



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:29 AM UTC

PDB ID : 7VA8 / pdb_00007va8
Title : Crystal structure of MiCGT
Authors : Zhong, L.; Zhang, Z.M.
Deposited on : 2021-08-27
Resolution : 2.85 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

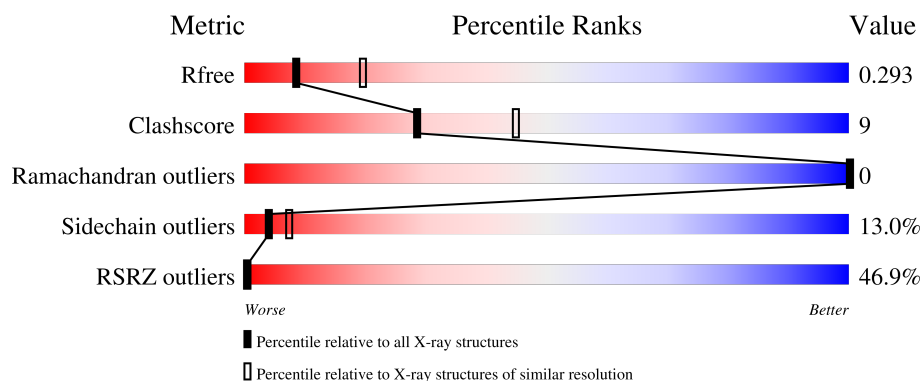
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	470	45% 70% 23% . .
1	B	470	44% 68% 21% . 7%

2 Entry composition [i](#)

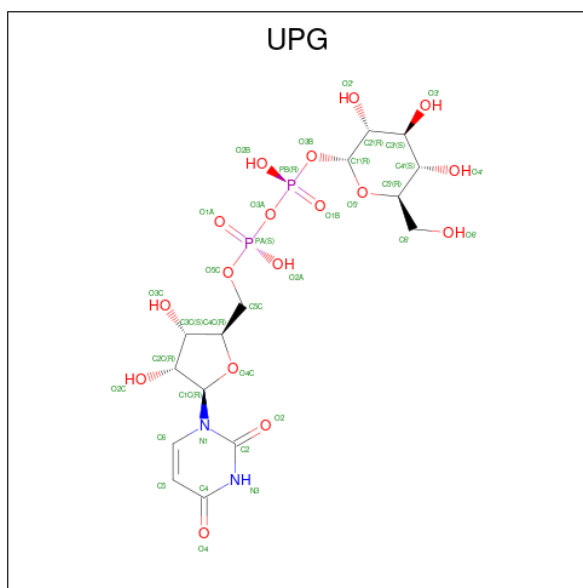
There are 2 unique types of molecules in this entry. The entry contains 6687 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-glycosyltransferase 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3510	2250	595	650	15			
1	B	439	Total	C	N	O	S	0	0	0
			3105	1997	527	567	14			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

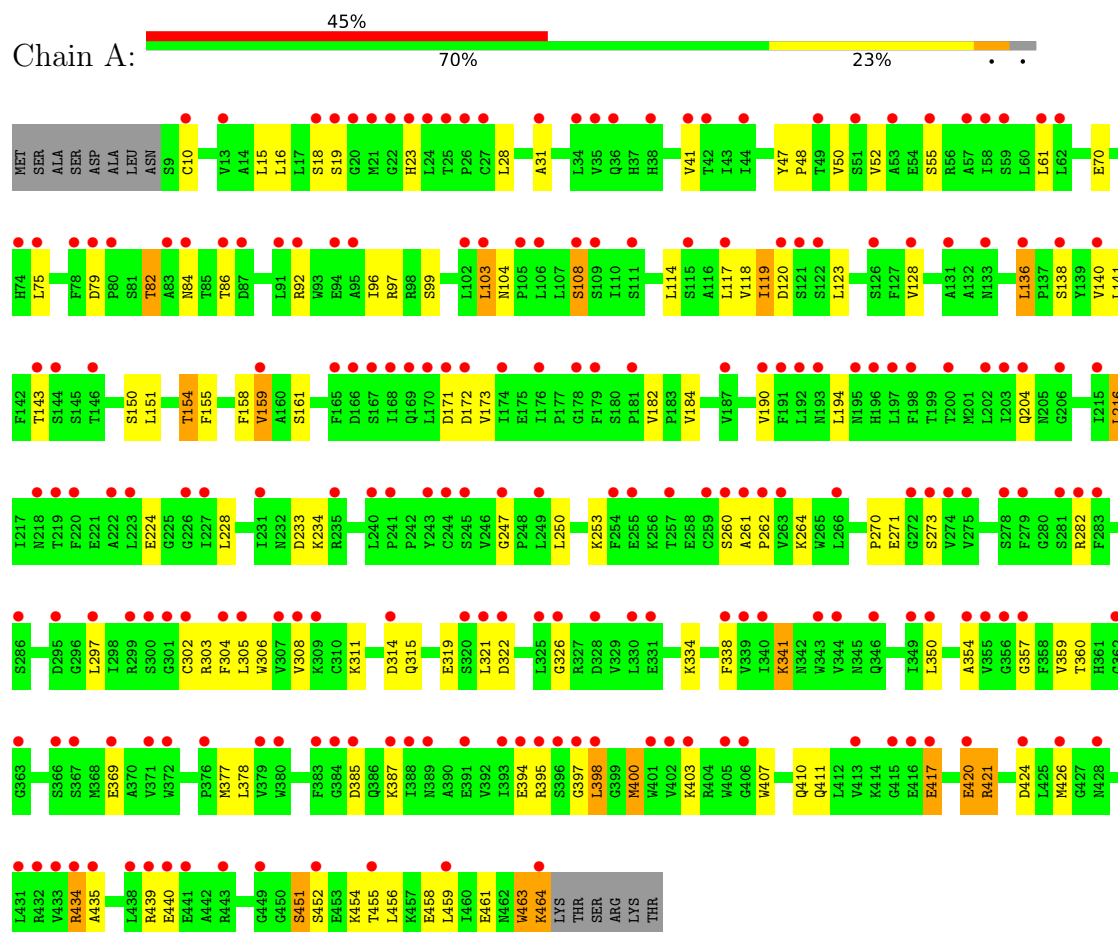


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

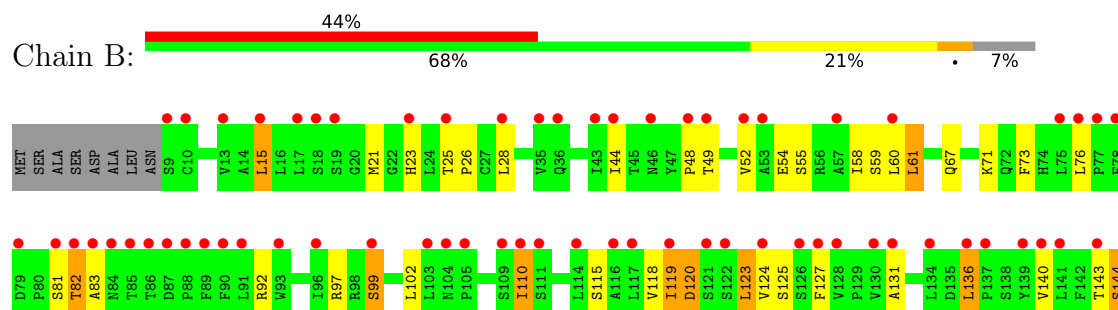
3 Residue-property plots

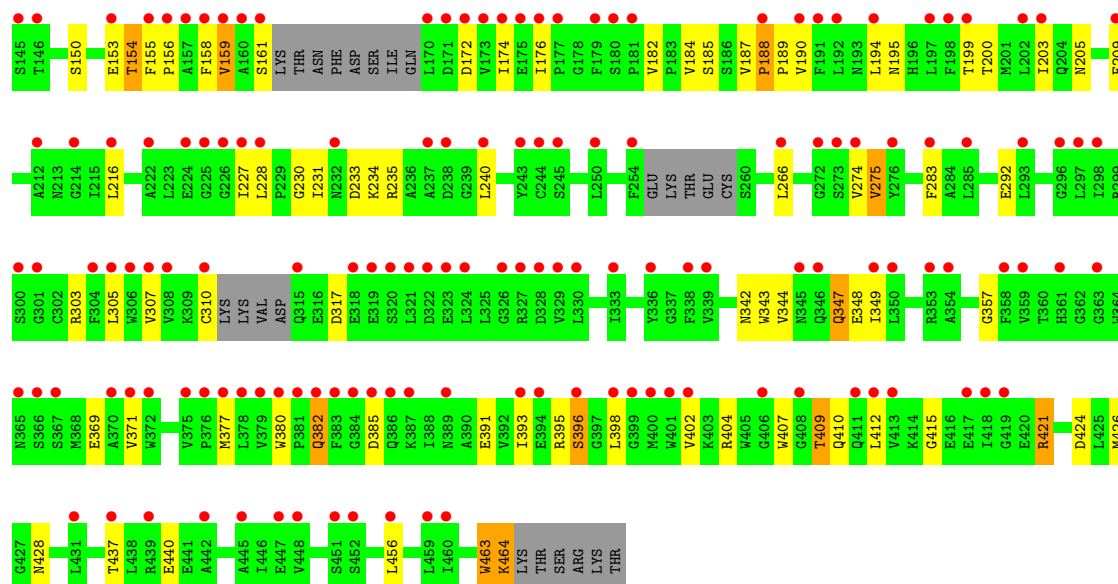
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-glycosyltransferase 13



• Molecule 1: UDP-glycosyltransferase 13





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.39Å 104.68Å 109.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.74 – 2.85 75.74 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (75.74-2.85) 94.2 (75.74-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.9_1692+SVN	Depositor
R, R_{free}	0.262 , 0.286 0.273 , 0.293	Depositor DCC
R_{free} test set	2006 reflections (7.86%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6687	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.36	0/3597	0.81	6/4900 (0.1%)
1	B	0.35	0/3182	0.83	3/4372 (0.1%)
All	All	0.36	0/6779	0.82	9/9272 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	463	TRP	N-CA-C	6.73	121.50	113.28
1	A	463	TRP	N-CA-C	6.66	121.63	112.90
1	A	173	VAL	N-CA-C	5.66	116.22	110.05
1	A	128	VAL	CA-C-N	-5.45	113.41	119.19
1	A	128	VAL	C-N-CA	-5.45	113.41	119.19
1	A	10	CYS	CA-C-N	5.39	125.70	119.93
1	A	10	CYS	C-N-CA	5.39	125.70	119.93
1	B	188	PRO	CA-C-N	5.26	125.31	119.32
1	B	188	PRO	C-N-CA	5.26	125.31	119.32

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	3510	0	3451	55	0
1	B	3105	0	2843	59	0
2	A	36	0	22	0	0
2	B	36	0	22	1	0
All	All	6687	0	6338	114	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 9.

All (114) 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:B:76:LEU:H	1:B:99:SER:HB3	1.53	0.73
1:B:463:TRP:N	1:B:464:LYS:HA	2.04	0.73
1:B:28:LEU:HD22	1:B:61:LEU:HD22	1.71	0.72
1:A:104:ASN:O	1:A:108:SER:OG	2.07	0.72
1:B:407:TRP:HB2	1:B:410:GLN:HB2	1.72	0.70
1:A:48:PRO:O	1:A:92:ARG:NH2	2.26	0.69
1:B:357:GLY:HA3	1:B:426:MET:HE1	1.75	0.69
1:B:342:ASN:OD1	1:B:343:TRP:N	2.28	0.67
1:A:150:SER:O	1:A:154:THR:OG1	2.11	0.67
1:B:380:TRP:O	1:B:382:GLN:NE2	2.28	0.66
1:B:150:SER:O	1:B:154:THR:OG1	2.12	0.66
1:B:153:GLU:HG3	1:B:209:PHE:HD2	1.62	0.65
1:B:144:SER:OG	1:B:385:ASP:OD2	2.14	0.65
1:B:174:ILE:HD12	1:B:187:VAL:HG21	1.79	0.65
1:B:48:PRO:O	1:B:92:ARG:NH2	2.30	0.65
1:B:421:ARG:NH1	1:B:424:ASP:OD2	2.30	0.64
1:A:421:ARG:NH1	1:A:424:ASP:OD2	2.31	0.64
1:A:97:ARG:NH2	1:A:204:GLN:OE1	2.31	0.64
1:B:23:HIS:ND1	1:B:120:ASP:OD2	2.31	0.64
1:B:115:SER:OG	1:B:463:TRP:O	2.15	0.63
1:A:23:HIS:HA	1:A:143:THR:HG21	1.79	0.63
1:B:153:GLU:OE1	1:B:235:ARG:NH2	2.32	0.62
1:A:15:LEU:HD22	1:A:118:VAL:HB	1.81	0.62
1:A:28:LEU:HD22	1:A:61:LEU:HD22	1.83	0.60
1:A:119:ILE:HD11	1:A:123:LEU:HB2	1.83	0.60
1:A:398:LEU:HD12	1:A:435:ALA:HA	1.84	0.60
1:A:463:TRP:N	1:A:464:LYS:HA	2.17	0.60
1:A:319:GLU:O	1:A:341:LYS:NZ	2.36	0.58
1:B:158:PHE:O	1:B:161:SER:OG	2.23	0.57
1:A:47:TYR:OH	1:A:70:GLU:OE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:THR:HG21	1:A:377:MET:HE3	1.86	0.56
1:A:387:LYS:HB2	1:A:407:TRP:CH2	2.41	0.55
1:A:417:GLU:HA	1:A:420:GLU:HG3	1.89	0.55
1:B:23:HIS:HA	1:B:143:THR:HG21	1.89	0.54
1:B:49:THR:OG1	1:B:55:SER:OG	2.24	0.53
1:B:172:ASP:O	1:B:184:VAL:HG23	2.09	0.53
1:A:23:HIS:ND1	1:A:120:ASP:OD1	2.40	0.53
1:B:125:SER:HB3	1:B:205:ASN:HA	1.91	0.52
1:A:357:GLY:HA3	1:A:426:MET:HE1	1.92	0.51
1:B:283:PHE:CZ	1:B:382:GLN:HG2	2.45	0.51
1:A:407:TRP:HB2	1:A:410:GLN:HG2	1.91	0.51
1:A:359:VAL:HG22	1:A:378:LEU:HD23	1.93	0.51
1:B:15:LEU:HD22	1:B:118:VAL:HB	1.93	0.51
1:B:199:THR:O	1:B:203:ILE:HG12	2.11	0.50
1:B:233:ASP:OD1	1:B:234:LYS:N	2.44	0.50
1:A:151:LEU:HD13	1:A:182:VAL:HG11	1.93	0.50
1:A:271:GLU:HA	1:A:354:ALA:HA	1.94	0.49
1:A:171:ASP:HA	1:A:184:VAL:HB	1.95	0.49
1:A:261:ALA:HA	1:A:264:LYS:HE3	1.95	0.49
1:A:385:ASP:OD1	1:A:385:ASP:N	2.45	0.49
1:B:82:THR:N	1:B:83:ALA:HB3	2.28	0.49
1:B:156:PRO:O	1:B:159:VAL:HG23	2.13	0.49
1:B:391:GLU:O	1:B:395:ARG:N	2.44	0.49
1:A:31:ALA:HB1	1:A:41:VAL:HG11	1.94	0.48
1:B:292:GLU:OE1	1:B:415:GLY:N	2.47	0.48
1:B:421:ARG:HD3	1:B:421:ARG:HA	1.66	0.47
1:B:119:ILE:HD11	1:B:123:LEU:C	2.40	0.47
1:B:393:ILE:O	1:B:396:SER:OG	2.25	0.47
1:B:67:GLN:OE1	1:B:67:GLN:N	2.42	0.47
1:B:227:ILE:O	1:B:231:ILE:HG13	2.15	0.47
1:A:52:VAL:HG23	1:A:315:GLN:HG3	1.96	0.47
1:B:235:ARG:HG2	1:B:240:LEU:HD12	1.97	0.47
1:A:50:VAL:CG2	1:A:92:ARG:HG3	2.44	0.47
1:A:117:LEU:HB2	1:A:136:LEU:HD13	1.96	0.47
1:B:176:ILE:HD11	1:B:182:VAL:HG12	1.97	0.47
1:B:131:ALA:HB1	1:B:136:LEU:O	2.15	0.46
1:A:378:LEU:HD13	1:A:400:MET:HE2	1.97	0.46
1:B:25:THR:HB	1:B:26:PRO:HD3	1.97	0.46
1:B:266:LEU:HD21	1:B:305:LEU:HD12	1.98	0.45
1:B:347:GLN:HG3	1:B:348:GLU:N	2.32	0.45
1:B:155:PHE:N	1:B:156:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:O	1:A:159:VAL:HG13	2.17	0.45
1:B:371:VAL:HG22	1:B:398:LEU:HD22	1.98	0.45
1:B:230:GLY:HA2	1:B:233:ASP:OD2	2.18	0.44
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.81	0.44
1:B:119:ILE:HD13	1:B:127:PHE:HB2	1.98	0.44
1:B:124:VAL:HG21	1:B:209:PHE:HE1	1.81	0.44
1:B:188:PRO:HA	1:B:189:PRO:HD3	1.82	0.44
1:A:16:LEU:HD23	1:A:119:ILE:HD13	1.99	0.44
1:B:275:VAL:HG23	1:B:303:ARG:O	2.16	0.44
1:B:110:ILE:H	1:B:110:ILE:HG12	1.54	0.44
1:B:310:CYS:HB2	1:B:317:ASP:OD1	2.18	0.44
1:A:306:TRP:CE2	1:A:308:VAL:HG22	2.53	0.44
1:B:382:GLN:O	1:B:409:THR:OG1	2.28	0.43
1:A:451:SER:O	1:A:455:THR:HG23	2.19	0.43
1:B:71:LYS:NZ	1:B:110:ILE:HD13	2.33	0.43
1:A:417:GLU:O	1:A:421:ARG:HG2	2.18	0.43
1:A:75:LEU:HD22	1:A:96:ILE:HA	2.00	0.43
1:A:270:PRO:O	1:A:273:SER:OG	2.31	0.43
1:A:305:LEU:HG	1:A:338:PHE:HB3	2.01	0.43
1:A:350:LEU:HD12	1:A:369:GLU:HB3	1.99	0.43
1:B:81:SER:C	1:B:83:ALA:HB3	2.43	0.43
1:B:275:VAL:HG13	1:B:426:MET:HE3	2.01	0.43
1:A:322:ASP:O	1:A:326:GLY:HA2	2.19	0.43
1:A:79:ASP:O	1:A:82:THR:OG1	2.37	0.43
1:A:247:GLY:O	1:A:452:SER:OG	2.24	0.43
1:B:44:ILE:HG22	1:B:73:PHE:HB2	2.01	0.43
1:A:216:LEU:HD11	1:A:459:LEU:HD11	2.01	0.42
1:A:314:ASP:OD1	1:A:315:GLN:N	2.53	0.42
1:B:369:GLU:OE1	2:B:501:UPG:O3C	2.35	0.42
1:A:261:ALA:N	1:A:262:PRO:HD2	2.34	0.42
1:A:397:GLY:O	1:A:434:ARG:NH2	2.53	0.42
1:A:439:ARG:NH2	1:A:440:GLU:OE2	2.53	0.42
1:B:136:LEU:HD22	1:B:136:LEU:HA	1.88	0.42
1:A:297:LEU:HD13	1:A:304:PHE:CD1	2.55	0.42
1:A:172:ASP:O	1:A:184:VAL:HG23	2.20	0.41
1:B:54:GLU:O	1:B:58:ILE:HG13	2.20	0.41
1:A:18:SER:HB3	1:A:123:LEU:HD11	2.03	0.41
1:A:302:CYS:SG	1:A:426:MET:HG3	2.60	0.41
1:B:176:ILE:HD11	1:B:182:VAL:CG1	2.50	0.41
1:A:459:LEU:HD23	1:A:459:LEU:HA	1.90	0.40
1:A:158:PHE:O	1:A:161:SER:OG	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASP:OD1	1:A:234:LYS:N	2.55	0.40
1:B:307:VAL:HG21	1:B:344:VAL:HG21	2.04	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	454/470 (97%)	444 (98%)	10 (2%)	0	100	100
1	B	431/470 (92%)	420 (97%)	11 (3%)	0	100	100
All	All	885/940 (94%)	864 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/411 (93%)	337 (88%)	46 (12%)	5	9
1	B	300/411 (73%)	257 (86%)	43 (14%)	3	6
All	All	683/822 (83%)	594 (87%)	89 (13%)	4	7

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	55	SER
1	A	82	THR
1	A	84	ASN
1	A	86	THR
1	A	99	SER
1	A	103	LEU
1	A	108	SER
1	A	114	LEU
1	A	119	ILE
1	A	136	LEU
1	A	138	SER
1	A	140	VAL
1	A	141	LEU
1	A	154	THR
1	A	159	VAL
1	A	190	VAL
1	A	194	LEU
1	A	216	LEU
1	A	224	GLU
1	A	228	LEU
1	A	250	LEU
1	A	253	LYS
1	A	260	SER
1	A	282	ARG
1	A	303	ARG
1	A	311	LYS
1	A	321	LEU
1	A	334	LYS
1	A	341	LYS
1	A	394	GLU
1	A	395	ARG
1	A	398	LEU
1	A	400	MET
1	A	403	LYS
1	A	411	GLN
1	A	417	GLU
1	A	420	GLU
1	A	421	ARG
1	A	434	ARG
1	A	451	SER
1	A	454	LYS
1	A	456	LEU

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Mol	Chain	Res	Type
1	A	458	GLU
1	A	461	GLU
1	A	464	LYS
1	B	15	LEU
1	B	21	MET
1	B	52	VAL
1	B	59	SER
1	B	60	LEU
1	B	61	LEU
1	B	82	THR
1	B	97	ARG
1	B	99	SER
1	B	102	LEU
1	B	110	ILE
1	B	119	ILE
1	B	120	ASP
1	B	123	LEU
1	B	136	LEU
1	B	140	VAL
1	B	144	SER
1	B	154	THR
1	B	159	VAL
1	B	185	SER
1	B	190	VAL
1	B	194	LEU
1	B	195	ASN
1	B	200	THR
1	B	216	LEU
1	B	228	LEU
1	B	274	VAL
1	B	275	VAL
1	B	347	GLN
1	B	349	ILE
1	B	377	MET
1	B	382	GLN
1	B	396	SER
1	B	402	VAL
1	B	404	ARG
1	B	409	THR
1	B	412	LEU
1	B	421	ARG
1	B	428	ASN

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Mol	Chain	Res	Type
1	B	437	THR
1	B	440	GLU
1	B	456	LEU
1	B	464	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	213	ASN
1	B	101	HIS
1	B	382	GLN
1	B	411	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UPG	A	501	-	37,38,38	3.14	14 (37%)	55,58,58	1.63	9 (16%)
2	UPG	B	501	-	37,38,38	3.12	14 (37%)	55,58,58	1.58	9 (16%)

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
2	UPG	A	501	-	-	8/23/59/59	0/3/3/3
2	UPG	B	501	-	-	9/23/59/59	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	UPG	O4C-C1C	7.11	1.58	1.42
2	B	501	UPG	O4C-C4C	-7.10	1.29	1.45
2	A	501	UPG	C2-N3	7.06	1.50	1.38
2	A	501	UPG	C3C-C2C	-7.06	1.34	1.53
2	B	501	UPG	O4C-C1C	7.02	1.58	1.42
2	A	501	UPG	O4C-C4C	-6.98	1.29	1.45
2	B	501	UPG	C3C-C2C	-6.94	1.34	1.53
2	B	501	UPG	C2-N3	6.89	1.50	1.38
2	A	501	UPG	C2-N1	5.87	1.47	1.38
2	B	501	UPG	C2-N1	5.72	1.47	1.38
2	A	501	UPG	C6-C5	5.60	1.48	1.35
2	B	501	UPG	C6-C5	5.55	1.47	1.35
2	B	501	UPG	C1C-N1	-5.23	1.32	1.47
2	A	501	UPG	C1C-N1	-5.18	1.32	1.47
2	B	501	UPG	C3C-C4C	3.87	1.62	1.53
2	A	501	UPG	C3C-C4C	3.81	1.62	1.53
2	B	501	UPG	O5'-C1'	3.51	1.50	1.41
2	A	501	UPG	O5'-C1'	3.46	1.50	1.41
2	B	501	UPG	O2C-C2C	3.01	1.50	1.43
2	A	501	UPG	O2C-C2C	2.95	1.50	1.43
2	B	501	UPG	C4-N3	2.55	1.43	1.38
2	B	501	UPG	O2-C2	-2.49	1.18	1.23
2	A	501	UPG	O2-C2	-2.47	1.18	1.23
2	B	501	UPG	C3'-C2'	-2.46	1.46	1.52
2	B	501	UPG	O3'-C3'	2.45	1.49	1.43
2	A	501	UPG	C4-N3	2.43	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	UPG	O3'-C3'	2.42	1.49	1.43
2	A	501	UPG	C3'-C2'	-2.39	1.46	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	UPG	C4-N3-C2	-5.50	119.78	126.61
2	B	501	UPG	C4-N3-C2	-5.46	119.84	126.61
2	A	501	UPG	N3-C2-N1	4.09	120.22	114.89
2	B	501	UPG	N3-C2-N1	3.82	119.86	114.89
2	B	501	UPG	C5-C4-N3	3.50	119.70	114.80
2	A	501	UPG	C5-C4-N3	3.49	119.69	114.80
2	A	501	UPG	C4C-O4C-C1C	-3.38	102.00	109.47
2	B	501	UPG	C4C-O4C-C1C	-3.13	102.55	109.47
2	B	501	UPG	O5'-C5'-C4'	3.13	115.33	109.70
2	A	501	UPG	O5'-C5'-C4'	3.11	115.31	109.70
2	A	501	UPG	O4-C4-C5	-2.94	120.10	125.16
2	B	501	UPG	O4-C4-C5	-2.87	120.22	125.16
2	A	501	UPG	O4C-C1C-C2C	-2.59	101.08	106.62
2	B	501	UPG	C2C-C3C-C4C	2.56	107.56	102.61
2	B	501	UPG	C1'-O5'-C5'	2.41	118.43	113.72
2	A	501	UPG	C1'-O5'-C5'	2.24	118.10	113.72
2	A	501	UPG	C2C-C3C-C4C	2.13	106.72	102.61
2	B	501	UPG	O2-C2-N1	-2.12	120.04	122.80

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	UPG	C5C-O5C-PA-O1A
2	A	501	UPG	C5C-O5C-PA-O2A
2	A	501	UPG	C5C-O5C-PA-O3A
2	A	501	UPG	PB-O3A-PA-O5C
2	A	501	UPG	O5'-C1'-O3B-PB
2	B	501	UPG	C5C-O5C-PA-O1A
2	B	501	UPG	C5C-O5C-PA-O2A
2	B	501	UPG	C5C-O5C-PA-O3A
2	B	501	UPG	PB-O3A-PA-O5C
2	B	501	UPG	O5'-C1'-O3B-PB
2	A	501	UPG	O5'-C5'-C6'-O6'
2	B	501	UPG	O5'-C5'-C6'-O6'
2	A	501	UPG	PA-O3A-PB-O2B

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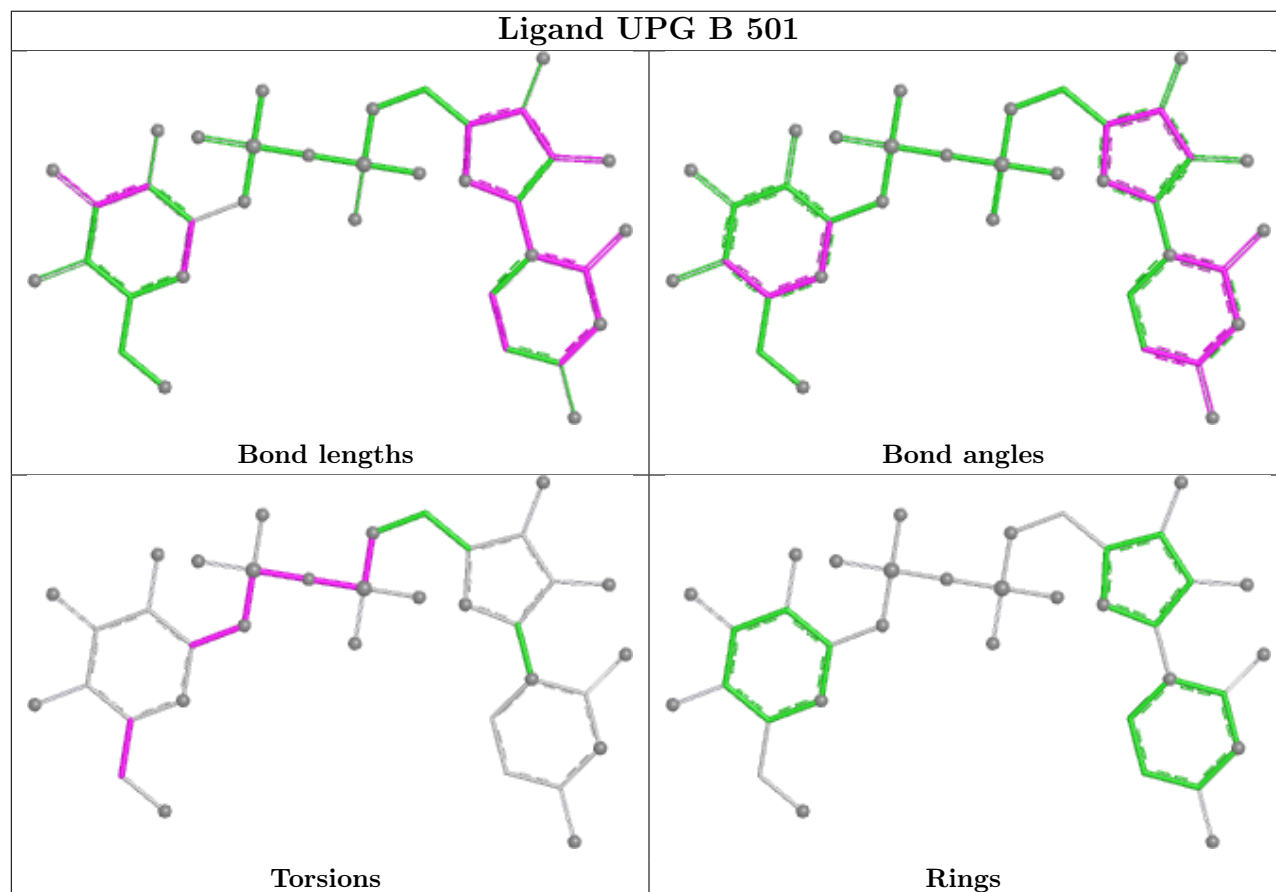
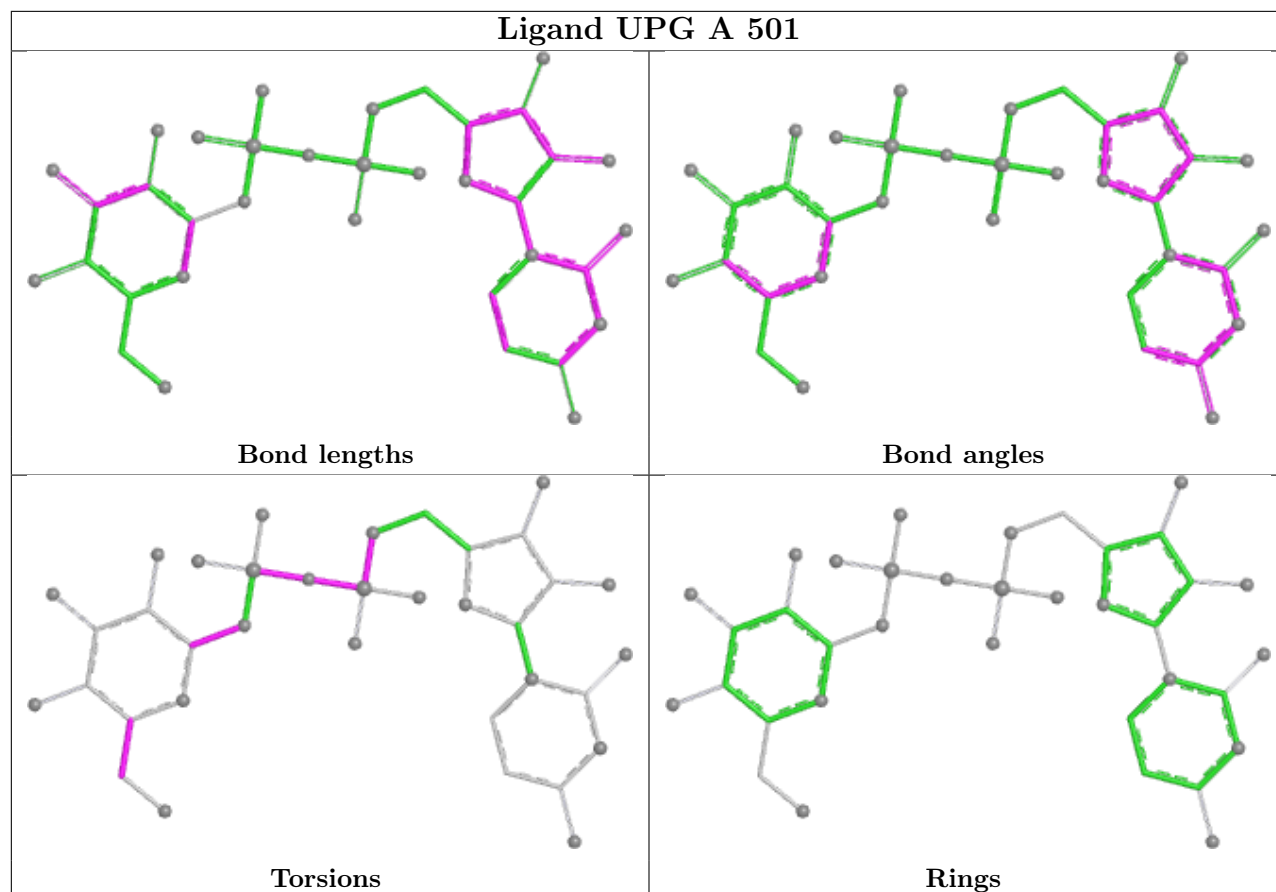
Mol	Chain	Res	Type	Atoms
2	B	501	UPG	PA-O3A-PB-O2B
2	B	501	UPG	C1'-O3B-PB-O1B
2	A	501	UPG	PA-O3A-PB-O1B
2	B	501	UPG	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	UPG	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.



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	456/470 (97%)	1.98	211 (46%) 0 0	23, 37, 60, 90	0
1	B	439/470 (93%)	2.07	209 (47%) 0 0	47, 68, 106, 121	0
All	All	895/940 (95%)	2.02	420 (46%) 0 0	23, 54, 98, 121	0

All (420) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	366	SER	6.1
1	B	175	GLU	5.8
1	B	320	SER	5.6
1	A	84	ASN	5.3
1	B	375	VAL	5.3
1	A	372	TRP	5.1
1	A	401	TRP	4.9
1	B	319	GLU	4.9
1	B	322	ASP	4.7
1	A	355	VAL	4.6
1	A	167	SER	4.6
1	A	281	SER	4.5
1	B	315	GLN	4.4
1	B	321	LEU	4.4
1	A	171	ASP	4.3
1	B	121	SER	4.2
1	A	363	GLY	4.2
1	B	228	LEU	4.1
1	B	10	CYS	4.1
1	A	19	SER	4.0
1	B	387	LYS	4.0
1	A	362	GLY	3.9
1	B	384	GLY	3.9
1	A	227	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	131	ALA	3.9
1	B	367	SER	3.9
1	A	279	PHE	3.9
1	B	328	ASP	3.9
1	B	127	PHE	3.8
1	B	17	LEU	3.8
1	A	140	VAL	3.8
1	A	266	LEU	3.8
1	B	153	GLU	3.8
1	B	232	ASN	3.7
1	A	302	CYS	3.7
1	A	406	GLY	3.7
1	B	84	ASN	3.7
1	B	155	PHE	3.6
1	A	275	VAL	3.6
1	B	103	LEU	3.6
1	B	19	SER	3.6
1	B	399	GLY	3.6
1	A	391	GLU	3.6
1	A	245	SER	3.5
1	B	318	GLU	3.5
1	A	439	ARG	3.5
1	A	115	SER	3.5
1	A	255	GLU	3.5
1	B	400	MET	3.5
1	A	181	PRO	3.5
1	A	169	GLN	3.5
1	B	174	ILE	3.5
1	B	78	PHE	3.4
1	B	398	LEU	3.4
1	A	83	ALA	3.4
1	B	53	ALA	3.4
1	A	176	ILE	3.4
1	A	307	VAL	3.4
1	A	379	VAL	3.4
1	B	141	LEU	3.4
1	B	111	SER	3.4
1	B	370	ALA	3.4
1	A	10	CYS	3.4
1	B	110	ILE	3.4
1	A	380	TRP	3.4
1	A	426	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	85	THR	3.4
1	A	193	ASN	3.3
1	A	38	HIS	3.3
1	A	354	ALA	3.3
1	B	198	PHE	3.3
1	B	346	GLN	3.3
1	B	266	LEU	3.3
1	A	257	THR	3.3
1	A	272	GLY	3.3
1	B	406	GLY	3.3
1	A	172	ASP	3.3
1	A	322	ASP	3.3
1	A	79	ASP	3.2
1	B	119	ILE	3.2
1	A	434	ARG	3.2
1	A	274	VAL	3.2
1	B	363	GLY	3.2
1	B	134	LEU	3.2
1	B	327	ARG	3.2
1	A	191	PHE	3.2
1	A	190	VAL	3.2
1	B	86	THR	3.2
1	B	25	THR	3.2
1	B	18	SER	3.2
1	B	15	LEU	3.2
1	B	371	VAL	3.2
1	B	298	ILE	3.2
1	B	354	ALA	3.1
1	B	361	HIS	3.1
1	B	197	LEU	3.1
1	A	165	PHE	3.1
1	B	124	VAL	3.1
1	B	156	PRO	3.1
1	A	305	LEU	3.1
1	B	293	LEU	3.1
1	A	428	ASN	3.1
1	B	431	LEU	3.1
1	B	336	TYR	3.1
1	B	130	VAL	3.1
1	B	338	PHE	3.0
1	B	171	ASP	3.0
1	A	413	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	383	PHE	3.0
1	A	166	ASP	3.0
1	A	340	ILE	3.0
1	B	244	CYS	3.0
1	B	310	CYS	3.0
1	A	416	GLU	3.0
1	B	380	TRP	3.0
1	A	397	GLY	3.0
1	B	203	ILE	3.0
1	B	365	ASN	3.0
1	B	408	GLY	3.0
1	B	216	LEU	3.0
1	B	146	THR	3.0
1	B	116	ALA	3.0
1	B	128	VAL	3.0
1	A	388	ILE	3.0
1	A	260	SER	3.0
1	B	413	VAL	3.0
1	A	120	ASP	2.9
1	A	195	ASN	2.9
1	B	126	SER	2.9
1	B	172	ASP	2.9
1	B	376	PRO	2.9
1	B	179	PHE	2.9
1	B	307	VAL	2.9
1	A	393	ILE	2.9
1	A	215	ILE	2.9
1	A	20	GLY	2.9
1	A	126	SER	2.9
1	B	190	VAL	2.9
1	A	443	ARG	2.9
1	B	439	ARG	2.9
1	B	381	PRO	2.9
1	A	464	LYS	2.9
1	B	57	ALA	2.9
1	A	396	SER	2.9
1	B	9	SER	2.9
1	A	350	LEU	2.9
1	B	306	TRP	2.8
1	B	83	ALA	2.8
1	B	79	ASP	2.8
1	A	42	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	102	LEU	2.8
1	A	325	LEU	2.8
1	B	139	TYR	2.8
1	A	415	GLY	2.8
1	A	309	LYS	2.8
1	B	212	ALA	2.8
1	A	367	SER	2.8
1	A	262	PRO	2.8
1	B	382	GLN	2.8
1	B	411	GLN	2.8
1	B	222	ALA	2.8
1	B	114	LEU	2.8
1	A	49	THR	2.8
1	B	245	SER	2.8
1	A	94	GLU	2.7
1	B	417	GLU	2.7
1	A	344	VAL	2.7
1	A	95	ALA	2.7
1	A	254	PHE	2.7
1	B	333	ILE	2.7
1	A	61	LEU	2.7
1	A	136	LEU	2.7
1	B	117	LEU	2.7
1	B	442	ALA	2.7
1	A	133	ASN	2.7
1	A	25	THR	2.7
1	A	22	GLY	2.7
1	A	424	ASP	2.7
1	B	226	GLY	2.7
1	B	304	PHE	2.7
1	A	27	CYS	2.7
1	A	366	SER	2.7
1	B	386	GLN	2.7
1	B	140	VAL	2.7
1	A	432	ARG	2.7
1	A	455	THR	2.7
1	A	346	GLN	2.7
1	A	394	GLU	2.7
1	B	159	VAL	2.7
1	A	24	LEU	2.7
1	A	59	SER	2.7
1	A	170	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	136	LEU	2.7
1	B	305	LEU	2.7
1	B	283	PHE	2.6
1	A	244	CYS	2.6
1	A	206	GLY	2.6
1	A	240	LEU	2.6
1	A	295	ASP	2.6
1	B	170	LEU	2.6
1	A	261	ALA	2.6
1	A	452	SER	2.6
1	B	191	PHE	2.6
1	B	451	SER	2.6
1	A	243	TYR	2.6
1	B	296	GLY	2.6
1	A	431	LEU	2.6
1	B	43	ILE	2.6
1	B	300	SER	2.6
1	B	452	SER	2.6
1	A	282	ARG	2.6
1	B	93	TRP	2.6
1	B	326	GLY	2.6
1	A	117	LEU	2.6
1	B	194	LEU	2.6
1	B	227	ILE	2.6
1	B	329	VAL	2.6
1	B	385	ASP	2.6
1	B	445	ALA	2.6
1	A	18	SER	2.6
1	B	81	SER	2.6
1	A	299	ARG	2.6
1	A	384	GLY	2.6
1	B	339	VAL	2.6
1	B	418	ILE	2.6
1	A	198	PHE	2.6
1	A	218	ASN	2.6
1	A	273	SER	2.5
1	A	103	LEU	2.5
1	A	202	LEU	2.5
1	A	226	GLY	2.5
1	A	330	LEU	2.5
1	B	324	LEU	2.5
1	A	187	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	203	ILE	2.5
1	B	358	PHE	2.5
1	A	235	ARG	2.5
1	B	214	GLY	2.5
1	A	308	VAL	2.5
1	B	158	PHE	2.5
1	B	87	ASP	2.5
1	B	161	SER	2.5
1	A	105	PRO	2.5
1	A	223	LEU	2.5
1	B	225	GLY	2.5
1	B	75	LEU	2.5
1	B	181	PRO	2.5
1	A	356	GLY	2.5
1	A	449	GLY	2.5
1	A	371	VAL	2.5
1	B	274	VAL	2.5
1	B	448	VAL	2.5
1	A	57	ALA	2.5
1	A	314	ASP	2.4
1	A	328	ASP	2.4
1	A	398	LEU	2.4
1	A	58	ILE	2.4
1	A	300	SER	2.4
1	B	122	SER	2.4
1	B	402	VAL	2.4
1	A	369	GLU	2.4
1	A	204	GLN	2.4
1	A	222	ALA	2.4
1	A	192	LEU	2.4
1	A	249	LEU	2.4
1	B	285	LEU	2.4
1	B	137	PRO	2.4
1	B	393	ILE	2.4
1	A	41	VAL	2.4
1	A	263	VAL	2.4
1	B	13	VAL	2.4
1	B	109	SER	2.4
1	A	441	GLU	2.4
1	A	197	LEU	2.4
1	B	353	ARG	2.4
1	A	109	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	278	SER	2.4
1	A	146	THR	2.4
1	A	23	HIS	2.4
1	B	377	MET	2.4
1	A	44	ILE	2.4
1	B	96	ILE	2.4
1	A	241	PRO	2.4
1	A	178	GLY	2.4
1	A	402	VAL	2.4
1	A	383	PHE	2.4
1	B	224	GLU	2.4
1	A	36	GLN	2.4
1	A	405	TRP	2.4
1	B	378	LEU	2.4
1	A	349	ILE	2.4
1	B	44	ILE	2.4
1	A	433	VAL	2.3
1	B	173	VAL	2.3
1	B	301	GLY	2.3
1	B	89	PHE	2.3
1	A	417	GLU	2.3
1	B	394	GLU	2.3
1	A	286	SER	2.3
1	A	320	SER	2.3
1	A	200	THR	2.3
1	B	91	LEU	2.3
1	B	35	VAL	2.3
1	B	308	VAL	2.3
1	B	90	PHE	2.3
1	A	440	GLU	2.3
1	A	144	SER	2.3
1	B	145	SER	2.3
1	B	176	ILE	2.3
1	B	276	TYR	2.3
1	A	92	ARG	2.3
1	B	48	PRO	2.3
1	A	35	VAL	2.3
1	A	31	ALA	2.3
1	A	420	GLU	2.3
1	A	385	ASP	2.3
1	B	459	LEU	2.3
1	A	108	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	349	ILE	2.3
1	B	401	TRP	2.3
1	A	128	VAL	2.3
1	B	77	PRO	2.3
1	A	338	PHE	2.3
1	A	459	LEU	2.3
1	B	330	LEU	2.3
1	B	412	LEU	2.3
1	B	188	PRO	2.3
1	B	389	ASN	2.2
1	B	143	THR	2.2
1	A	55	SER	2.2
1	A	91	LEU	2.2
1	A	403	LYS	2.2
1	A	159	VAL	2.2
1	A	259	CYS	2.2
1	A	343	TRP	2.2
1	B	272	GLY	2.2
1	A	78	PHE	2.2
1	B	209	PHE	2.2
1	A	75	LEU	2.2
1	B	460	ILE	2.2
1	A	74	HIS	2.2
1	A	196	HIS	2.2
1	B	379	VAL	2.2
1	A	51	SER	2.2
1	A	138	SER	2.2
1	A	283	PHE	2.2
1	A	304	PHE	2.2
1	A	387	LYS	2.2
1	A	34	LEU	2.2
1	A	106	LEU	2.2
1	A	297	LEU	2.2
1	B	350	LEU	2.2
1	A	174	ILE	2.2
1	B	52	VAL	2.2
1	A	179	PHE	2.2
1	A	62	LEU	2.2
1	B	202	LEU	2.2
1	B	240	LEU	2.2
1	B	250	LEU	2.2
1	B	157	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	447	GLU	2.2
1	A	376	PRO	2.1
1	B	105	PRO	2.1
1	A	21	MET	2.1
1	A	326	GLY	2.1
1	B	49	THR	2.1
1	A	122	SER	2.1
1	B	99	SER	2.1
1	A	331	GLU	2.1
1	A	395	ARG	2.1
1	B	46	ASN	2.1
1	A	80	PRO	2.1
1	A	87	ASP	2.1
1	A	143	THR	2.1
1	A	357	GLY	2.1
1	B	199	THR	2.1
1	A	220	PHE	2.1
1	B	237	ALA	2.1
1	B	104	ASN	2.1
1	B	177	PRO	2.1
1	B	345	ASN	2.1
1	A	247	GLY	2.1
1	A	86	THR	2.1
1	A	219	THR	2.1
1	B	238	ASP	2.1
1	A	435	ALA	2.1
1	B	160	ALA	2.1
1	B	180	SER	2.1
1	A	26	PRO	2.1
1	A	321	LEU	2.1
1	A	438	LEU	2.1
1	B	456	LEU	2.1
1	A	301	GLY	2.1
1	B	254	PHE	2.1
1	A	53	ALA	2.1
1	A	131	ALA	2.1
1	A	231	ILE	2.1
1	B	372	TRP	2.1
1	B	323	GLU	2.1
1	A	111	SER	2.0
1	B	396	SER	2.0
1	B	23	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	389	ASN	2.0
1	B	60	LEU	2.0
1	B	192	LEU	2.0
1	B	297	LEU	2.0
1	B	419	GLY	2.0
1	B	437	THR	2.0
1	A	121	SER	2.0
1	A	339	VAL	2.0
1	B	36	GLN	2.0
1	B	273	SER	2.0
1	B	359	VAL	2.0
1	B	88	PRO	2.0
1	B	28	LEU	2.0
1	B	76	LEU	2.0
1	A	168	ILE	2.0
1	B	82	THR	2.0
1	B	243	TYR	2.0
1	A	13	VAL	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 oligosaccharides 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.

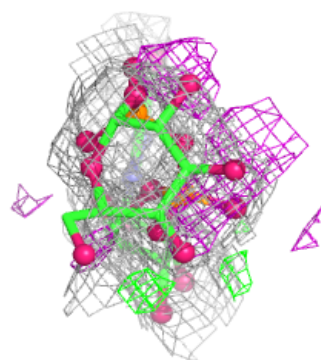
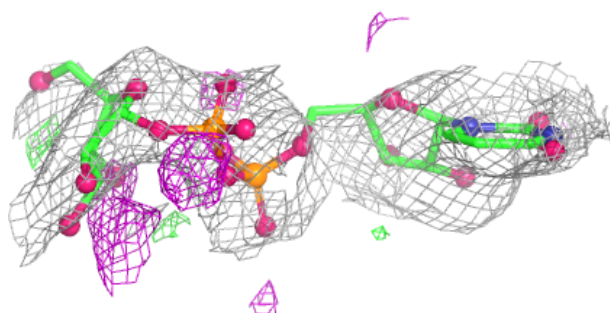
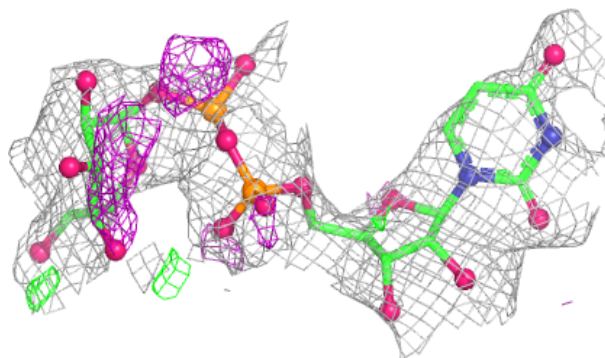
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UPG	B	501	36/36	0.70	0.20	51,67,73,83	0
2	UPG	A	501	36/36	0.85	0.17	25,30,42,46	0

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.

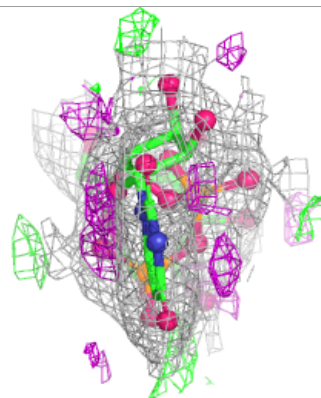
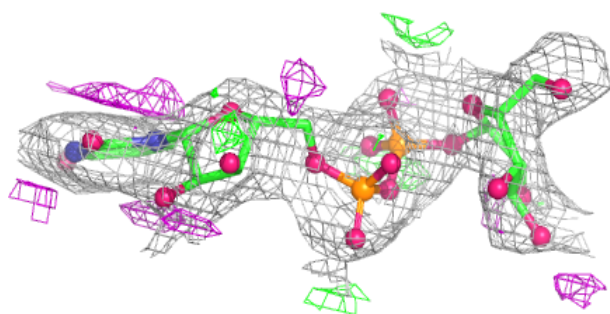
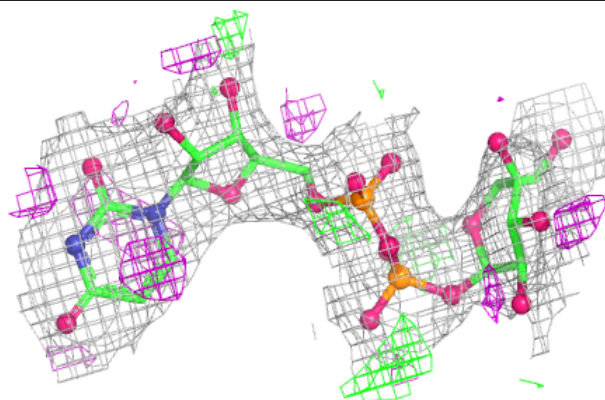
Electron density around UPG B 501:

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



Electron density around UPG A 501:

$2mF_o-DF_c$ (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.