ASN
2	B	386	GLN
1	C	445	ASN
1	C	473	ASN
2	D	562	GLN
2	D	563	GLN
2	D	582	HIS
2	D	596	HIS
2	D	612	GLN
2	D	671	GLN
2	D	701	GLN
2	D	707	ASN
2	D	712	ASN
2	D	738	ASN
2	D	767	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)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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	$\#\|Z\| > 2$
4	PG4	C	814	-	12,12,12	0.52	0	11,11,11	0.19	0
4	PG4	A	813	-	12,12,12	0.55	0	11,11,11	0.29	0
8	UDP	B	811	-	24,26,26	1.26	2 (8%)	37,40,40	1.47	7 (18%)
8	UDP	D	812	-	24,26,26	1.26	3 (12%)	37,40,40	1.48	7 (18%)
7	UPG	D	810	6	35,38,38	1.67	6 (17%)	53,58,58	2.32	16 (30%)
5	MES	A	815	-	12,12,12	1.52	3 (25%)	14,16,16	0.85	0
7	UPG	B	809	6	35,38,38	1.37	6 (17%)	53,58,58	2.24	14 (26%)

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
4	PG4	C	814	-	-	3/10/10/10	-
4	PG4	A	813	-	-	6/10/10/10	-
8	UDP	B	811	-	-	2/16/32/32	0/2/2/2
8	UDP	D	812	-	-	3/16/32/32	0/2/2/2
7	UPG	D	810	6	-	3/23/59/59	0/3/3/3
5	MES	A	815	-	-	2/6/14/14	0/1/1/1
7	UPG	B	809	6	-	3/23/59/59	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	810	UPG	O5'-C1'	4.31	1.52	1.41
7	D	810	UPG	C1'-C2'	4.02	1.64	1.52
7	D	810	UPG	PB-O3B	-3.86	1.50	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	812	UDP	PB-O1B	3.58	1.62	1.50
7	B	809	UPG	PB-O3B	-3.53	1.51	1.60
8	B	811	UDP	PB-O1B	3.45	1.61	1.50
7	B	809	UPG	O5'-C1'	2.86	1.49	1.41
5	A	815	MES	C5-N4	2.70	1.54	1.46
7	D	810	UPG	O4'-C4'	-2.67	1.36	1.43
7	B	809	UPG	C1'-C2'	2.66	1.60	1.52
7	D	810	UPG	O5'-C5'	2.59	1.50	1.44
7	B	809	UPG	O4'-C4'	-2.52	1.37	1.43
8	B	811	UDP	C2-N1	2.50	1.42	1.38
5	A	815	MES	C7-N4	2.36	1.52	1.47
7	D	810	UPG	PB-O1B	2.30	1.59	1.50
5	A	815	MES	C3-N4	2.27	1.53	1.46
7	B	809	UPG	C3C-C2C	-2.25	1.47	1.53
8	D	812	UDP	C2-N1	2.12	1.41	1.38
7	B	809	UPG	O5'-C5'	2.08	1.49	1.44
8	D	812	UDP	C4-N3	2.04	1.42	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	810	UPG	O4'-C4'-C3'	6.95	126.42	110.35
7	B	809	UPG	O5'-C5'-C6'	-6.87	89.36	106.44
7	D	810	UPG	C4'-C3'-C2'	-6.27	99.89	110.82
7	B	809	UPG	O4'-C4'-C3'	5.99	124.19	110.35
7	B	809	UPG	O3B-PB-O1B	5.66	130.72	109.47
7	D	810	UPG	O3B-PB-O1B	5.51	130.16	109.47
7	D	810	UPG	O5'-C5'-C4'	-5.51	99.69	109.69
7	B	809	UPG	O5'-C1'-O3B	5.44	118.47	111.36
7	B	809	UPG	C4'-C3'-C2'	-5.16	101.82	110.82
7	D	810	UPG	O5'-C1'-O3B	5.04	117.95	111.36
8	B	811	UDP	O3B-PB-O1B	3.96	126.18	110.68
8	D	812	UDP	O3B-PB-O1B	3.79	125.53	110.68
7	D	810	UPG	O4C-C4C-C3C	-3.55	98.08	105.11
8	B	811	UDP	O5'-C5'-C4'	3.40	120.68	108.99
7	B	809	UPG	O4C-C4C-C3C	-3.25	98.68	105.11
7	B	809	UPG	C3'-C4'-C5'	3.16	115.87	110.24
7	D	810	UPG	O2-C2-N1	-3.01	118.78	122.79
8	D	812	UDP	O2-C2-N1	-3.00	118.80	122.79
8	D	812	UDP	C2'-C1'-N1	2.78	121.09	113.22
8	D	812	UDP	O5'-C5'-C4'	2.74	118.43	108.99
7	D	810	UPG	O3A-PB-O3B	2.68	107.89	102.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	811	UDP	C2'-C1'-N1	2.65	120.72	113.22
7	B	809	UPG	O5'-C5'-C4'	-2.61	104.96	109.69
7	D	810	UPG	C6'-C5'-C4'	2.60	119.09	113.00
7	D	810	UPG	O4'-C4'-C5'	2.59	115.72	109.30
7	B	809	UPG	O3'-C3'-C4'	-2.57	104.41	110.35
8	B	811	UDP	O2-C2-N1	-2.54	119.40	122.79
7	B	809	UPG	O2-C2-N1	-2.53	119.43	122.79
7	D	810	UPG	PB-O3B-C1'	2.50	129.40	119.74
7	D	810	UPG	C2C-C1C-N1	2.50	120.28	113.22
8	D	812	UDP	O2-C2-N3	2.48	126.12	121.50
7	D	810	UPG	O2'-C2'-C3'	-2.36	104.88	110.35
8	B	811	UDP	O2-C2-N3	2.34	125.86	121.50
8	D	812	UDP	O3A-PB-O1B	-2.31	98.38	111.19
8	B	811	UDP	O4'-C4'-C3'	-2.30	100.57	105.11
7	D	810	UPG	C1'-O5'-C5'	-2.26	109.25	113.69
7	B	809	UPG	PB-O3B-C1'	2.26	128.46	119.74
8	D	812	UDP	O4'-C4'-C3'	-2.25	100.66	105.11
8	B	811	UDP	O3A-PB-O1B	-2.24	98.77	111.19
7	D	810	UPG	O2-C2-N3	2.19	125.57	121.50
7	B	809	UPG	O2A-PA-O5C	2.12	117.61	107.75
7	B	809	UPG	C2C-C1C-N1	2.07	119.09	113.22
7	B	809	UPG	O2-C2-N3	2.04	125.31	121.50
7	D	810	UPG	O5'-C5'-C6'	-2.02	101.40	106.44

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	809	UPG	O5'-C1'-O3B-PB
7	D	810	UPG	O5'-C1'-O3B-PB
8	B	811	UDP	C3'-C4'-C5'-O5'
8	B	811	UDP	O4'-C4'-C5'-O5'
8	D	812	UDP	O4'-C4'-C5'-O5'
8	D	812	UDP	C5'-O5'-PA-O1A
8	D	812	UDP	C5'-O5'-PA-O3A
4	A	813	PG4	O3-C5-C6-O4
7	D	810	UPG	O5'-C5'-C6'-O6'
4	C	814	PG4	O4-C7-C8-O5
7	B	809	UPG	C1'-O3B-PB-O3A
7	D	810	UPG	C1'-O3B-PB-O3A
4	A	813	PG4	O2-C3-C4-O3
4	A	813	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	A	813	PG4	C3-C4-O3-C5
4	C	814	PG4	C8-C7-O4-C6
4	A	813	PG4	C1-C2-O2-C3
4	A	813	PG4	O4-C7-C8-O5
5	A	815	MES	C8-C7-N4-C5
4	C	814	PG4	C4-C3-O2-C2
7	B	809	UPG	PA-O3A-PB-O2B
5	A	815	MES	C8-C7-N4-C3

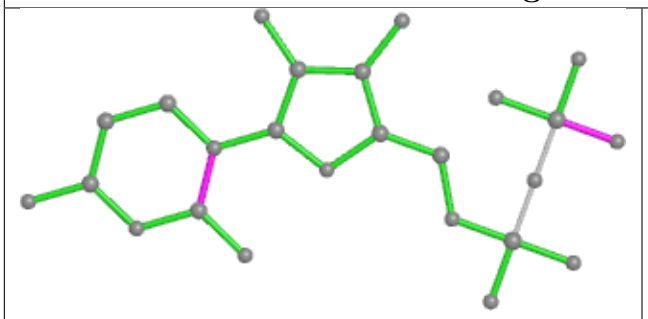
There are no ring outliers.

6 monomers are involved in 24 short contacts:

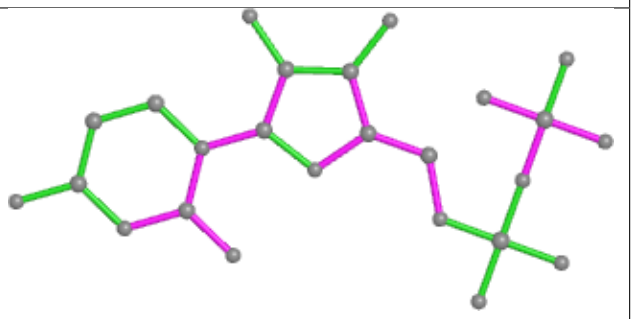
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	814	PG4	3	0
8	B	811	UDP	1	0
8	D	812	UDP	1	0
7	D	810	UPG	6	0
5	A	815	MES	11	0
7	B	809	UPG	2	0

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.

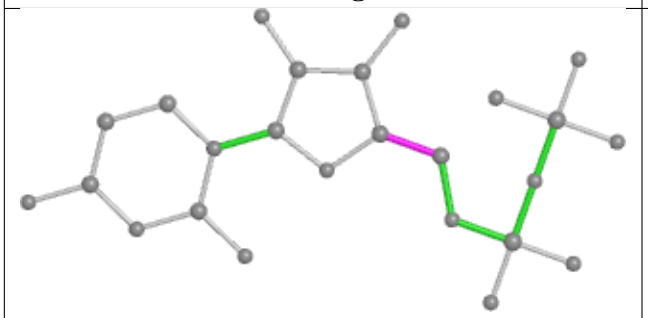
Ligand UDP B 811



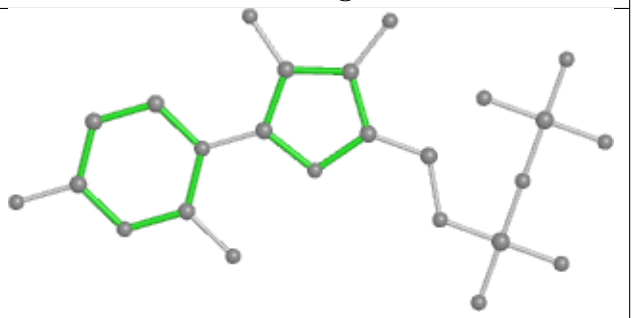
Bond lengths



Bond angles

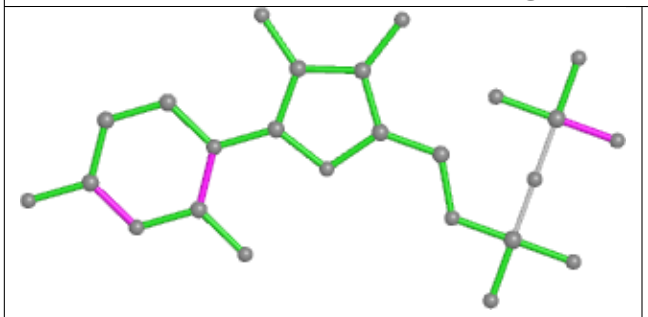


Torsions

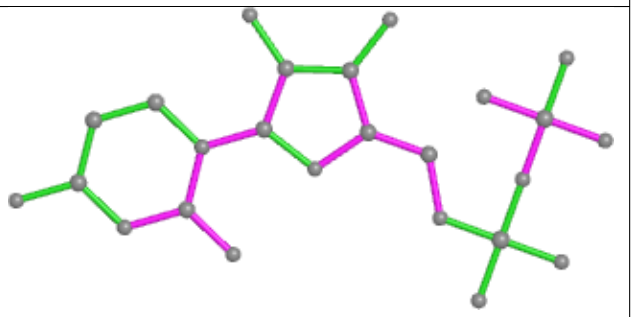


Rings

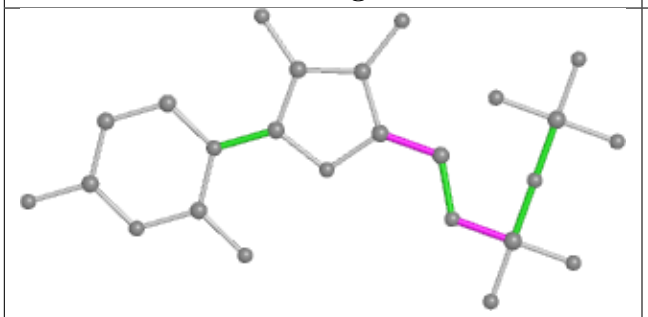
Ligand UDP D 812



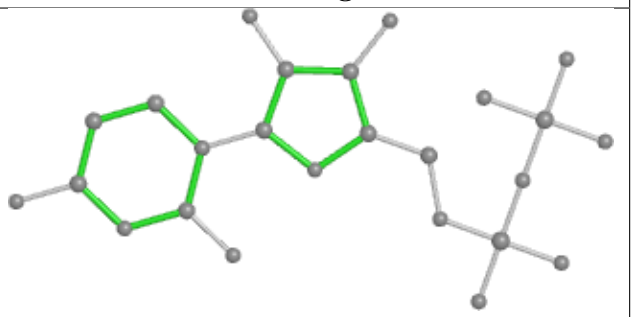
Bond lengths



Bond angles

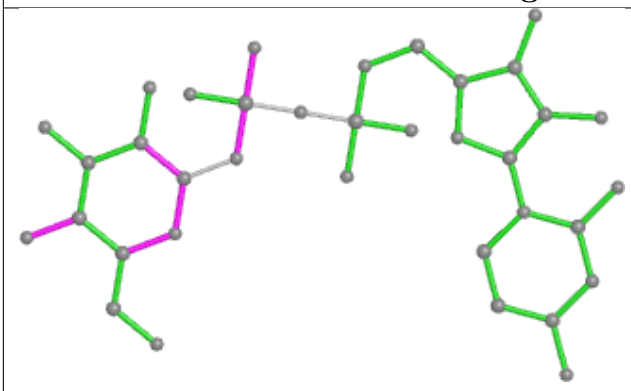


Torsions

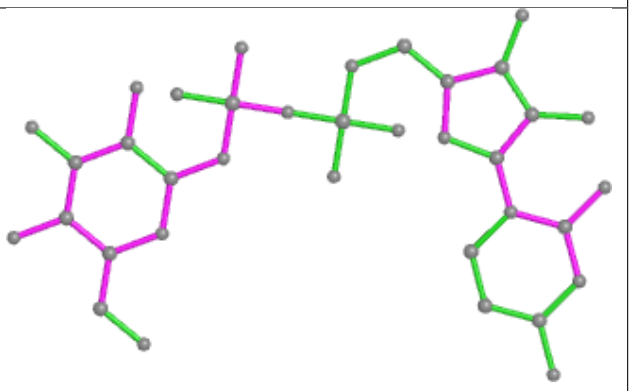


Rings

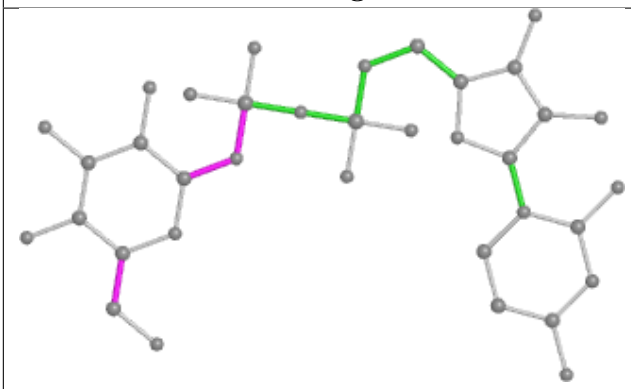
Ligand UPG D 810



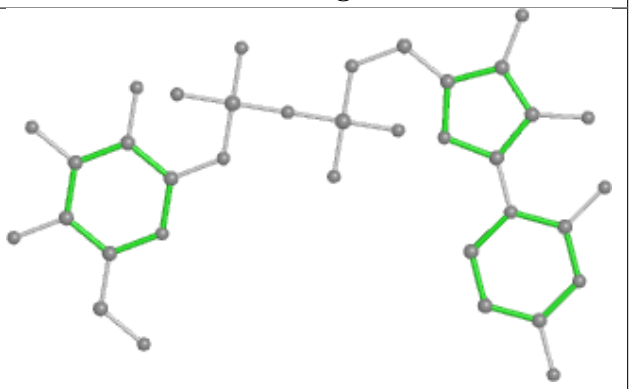
Bond lengths



Bond angles

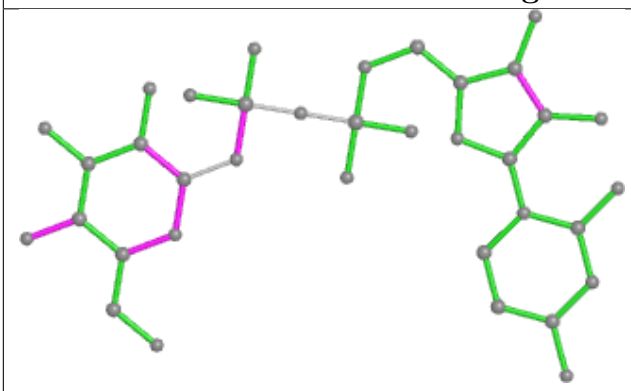


Torsions

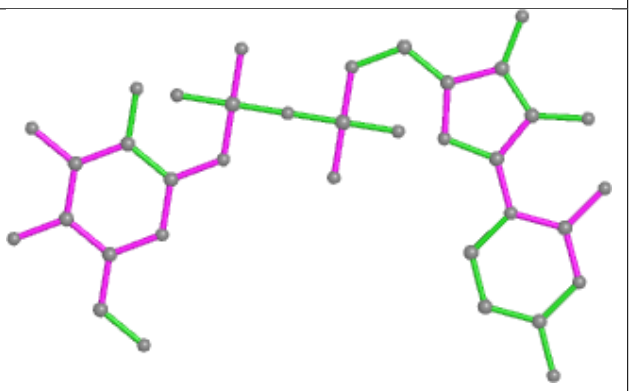


Rings

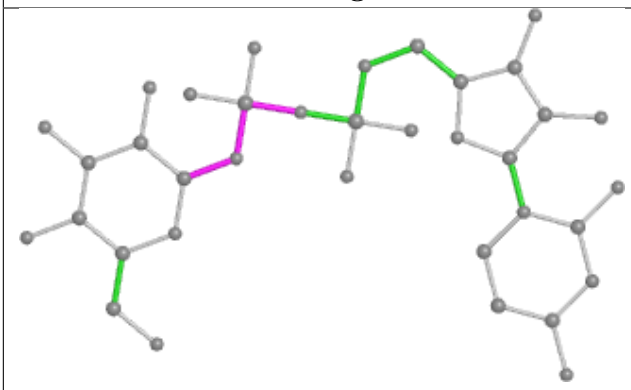
Ligand UPG B 809



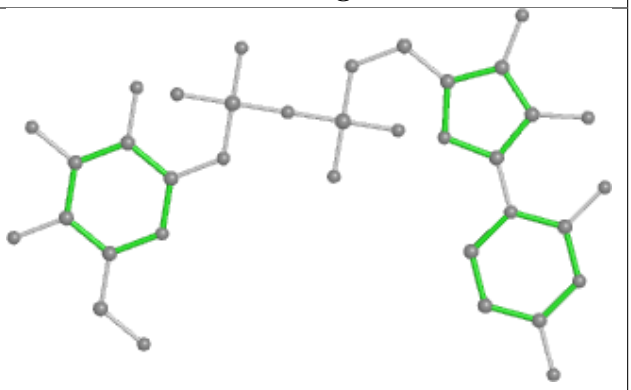
Bond lengths



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 (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	123/123 (100%)	0.06	8 (6%)	18	24	31, 45, 71, 91	0
1	C	123/123 (100%)	-0.04	5 (4%)	37	44	29, 40, 66, 107	0
2	B	272/286 (95%)	-0.10	6 (2%)	62	69	29, 44, 69, 81	0
2	D	272/286 (95%)	-0.08	7 (2%)	56	63	33, 46, 67, 83	0
All	All	790/818 (96%)	-0.06	26 (3%)	46	53	29, 45, 69, 107	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	525	PRO	9.4
2	D	804	SER	5.0
2	B	402	SER	4.8
1	A	68	GLU	4.1
2	D	534	THR	4.0
2	D	533	LEU	3.7
1	C	524	LYS	3.3
1	A	66	PHE	3.3
2	D	576	MET	3.2
2	B	160	GLN	3.1
1	C	470	GLU	3.1
1	A	67	PRO	3.0
1	A	123	PRO	3.0
2	D	748	ARG	2.9
1	C	448	GLY	2.7
2	D	773	LEU	2.7
2	B	346	ARG	2.6
1	A	122	LYS	2.5
1	A	64	SER	2.4
2	B	131	LEU	2.3
2	D	553	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	432	LEU	2.2
1	A	45	ASN	2.2
2	B	229	ALA	2.2
2	B	150	ASN	2.1
1	A	65	GLU	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)

There are no monosaccharides in this entry.

6.4 Ligands (i)

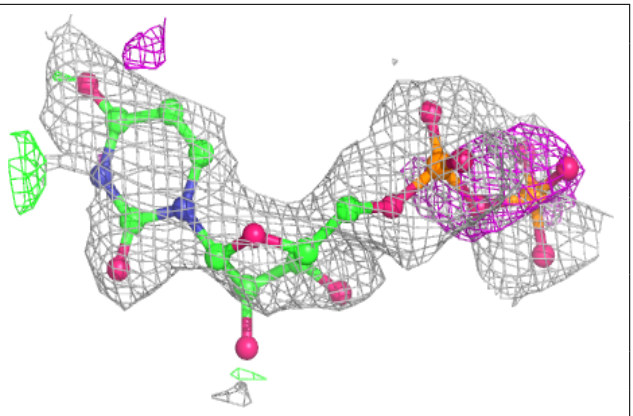
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

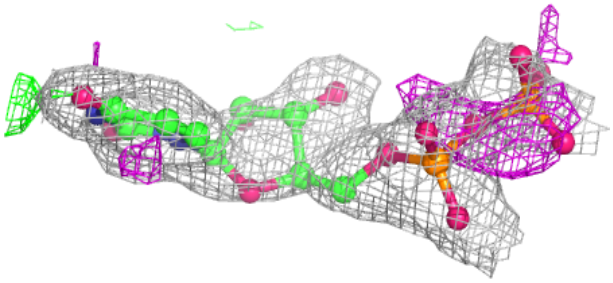
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	UDP	D	812	25/25	0.61	0.32	80,95,111,112	0
5	MES	A	815	12/12	0.68	0.38	75,79,93,94	0
4	PG4	C	814	13/13	0.70	0.32	79,82,83,83	0
8	UDP	B	811	25/25	0.74	0.26	82,96,116,117	0
4	PG4	A	813	13/13	0.78	0.30	67,75,82,83	0
7	UPG	B	809	36/36	0.96	0.12	38,44,47,48	0
7	UPG	D	810	36/36	0.96	0.12	37,44,55,58	0
3	CA	C	806	1/1	0.98	0.05	36,36,36,36	0
3	CA	A	805	1/1	0.98	0.06	42,42,42,42	0
6	MN	B	807	1/1	0.99	0.05	40,40,40,40	0
6	MN	D	808	1/1	1.00	0.08	37,37,37,37	0

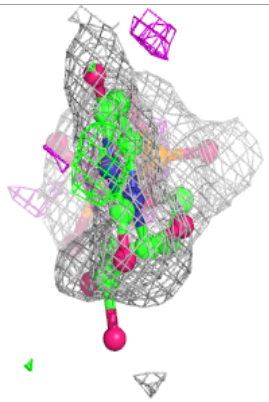
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UDP D 812:

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

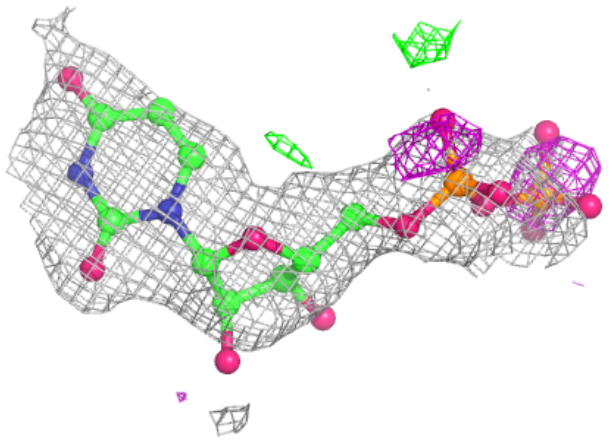


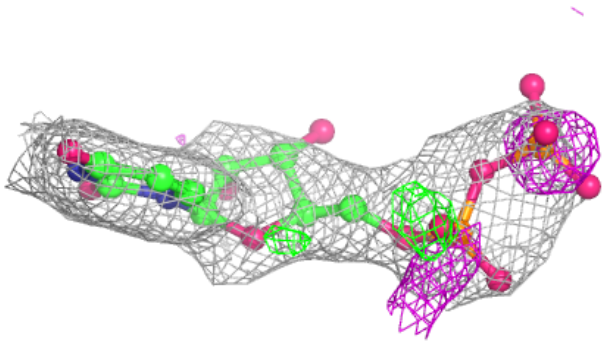


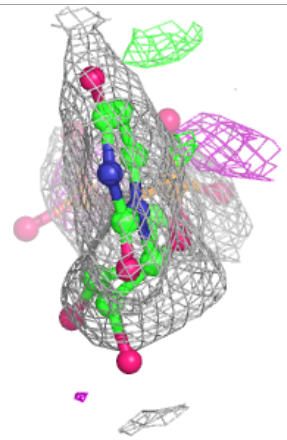


Electron density around UDP B 811:

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

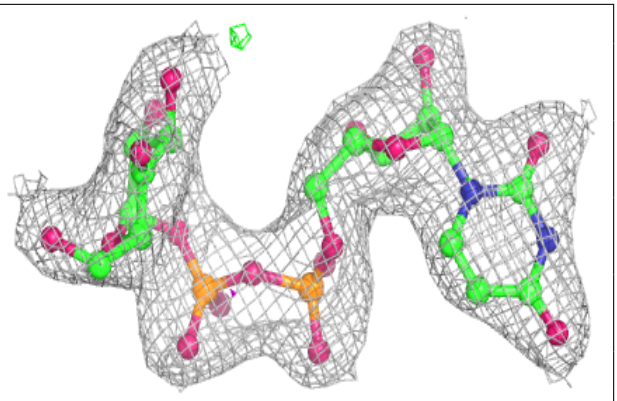


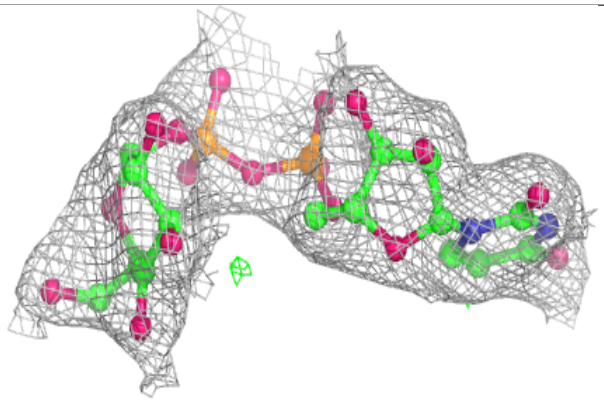


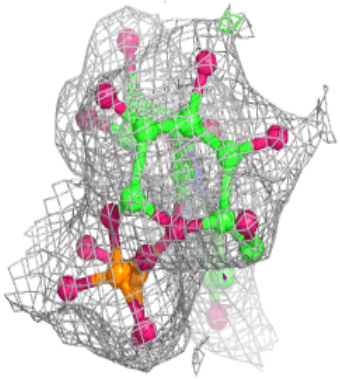


Electron density around UPG B 809:

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







Electron density around UPG D 810:

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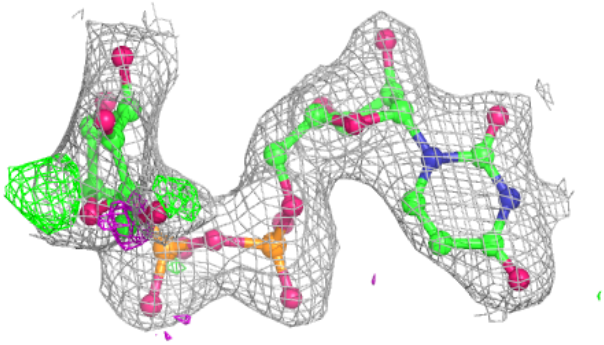
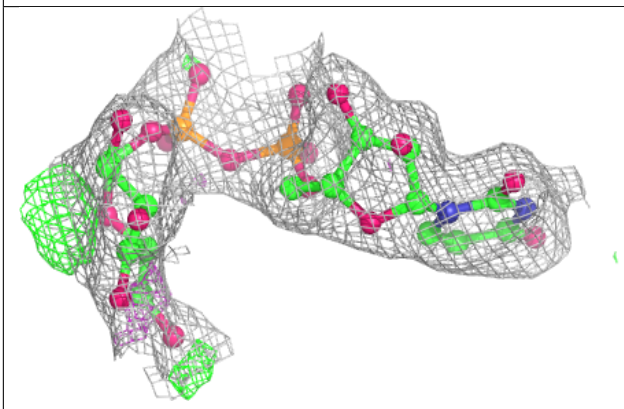
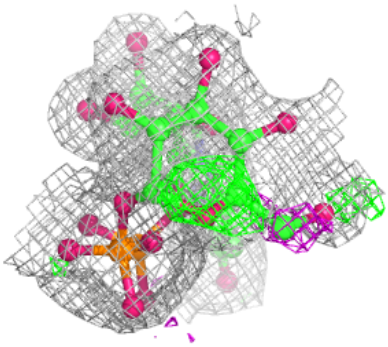
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.