



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:18 PM UTC

PDB ID : 3GG2 / pdb_00003gg2
Title : Crystal structure of UDP-glucose 6-dehydrogenase from Porphyromonas gingivalis bound to product UDP-glucuronate
Authors : Bonanno, J.B.; Freeman, J.; Bain, K.T.; Chang, S.; Sampathkumar, P.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-02-27
Resolution : 1.70 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](#) ①) 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

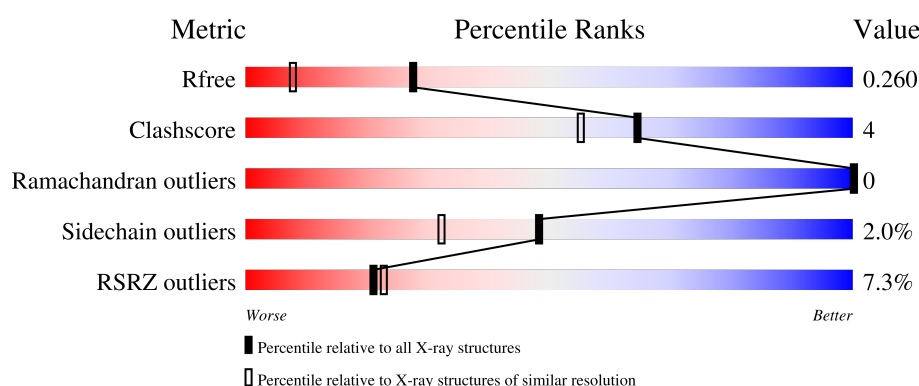
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	450	5% 87% 8% • •
1	B	450	12% 84% 9% • 6%
1	C	450	6% 85% 8% • 7%
1	D	450	5% 88% 6% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14679 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 Sugar dehydrogenase, UDP-glucose/GDP-mannose dehydrogenase family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	8	0
			3360	2136	570	631	23			
1	B	425	Total	C	N	O	S	0	2	0
			3256	2065	551	617	23			
1	C	420	Total	C	N	O	S	0	3	0
			3229	2048	545	613	23			
1	D	427	Total	C	N	O	S	0	4	0
			3305	2101	561	620	23			

There are 60 discrepancies between the modelled and reference sequences:

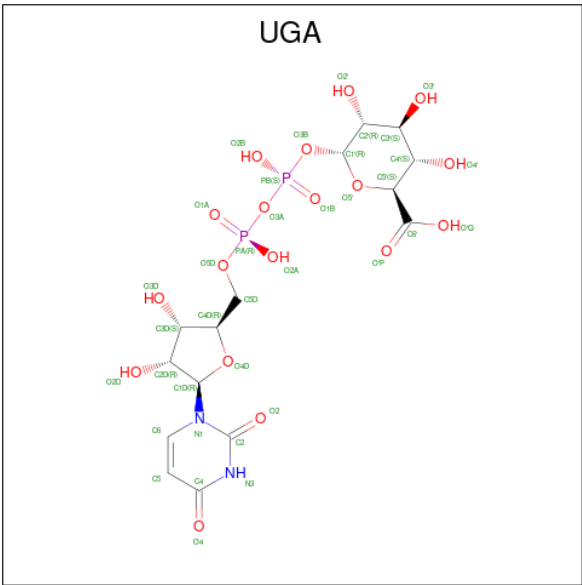
Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	expression tag	UNP Q7MVC7
A	78	SER	-	expression tag	UNP Q7MVC7
A	79	LEU	-	expression tag	UNP Q7MVC7
A	158	ILE	VAL	engineered mutation	UNP Q7MVC7
A	175	SER	GLY	engineered mutation	UNP Q7MVC7
A	211	ALA	VAL	engineered mutation	UNP Q7MVC7
A	485	ALA	THR	engineered mutation	UNP Q7MVC7
A	519	GLU	-	expression tag	UNP Q7MVC7
A	520	GLY	-	expression tag	UNP Q7MVC7
A	521	HIS	-	expression tag	UNP Q7MVC7
A	522	HIS	-	expression tag	UNP Q7MVC7
A	523	HIS	-	expression tag	UNP Q7MVC7
A	524	HIS	-	expression tag	UNP Q7MVC7
A	525	HIS	-	expression tag	UNP Q7MVC7
A	526	HIS	-	expression tag	UNP Q7MVC7
B	77	MET	-	expression tag	UNP Q7MVC7
B	78	SER	-	expression tag	UNP Q7MVC7
B	79	LEU	-	expression tag	UNP Q7MVC7
B	158	ILE	VAL	engineered mutation	UNP Q7MVC7
B	175	SER	GLY	engineered mutation	UNP Q7MVC7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	211	ALA	VAL	engineered mutation	UNP Q7MVC7
B	485	ALA	THR	engineered mutation	UNP Q7MVC7
B	519	GLU	-	expression tag	UNP Q7MVC7
B	520	GLY	-	expression tag	UNP Q7MVC7
B	521	HIS	-	expression tag	UNP Q7MVC7
B	522	HIS	-	expression tag	UNP Q7MVC7
B	523	HIS	-	expression tag	UNP Q7MVC7
B	524	HIS	-	expression tag	UNP Q7MVC7
B	525	HIS	-	expression tag	UNP Q7MVC7
B	526	HIS	-	expression tag	UNP Q7MVC7
C	77	MET	-	expression tag	UNP Q7MVC7
C	78	SER	-	expression tag	UNP Q7MVC7
C	79	LEU	-	expression tag	UNP Q7MVC7
C	158	ILE	VAL	engineered mutation	UNP Q7MVC7
C	175	SER	GLY	engineered mutation	UNP Q7MVC7
C	211	ALA	VAL	engineered mutation	UNP Q7MVC7
C	485	ALA	THR	engineered mutation	UNP Q7MVC7
C	519	GLU	-	expression tag	UNP Q7MVC7
C	520	GLY	-	expression tag	UNP Q7MVC7
C	521	HIS	-	expression tag	UNP Q7MVC7
C	522	HIS	-	expression tag	UNP Q7MVC7
C	523	HIS	-	expression tag	UNP Q7MVC7
C	524	HIS	-	expression tag	UNP Q7MVC7
C	525	HIS	-	expression tag	UNP Q7MVC7
C	526	HIS	-	expression tag	UNP Q7MVC7
D	77	MET	-	expression tag	UNP Q7MVC7
D	78	SER	-	expression tag	UNP Q7MVC7
D	79	LEU	-	expression tag	UNP Q7MVC7
D	158	ILE	VAL	engineered mutation	UNP Q7MVC7
D	175	SER	GLY	engineered mutation	UNP Q7MVC7
D	211	ALA	VAL	engineered mutation	UNP Q7MVC7
D	485	ALA	THR	engineered mutation	UNP Q7MVC7
D	519	GLU	-	expression tag	UNP Q7MVC7
D	520	GLY	-	expression tag	UNP Q7MVC7
D	521	HIS	-	expression tag	UNP Q7MVC7
D	522	HIS	-	expression tag	UNP Q7MVC7
D	523	HIS	-	expression tag	UNP Q7MVC7
D	524	HIS	-	expression tag	UNP Q7MVC7
D	525	HIS	-	expression tag	UNP Q7MVC7
D	526	HIS	-	expression tag	UNP Q7MVC7

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (CCD ID: UGA) (formula: C₁₅H₂₂N₂O₁₈P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	A	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	B	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	C	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	D	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	D	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

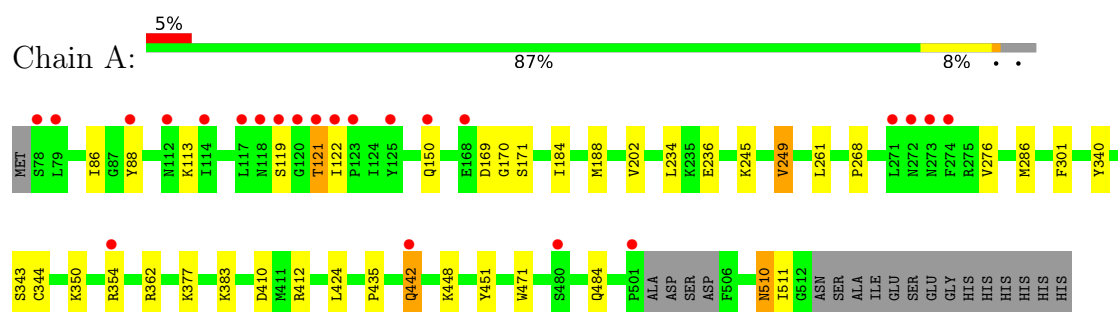
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	362	Total	O	0	0
			362	362		
3	B	295	Total	O	0	0
			295	295		
3	C	366	Total	O	0	0
			366	366		
3	D	284	Total	O	0	0
			284	284		

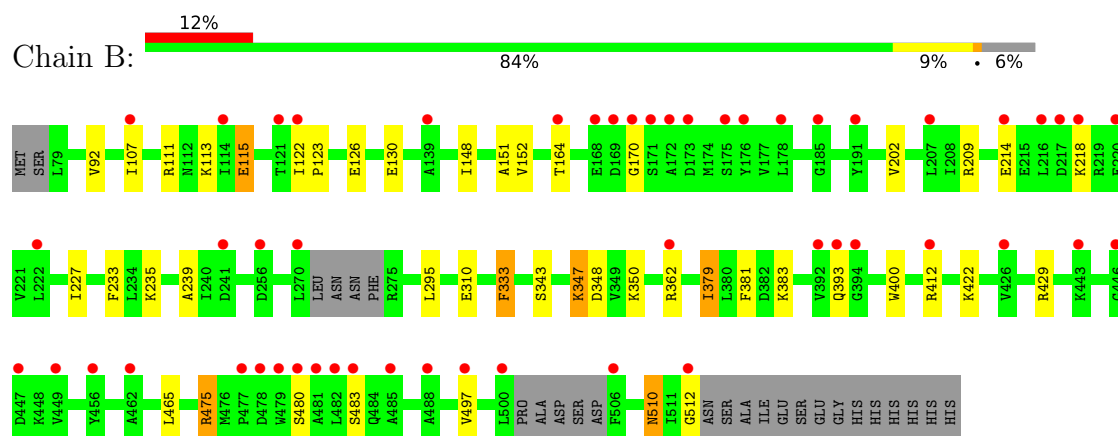
3 Residue-property plots [i](#)

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.

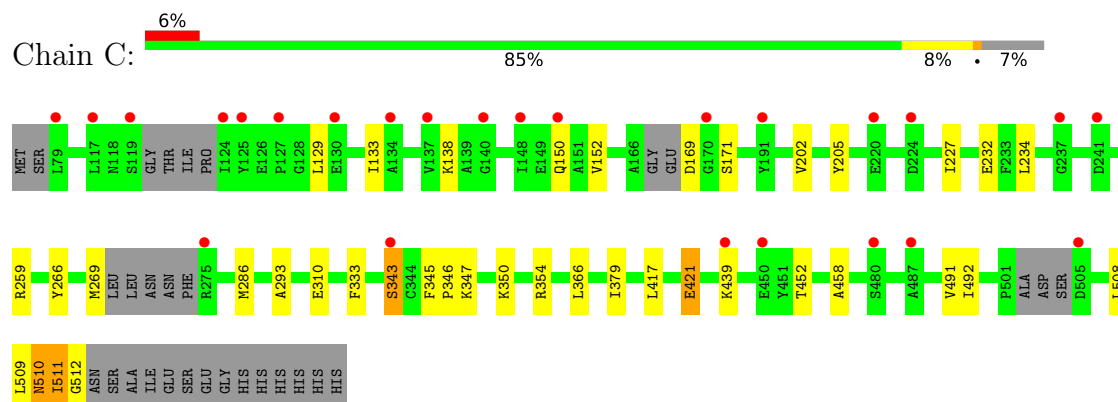
- Molecule 1: Sugar dehydrogenase, UDP-glucose/GDP-mannose dehydrogenase family



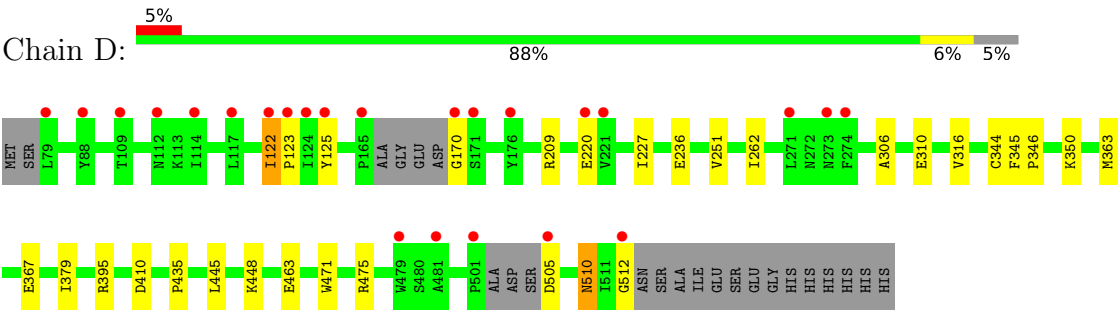
- Molecule 1: Sugar dehydrogenase, UDP-glucose/GDP-mannose dehydrogenase family



- Molecule 1: Sugar dehydrogenase, UDP-glucose/GDP-mannose dehydrogenase family



● Molecule 1: Sugar dehydrogenase, UDP-glucose/GDP-mannose dehydrogenase family



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.36Å 143.49Å 85.50Å 90.00° 112.46° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.7 (20.00-1.70) 93.2 (20.00-1.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.256 0.219 , 0.260	Depositor DCC
R_{free} test set	9495 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14679	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.88	0/3438	0.95	1/4642 (0.0%)
1	B	0.81	1/3312 (0.0%)	0.95	3/4476 (0.1%)
1	C	0.86	0/3286	0.95	2/4438 (0.0%)
1	D	0.85	0/3370	0.91	1/4553 (0.0%)
All	All	0.85	1/13406 (0.0%)	0.94	7/18109 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	VAL	CA-CB	7.23	1.57	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	CYS	N-CA-C	8.29	120.23	111.03
1	D	344	CYS	N-CA-C	7.33	119.17	111.03
1	B	126	GLU	CA-C-N	6.38	126.75	119.93
1	B	126	GLU	C-N-CA	6.38	126.75	119.93
1	B	475	ARG	N-CA-C	6.14	118.95	111.82
1	C	152	VAL	CA-C-N	-5.41	114.24	119.87
1	C	152	VAL	C-N-CA	-5.41	114.24	119.87

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	3360	0	3402	31	0
1	B	3256	0	3256	29	1
1	C	3229	0	3222	26	0
1	D	3305	0	3322	17	0
2	A	74	0	38	1	0
2	B	37	0	19	0	0
2	C	37	0	19	0	0
2	D	74	0	38	1	0
3	A	362	0	0	4	0
3	B	295	0	0	4	0
3	C	366	0	0	5	0
3	D	284	0	0	1	1
All	All	14679	0	13316	103	1

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 4.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LYS:HG3	3:A:1815:HOH:O	1.65	0.94
1:C:202:VAL:HG23	3:C:560:HOH:O	1.74	0.87
1:B:107:ILE:HD11	1:B:151:ALA:HB2	1.61	0.82
1:B:107:ILE:HD11	1:B:151:ALA:CB	2.10	0.81
1:B:233:PHE:O	3:B:2215:HOH:O	2.02	0.78
1:A:86:ILE:HD12	1:A:113:LYS:HD3	1.65	0.77
1:C:232[A]:GLU:CG	1:C:234:LEU:HG	2.16	0.75
1:C:439:LYS:HG3	3:C:33:HOH:O	1.89	0.72
1:A:170:GLY:HA3	1:A:350:LYS:HE2	1.74	0.70
1:B:113:LYS:HD2	1:B:123:PRO:HB3	1.75	0.69
1:A:249[A]:VAL:HG13	1:A:276:VAL:HA	1.75	0.68
1:C:343:SER:O	1:C:347:LYS:HG2	1.95	0.67
1:B:310:GLU:HG3	1:B:512:GLY:HA2	1.78	0.66
1:A:383:LYS:HE3	1:A:511:ILE:HD13	1.78	0.66
1:D:445:LEU:O	1:D:448:LYS:HG2	1.99	0.63
1:B:475:ARG:HD3	1:B:497:VAL:HG11	1.80	0.62
1:B:379:ILE:O	1:B:383:LYS:HG2	2.00	0.62
1:C:232[A]:GLU:HG3	1:C:234:LEU:HG	1.80	0.62
1:C:171:SER:HB3	1:C:354:ARG:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ARG:HB2	1:D:227:ILE:HD13	1.83	0.60
1:B:209:ARG:HB2	1:B:227:ILE:HD13	1.84	0.60
1:C:202:VAL:HG21	1:C:286:MET:HE2	1.85	0.58
1:B:113:LYS:HD2	1:B:123:PRO:CB	2.33	0.57
1:C:510:ASN:HD22	1:C:510:ASN:C	2.11	0.56
1:B:202:VAL:HG23	3:B:1220:HOH:O	2.04	0.56
1:A:119:SER:HB2	1:A:121:THR:HG22	1.88	0.56
1:A:249[A]:VAL:CG1	1:A:276:VAL:HG22	2.36	0.56
1:A:88[B]:TYR:HD1	1:A:234:LEU:HD11	1.71	0.55
1:C:350:LYS:HG3	3:C:540:HOH:O	2.06	0.55
1:B:343:SER:OG	1:B:412:ARG:NE	2.39	0.55
1:B:107:ILE:HD13	1:B:148:ILE:HA	1.89	0.55
1:D:510:ASN:C	1:D:510:ASN:HD22	2.15	0.54
1:B:164:THR:O	1:B:347:LYS:HE3	2.07	0.54
1:A:86:ILE:CD1	1:A:113:LYS:HD3	2.35	0.53
1:B:510:ASN:C	1:B:510:ASN:HD22	2.18	0.51
1:C:232[A]:GLU:HG2	1:C:234:LEU:HG	1.89	0.50
1:B:343:SER:OG	1:B:412:ARG:CZ	2.60	0.50
1:C:417:LEU:O	1:C:421:GLU:HG2	2.12	0.50
1:A:249[A]:VAL:HG11	1:A:276:VAL:HG22	1.94	0.49
1:A:202:VAL:HG21	1:A:286:MET:HE2	1.94	0.49
1:A:442:GLN:NE2	3:A:815:HOH:O	2.39	0.49
1:A:113:LYS:HE2	1:A:122:ILE:HD13	1.94	0.49
1:B:381:PHE:CG	1:B:422:LYS:HG3	2.47	0.48
1:A:171:SER:HB3	1:A:354:ARG:HG2	1.94	0.48
1:A:510:ASN:C	1:A:510:ASN:HD22	2.22	0.47
1:A:88[B]:TYR:CD1	1:A:234:LEU:HD11	2.49	0.47
1:C:259:ARG:NH1	3:C:2896:HOH:O	2.39	0.47
1:D:435:PRO:HG2	1:D:471:TRP:CD2	2.49	0.47
1:B:113:LYS:HD3	3:B:1759:HOH:O	2.13	0.47
1:B:347:LYS:HE2	1:B:348:ASP:OD1	2.15	0.47
1:C:492:ILE:HG12	1:C:509:LEU:HD12	1.97	0.47
1:D:345:PHE:HB2	1:D:346:PRO:HD3	1.97	0.46
1:D:251:VAL:HG21	1:D:262:ILE:HG21	1.97	0.46
1:A:121:THR:O	1:A:121:THR:OG1	2.34	0.46
1:B:381:PHE:CD1	1:B:422:LYS:HG3	2.51	0.45
1:A:424:LEU:HD13	1:A:448:LYS:HE2	1.98	0.45
1:C:345:PHE:HB2	1:C:346:PRO:HD3	1.97	0.45
1:D:310:GLU:HG3	1:D:512:GLY:HA2	1.98	0.45
1:B:111:ARG:O	1:B:115:GLU:HB2	2.17	0.45
1:D:395:ARG:NH1	1:D:463:GLU:OE1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:GLY:HA3	1:B:350:LYS:HE3	1.99	0.45
1:C:205:TYR:HB2	1:C:227:ILE:HD12	1.99	0.45
1:A:234:LEU:C	1:A:234:LEU:HD12	2.43	0.44
1:B:122:ILE:HG23	1:B:130:GLU:HG3	1.99	0.44
1:B:475:ARG:CD	1:B:497:VAL:HG11	2.47	0.44
1:D:122:ILE:HG13	1:D:123:PRO:HD2	1.99	0.44
1:C:343:SER:OG	3:C:692:HOH:O	2.20	0.44
1:A:169:ASP:CB	3:A:1763:HOH:O	2.66	0.44
1:C:491:VAL:HG13	1:C:508:LEU:HD12	2.00	0.44
1:C:169:ASP:OD2	1:C:354:ARG:NH1	2.50	0.43
1:C:379:ILE:HG21	1:C:511:ILE:HD13	1.99	0.43
1:D:306:ALA:HB2	1:D:316:VAL:HG21	2.01	0.43
2:A:6000:UGA:O3D	2:D:4000:UGA:H2A1	2.18	0.43
1:C:310:GLU:HG3	1:C:512:GLY:HA2	2.00	0.43
1:C:491:VAL:HG13	1:C:508:LEU:CD1	2.49	0.43
1:A:184:ILE:O	1:A:188:MET:HG3	2.19	0.42
1:A:202:VAL:HG23	3:A:1099:HOH:O	2.19	0.42
1:A:268:PRO:HB3	1:D:475:ARG:HG3	2.01	0.42
1:A:245:LYS:HE3	1:A:245:LYS:HB3	1.75	0.42
1:A:249[A]:VAL:HG13	1:A:276:VAL:HG22	2.01	0.42
1:A:435:PRO:HG2	1:A:471:TRP:CD2	2.53	0.42
1:B:295:LEU:HB3	1:B:333:PHE:CE2	2.54	0.42
1:A:343:SER:HB3	1:A:412:ARG:HD2	2.00	0.42
1:B:400:TRP:CG	1:B:465:LEU:HD11	2.55	0.42
1:D:363:MET:O	1:D:367:GLU:HG3	2.20	0.42
1:D:379:ILE:HD13	3:D:574:HOH:O	2.19	0.42
1:C:452:THR:HG21	1:C:458:ALA:HA	2.02	0.42
1:D:236:GLU:OE2	1:D:410:ASP:OD2	2.37	0.42
1:B:92:VAL:HG21	1:B:239:ALA:HB3	2.02	0.41
1:B:214:GLU:O	1:B:218:LYS:HG3	2.20	0.41
1:B:235:LYS:HB2	1:B:235:LYS:HE2	1.84	0.41
1:C:266:TYR:HD1	1:C:269:MET:HE3	1.85	0.41
1:A:236:GLU:OE2	1:A:410:ASP:OD2	2.39	0.41
1:A:442:GLN:HA	1:A:451:TYR:OH	2.20	0.41
1:B:347:LYS:HE3	3:B:618:HOH:O	2.20	0.41
1:C:293:ALA:HB1	1:C:366:LEU:HD21	2.03	0.41
1:A:301:PHE:CD2	1:A:301:PHE:C	2.98	0.41
1:A:340:TYR:O	1:A:377[A]:LYS:HE3	2.21	0.41
1:D:170:GLY:HA3	1:D:350:LYS:HG3	2.03	0.41
1:C:129:LEU:O	1:C:133:ILE:HG13	2.22	0.40
1:D:310:GLU:CG	1:D:512:GLY:HA2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:TYR:CD1	1:C:269:MET:HE3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ARG:NH2	3:D:1429:HOH:O[1_655]	2.13	0.07

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	435/450 (97%)	430 (99%)	5 (1%)	0	100	100
1	B	421/450 (94%)	416 (99%)	5 (1%)	0	100	100
1	C	413/450 (92%)	406 (98%)	7 (2%)	0	100	100
1	D	425/450 (94%)	419 (99%)	6 (1%)	0	100	100
All	All	1694/1800 (94%)	1671 (99%)	23 (1%)	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	360/374 (96%)	351 (98%)	9 (2%)	42	24
1	B	343/374 (92%)	334 (97%)	9 (3%)	40	23
1	C	341/374 (91%)	334 (98%)	7 (2%)	47	30
1	D	351/374 (94%)	347 (99%)	4 (1%)	65	54
All	All	1395/1496 (93%)	1366 (98%)	29 (2%)	48	30

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	THR
1	A	150	GLN
1	A	249[A]	VAL
1	A	249[B]	VAL
1	A	261	LEU
1	A	362	ARG
1	A	442	GLN
1	A	484	GLN
1	A	510	ASN
1	B	115	GLU
1	B	333	PHE
1	B	347	LYS
1	B	379	ILE
1	B	393	GLN
1	B	429	ARG
1	B	480	SER
1	B	483	SER
1	B	510	ASN
1	C	138	LYS
1	C	150	GLN
1	C	333	PHE
1	C	343	SER
1	C	421	GLU
1	C	510	ASN
1	C	511	ILE
1	D	122	ILE
1	D	220	GLU
1	D	505	ASP
1	D	510	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	272	ASN
1	A	393	GLN
1	A	442	GLN
1	A	510	ASN
1	B	112	ASN
1	B	393	GLN
1	B	510	ASN
1	C	116	GLN
1	C	150	GLN
1	C	230	ASN
1	C	510	ASN
1	D	272	ASN
1	D	273	ASN
1	D	442	GLN
1	D	510	ASN

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](#)

6 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	UGA	A	6000	-	38,39,39	1.10	2 (5%)	56,60,60	1.45	7 (12%)
2	UGA	A	1000	-	38,39,39	1.18	3 (7%)	56,60,60	1.64	8 (14%)
2	UGA	D	5000	-	38,39,39	1.04	2 (5%)	56,60,60	1.26	4 (7%)
2	UGA	D	4000	-	38,39,39	1.21	4 (10%)	56,60,60	1.43	6 (10%)
2	UGA	C	3000	-	38,39,39	1.09	2 (5%)	56,60,60	1.69	7 (12%)
2	UGA	B	2000	-	38,39,39	1.02	3 (7%)	56,60,60	1.57	8 (14%)

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	UGA	A	6000	-	-	0/25/61/61	0/3/3/3
2	UGA	A	1000	-	-	3/25/61/61	0/3/3/3
2	UGA	D	5000	-	-	1/25/61/61	0/3/3/3
2	UGA	D	4000	-	-	3/25/61/61	0/3/3/3
2	UGA	C	3000	-	-	3/25/61/61	0/3/3/3
2	UGA	B	2000	-	-	3/25/61/61	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4000	UGA	PA-O3A	3.50	1.63	1.59
2	A	6000	UGA	PB-O3A	3.32	1.63	1.59
2	A	1000	UGA	PB-O3A	3.08	1.62	1.59
2	C	3000	UGA	C6-C5	2.77	1.41	1.35
2	A	6000	UGA	PA-O3A	2.59	1.62	1.59
2	D	5000	UGA	C6-C5	2.25	1.40	1.35
2	A	1000	UGA	PA-O3A	2.24	1.61	1.59
2	D	4000	UGA	C2-N1	-2.21	1.35	1.38
2	B	2000	UGA	C6-C5	2.17	1.40	1.35
2	C	3000	UGA	C4-N3	-2.16	1.34	1.38
2	A	1000	UGA	C4-N3	-2.09	1.35	1.38
2	B	2000	UGA	C4-N3	-2.09	1.35	1.38
2	D	4000	UGA	C4-N3	-2.07	1.35	1.38
2	D	4000	UGA	O2-C2	2.05	1.26	1.23
2	D	5000	UGA	PB-O3A	2.04	1.61	1.59
2	B	2000	UGA	C2-N3	-2.02	1.34	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3000	UGA	C4-N3-C2	-5.85	119.35	126.61
2	C	3000	UGA	N3-C2-N1	5.43	121.96	114.89
2	A	1000	UGA	C4-N3-C2	-5.20	120.16	126.61
2	A	6000	UGA	C4-N3-C2	-4.91	120.51	126.61
2	A	1000	UGA	C5-C4-N3	4.83	121.57	114.80
2	C	3000	UGA	C5-C4-N3	4.74	121.44	114.80
2	B	2000	UGA	C4-N3-C2	-4.45	121.09	126.61
2	B	2000	UGA	C5-C4-N3	4.44	121.01	114.80
2	B	2000	UGA	N3-C2-N1	4.43	120.65	114.89
2	D	4000	UGA	C4-N3-C2	-4.27	121.31	126.61
2	A	1000	UGA	N3-C2-N1	4.02	120.13	114.89
2	D	4000	UGA	N3-C2-N1	3.93	120.01	114.89
2	A	6000	UGA	N3-C2-N1	3.84	119.89	114.89
2	D	4000	UGA	C5-C4-N3	3.75	120.05	114.80
2	D	5000	UGA	C4-N3-C2	-3.71	122.00	126.61
2	A	6000	UGA	C5-C4-N3	3.69	119.97	114.80
2	D	5000	UGA	N3-C2-N1	3.56	119.52	114.89
2	A	6000	UGA	O4-C4-C5	-3.54	119.05	125.16
2	A	1000	UGA	O4-C4-C5	-3.35	119.39	125.16
2	D	5000	UGA	C5-C4-N3	3.29	119.41	114.80
2	D	4000	UGA	O4-C4-C5	-3.21	119.62	125.16
2	A	1000	UGA	O5'-C1'-O3B	-3.10	107.31	111.36
2	B	2000	UGA	C4'-C3'-C2'	-2.96	105.63	110.83
2	C	3000	UGA	O4-C4-C5	-2.81	120.32	125.16
2	D	5000	UGA	O4-C4-C5	-2.75	120.41	125.16
2	B	2000	UGA	O4-C4-C5	-2.65	120.59	125.16
2	A	6000	UGA	C3'-C4'-C5'	2.59	113.75	109.30
2	C	3000	UGA	O2-C2-N3	-2.58	116.72	121.49
2	C	3000	UGA	O3D-C3D-C4D	-2.55	103.75	111.08
2	A	1000	UGA	O5'-C5'-C6'	2.51	113.98	106.14
2	D	4000	UGA	O3A-PA-O1A	-2.27	103.88	110.70
2	D	4000	UGA	O2A-PA-O1A	2.25	122.92	112.44
2	C	3000	UGA	C4'-C3'-C2'	-2.22	106.93	110.83
2	A	1000	UGA	O2-C2-N3	-2.14	117.53	121.49
2	B	2000	UGA	C1D-N1-C2	2.13	121.41	117.59
2	B	2000	UGA	O2B-PB-O3A	-2.10	101.58	107.27
2	A	6000	UGA	O4D-C1D-N1	2.09	113.09	108.36
2	B	2000	UGA	C6-C5-C4	-2.06	116.91	119.53
2	A	6000	UGA	O2A-PA-O1A	2.02	121.85	112.44
2	A	1000	UGA	O2A-PA-O3A	2.01	112.72	107.27

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	UGA	PA-O3A-PB-O3B
2	B	2000	UGA	PA-O3A-PB-O3B
2	D	4000	UGA	C1'-O3B-PB-O3A
2	C	3000	UGA	PA-O3A-PB-O3B
2	D	4000	UGA	PA-O3A-PB-O3B
2	D	5000	UGA	PA-O3A-PB-O3B
2	B	2000	UGA	PB-O3A-PA-O1A
2	C	3000	UGA	PB-O3A-PA-O1A
2	A	1000	UGA	PB-O3A-PA-O1A
2	B	2000	UGA	PB-O3A-PA-O2A
2	C	3000	UGA	PB-O3A-PA-O2A
2	A	1000	UGA	PB-O3A-PA-O2A
2	D	4000	UGA	PB-O3A-PA-O2A

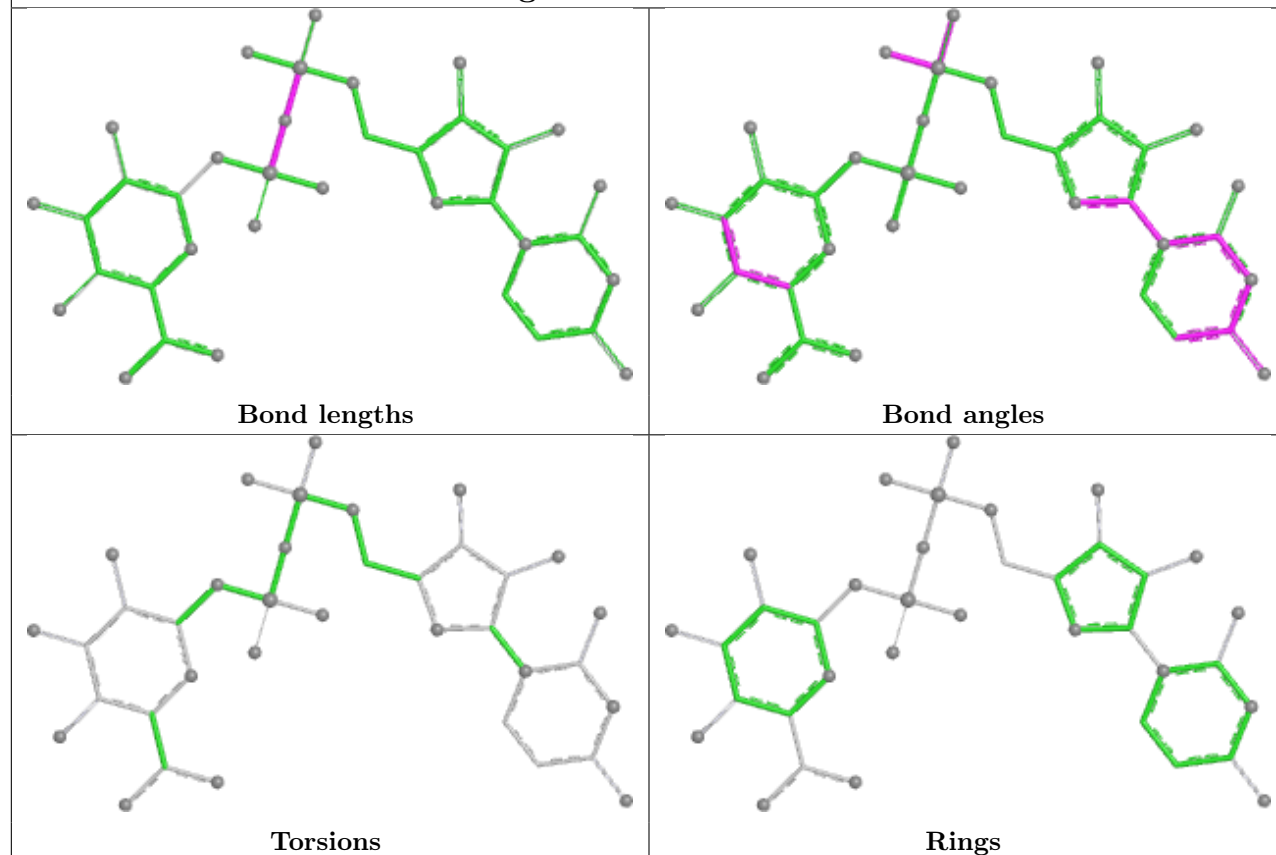
There are no ring outliers.

2 monomers are involved in 1 short contact:

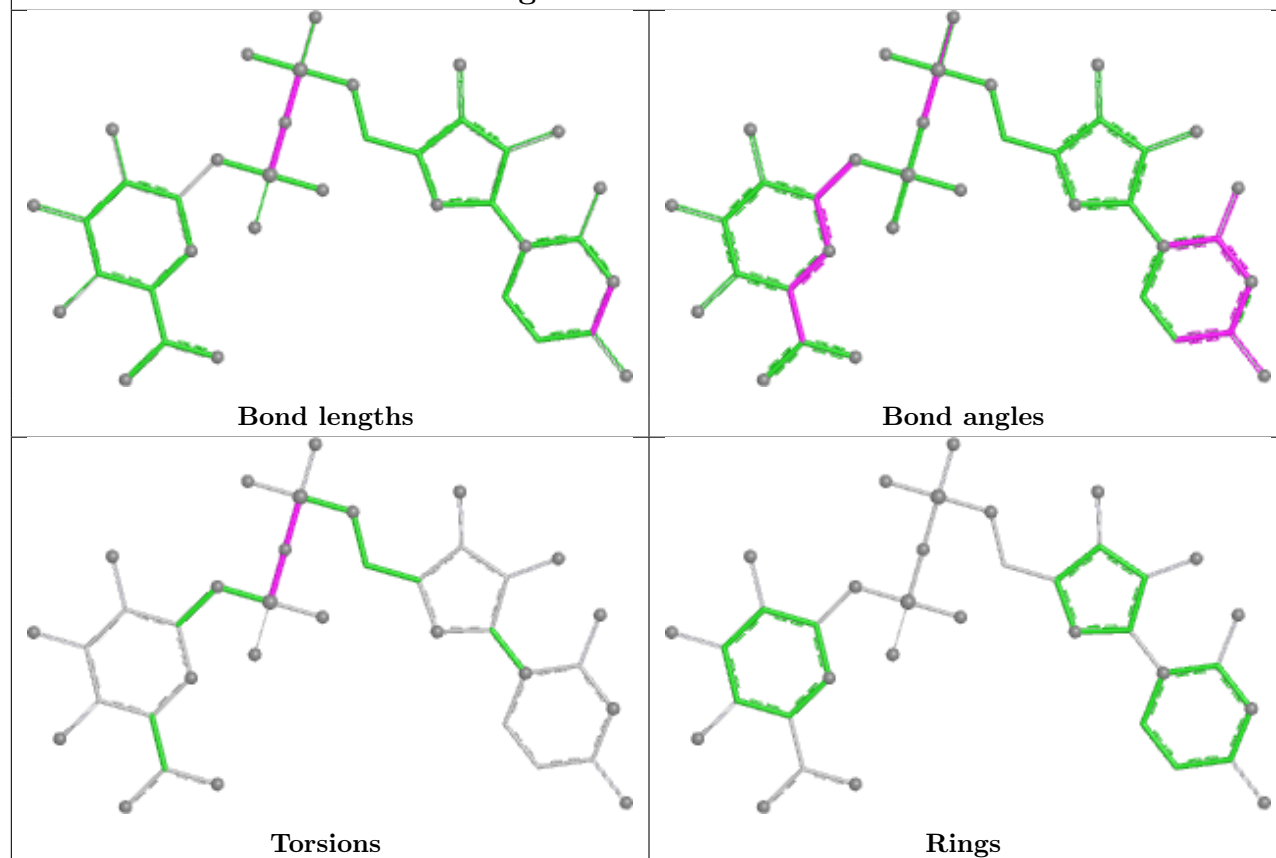
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6000	UGA	1	0
2	D	4000	UGA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

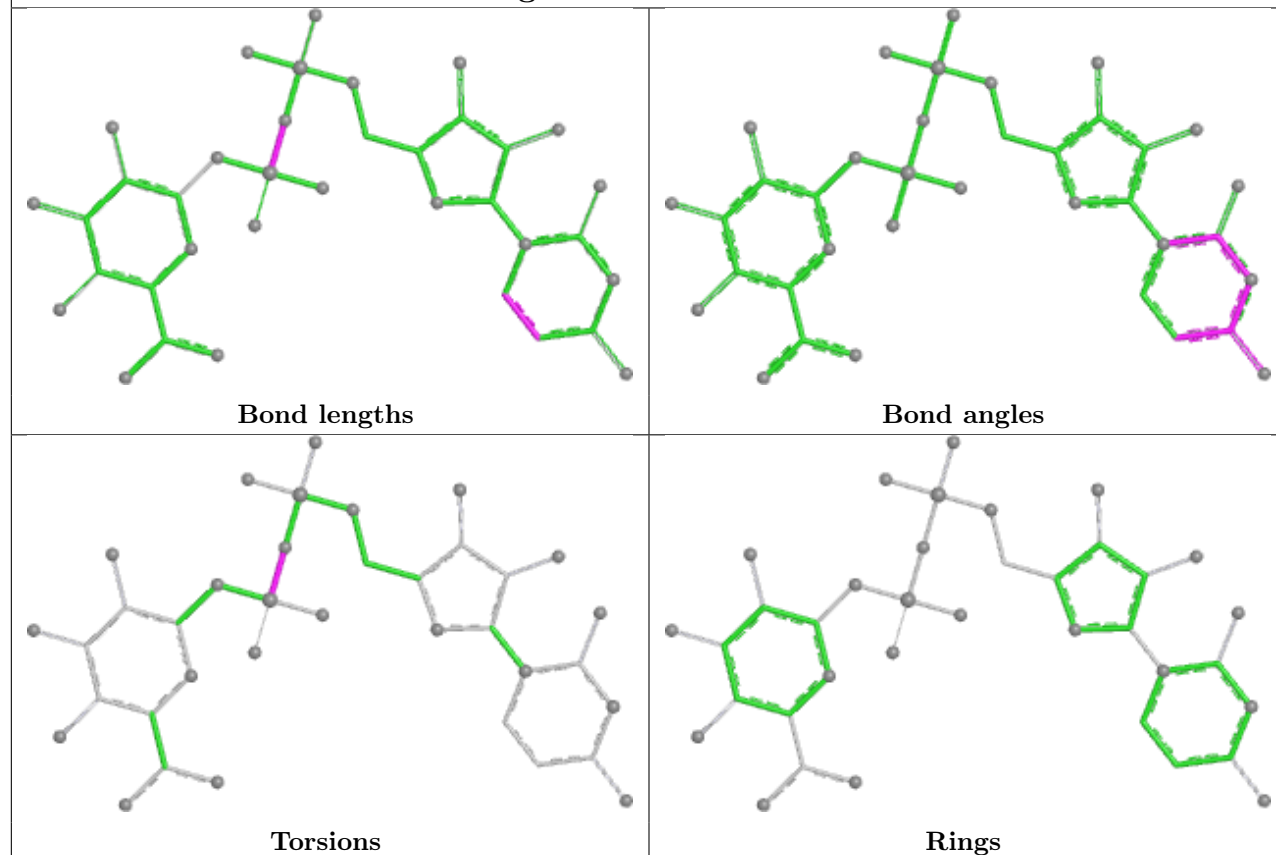
Ligand UGA A 6000



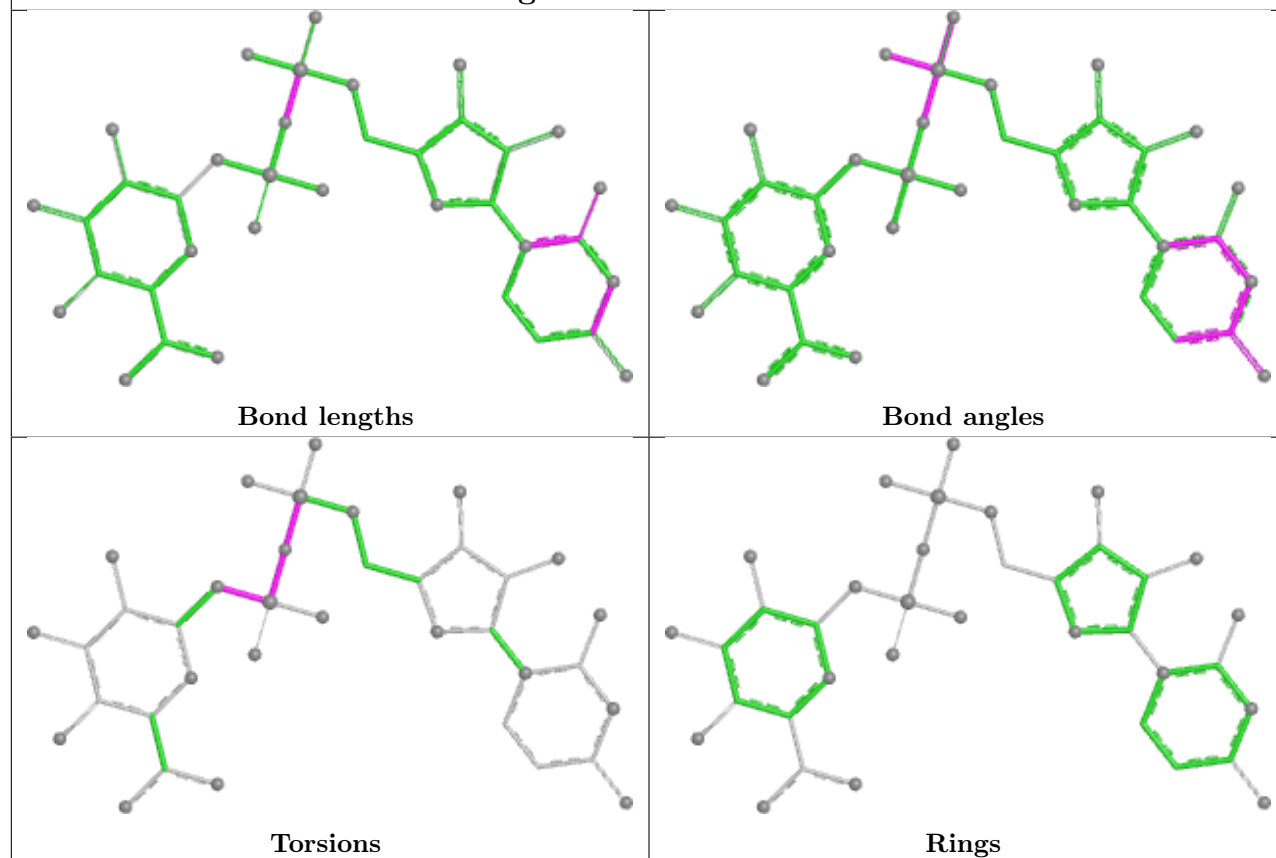
Ligand UGA A 1000

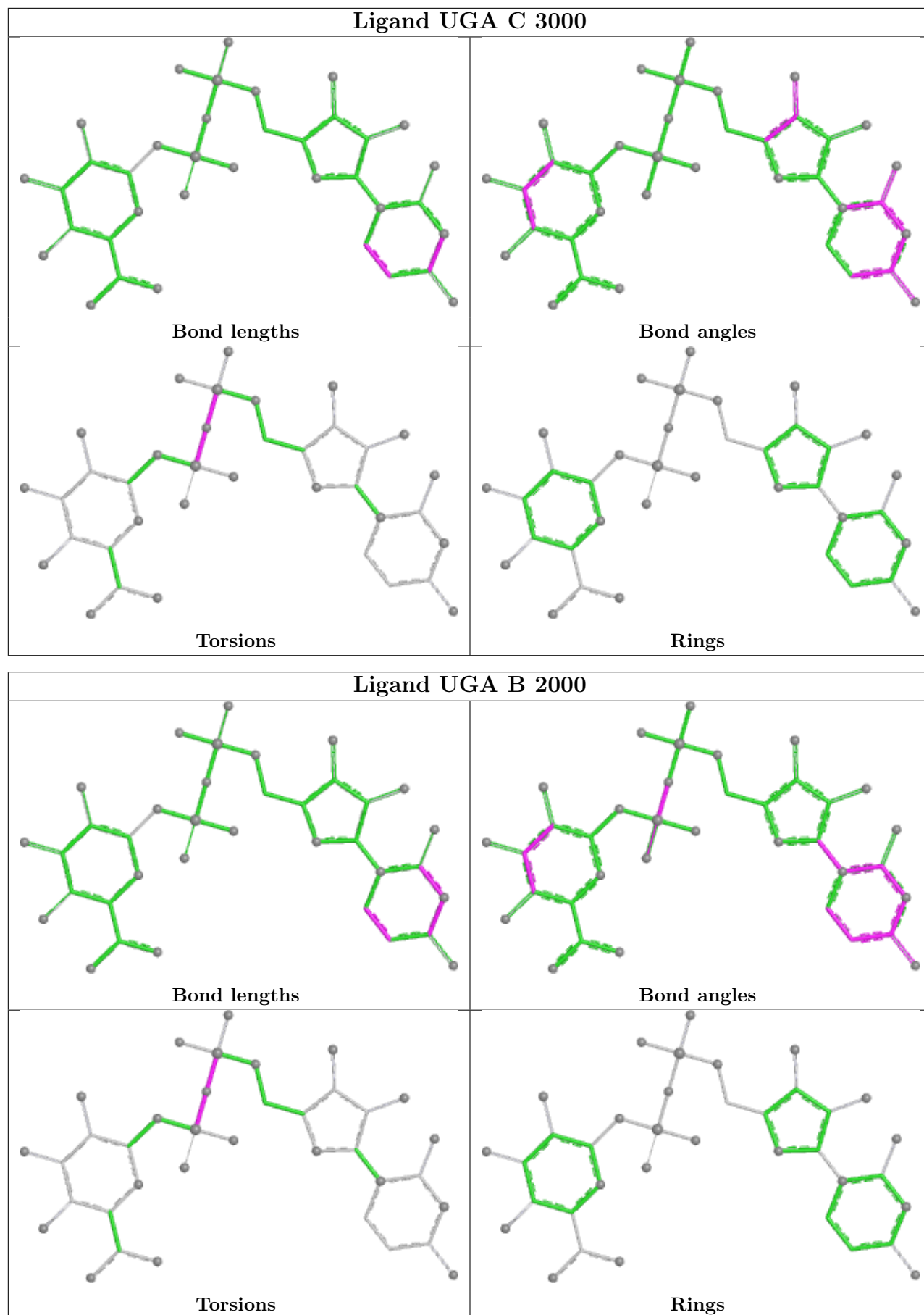


Ligand UGA D 5000



Ligand UGA D 4000





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	431/450 (95%)	0.39	23 (5%) 32 35	11, 23, 35, 41	8 (1%)
1	B	425/450 (94%)	0.96	52 (12%) 8 8	13, 30, 42, 47	2 (0%)
1	C	420/450 (93%)	0.69	25 (5%) 27 30	12, 27, 38, 44	3 (0%)
1	D	427/450 (94%)	0.48	24 (5%) 30 33	13, 24, 36, 43	4 (0%)
All	All	1703/1800 (94%)	0.63	124 (7%) 21 23	11, 26, 39, 47	17 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	125[A]	TYR	5.8
1	B	121	THR	4.6
1	B	185	GLY	4.3
1	D	505	ASP	4.3
1	A	274	PHE	4.3
1	D	170	GLY	4.2
1	A	78	SER	4.1
1	B	170	GLY	4.1
1	A	122	ILE	3.8
1	D	88	TYR	3.7
1	A	271	LEU	3.7
1	C	125	TYR	3.5
1	A	123	PRO	3.5
1	B	392	VAL	3.5
1	B	446	GLY	3.5
1	B	479	TRP	3.4
1	D	479	TRP	3.4
1	C	224	ASP	3.4
1	C	124	ILE	3.3
1	B	482	LEU	3.3
1	B	500	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	512	GLY	3.2
1	A	121	THR	3.2
1	B	114	ILE	3.1
1	B	216	LEU	3.1
1	A	125	TYR	3.1
1	B	488	ALA	3.1
1	A	118	ASN	3.0
1	C	148	ILE	3.0
1	D	123	PRO	3.0
1	C	343	SER	3.0
1	C	119	SER	2.9
1	B	481	ALA	2.9
1	A	79	LEU	2.9
1	D	124	ILE	2.9
1	C	79	LEU	2.9
1	B	176	TYR	2.8
1	B	480	SER	2.8
1	B	172	ALA	2.8
1	A	88[A]	TYR	2.8
1	C	505	ASP	2.8
1	D	176	TYR	2.7
1	D	114	ILE	2.7
1	D	109	THR	2.7
1	A	112	ASN	2.7
1	C	134	ALA	2.7
1	C	237	GLY	2.7
1	B	218	LYS	2.7
1	B	462	ALA	2.7
1	D	501	PRO	2.6
1	D	271	LEU	2.6
1	B	122	ILE	2.6
1	C	117	LEU	2.6
1	D	79	LEU	2.6
1	B	485	ALA	2.6
1	D	112	ASN	2.6
1	C	241	ASP	2.5
1	B	497	VAL	2.5
1	B	168	GLU	2.5
1	A	119	SER	2.5
1	B	393	GLN	2.5
1	B	217	ASP	2.5
1	A	501	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	480	SER	2.5
1	B	178	LEU	2.4
1	A	120	GLY	2.4
1	C	127	PRO	2.4
1	D	122	ILE	2.4
1	D	171	SER	2.4
1	C	170	GLY	2.4
1	B	107	ILE	2.4
1	B	214	GLU	2.4
1	D	221	VAL	2.4
1	B	483	SER	2.3
1	A	117	LEU	2.3
1	D	274	PHE	2.3
1	C	137	VAL	2.3
1	B	164	THR	2.3
1	B	175	SER	2.3
1	A	273	ASN	2.3
1	B	171	SER	2.3
1	B	443	LYS	2.3
1	C	439	LYS	2.3
1	B	426	VAL	2.3
1	C	487	ALA	2.2
1	C	480	SER	2.2
1	C	140	GLY	2.2
1	C	150	GLN	2.2
1	C	450	GLU	2.2
1	D	165	PRO	2.2
1	A	272	ASN	2.2
1	A	150	GLN	2.2
1	A	114	ILE	2.2
1	B	412	ARG	2.2
1	B	169	ASP	2.2
1	B	241	ASP	2.2
1	B	394	GLY	2.2
1	B	506	PHE	2.2
1	B	191	TYR	2.2
1	B	173	ASP	2.1
1	B	447	ASP	2.1
1	B	207	LEU	2.1
1	B	222	LEU	2.1
1	B	270	LEU	2.1
1	C	220	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	481	ALA	2.1
1	D	273	ASN	2.1
1	A	168	GLU	2.1
1	A	442	GLN	2.1
1	B	256	ASP	2.1
1	B	362	ARG	2.1
1	B	477	PRO	2.1
1	C	191	TYR	2.1
1	A	354	ARG	2.1
1	C	275	ARG	2.1
1	D	117	LEU	2.1
1	B	512	GLY	2.0
1	D	220	GLU	2.0
1	B	478	ASP	2.0
1	B	220	GLU	2.0
1	C	130	GLU	2.0
1	B	456	TYR	2.0
1	B	139	ALA	2.0
1	B	449	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($\text{\AA}^2$)	Q<0.9
2	UGA	A	6000	37/37	0.86	0.12	30,36,44,46	0
2	UGA	D	5000	37/37	0.93	0.10	25,29,35,39	0
2	UGA	C	3000	37/37	0.97	0.06	17,21,24,26	0
2	UGA	B	2000	37/37	0.97	0.06	17,22,26,28	0

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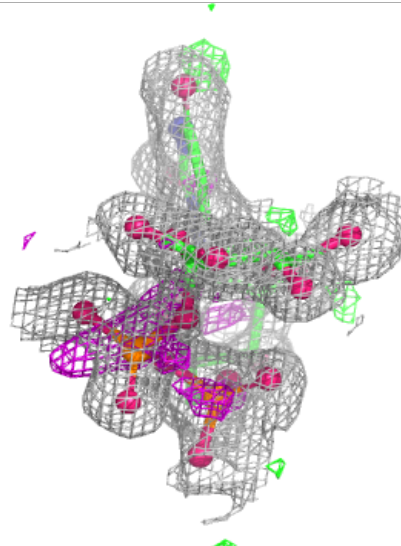
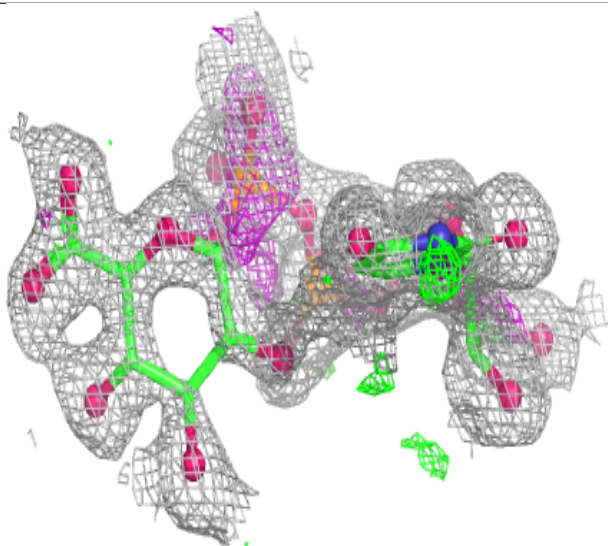
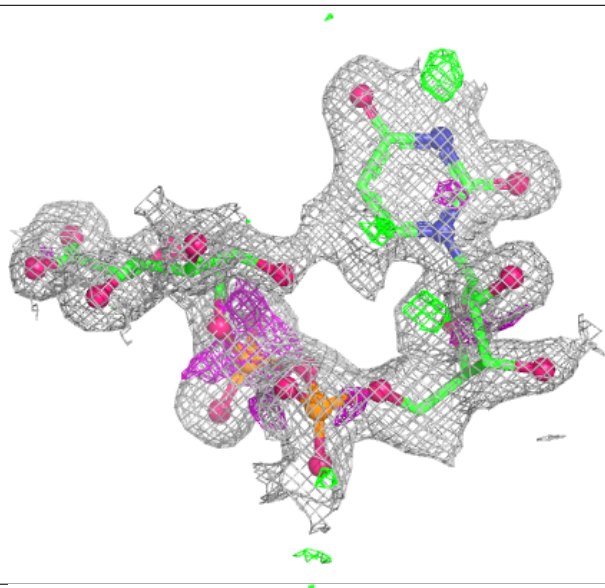
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UGA	D	4000	37/37	0.98	0.06	16,19,24,27	0
2	UGA	A	1000	37/37	0.98	0.06	12,18,22,25	0

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.

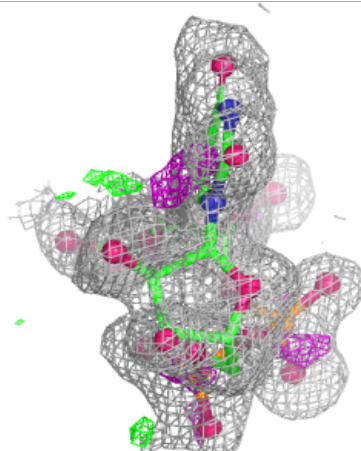
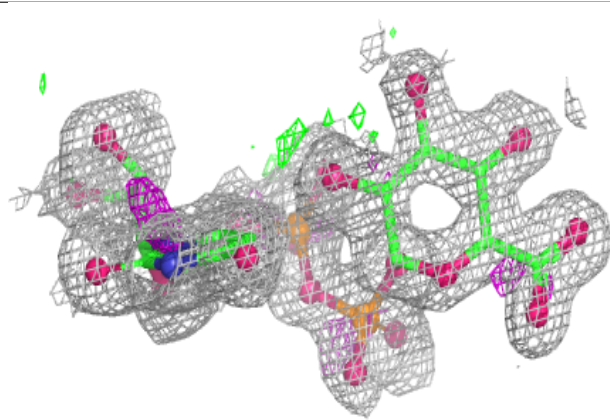
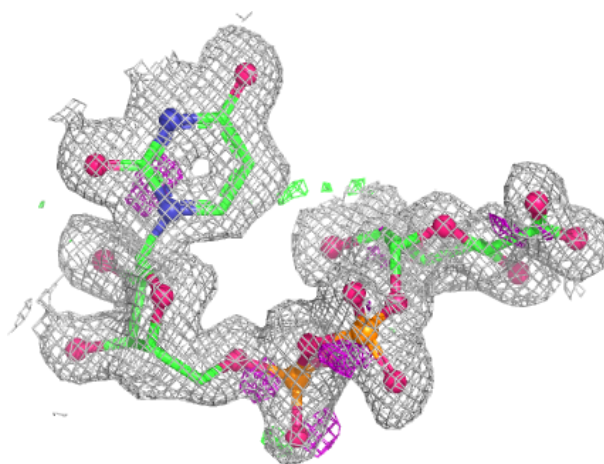
Electron density around UGA A 6000:

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



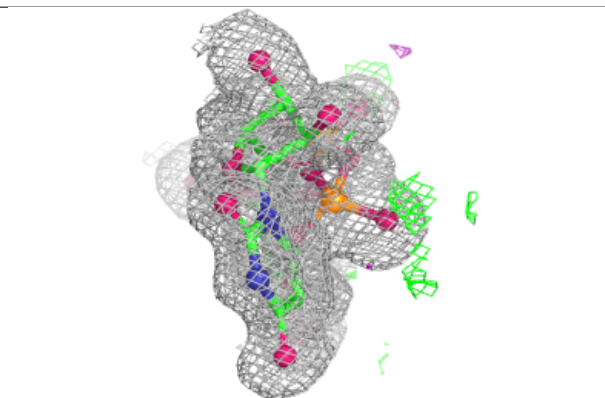
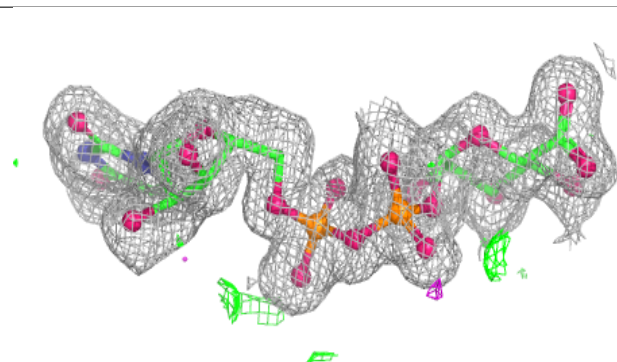
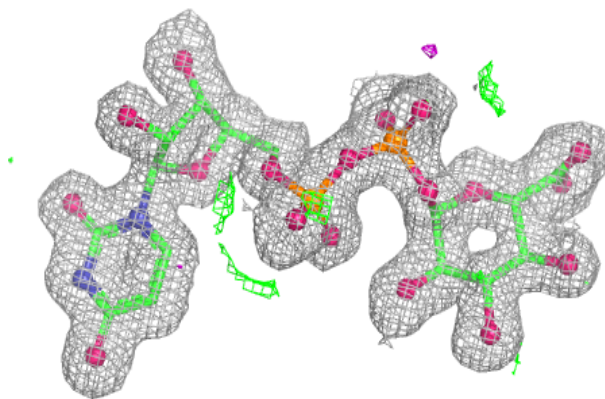
Electron density around UGA D 5000:

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

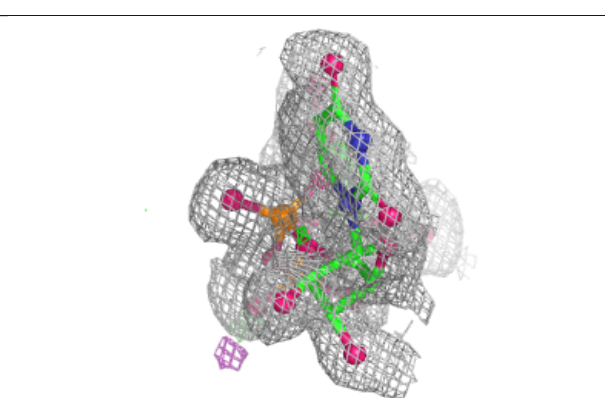
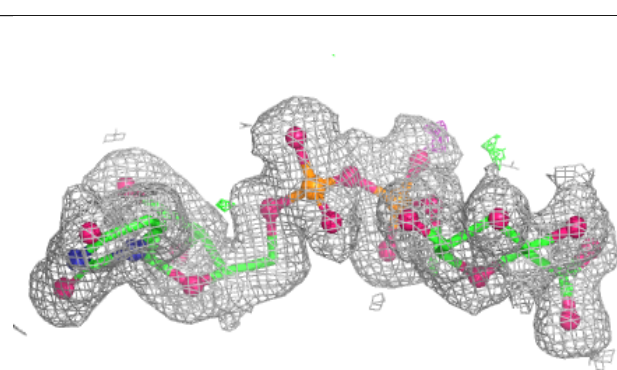
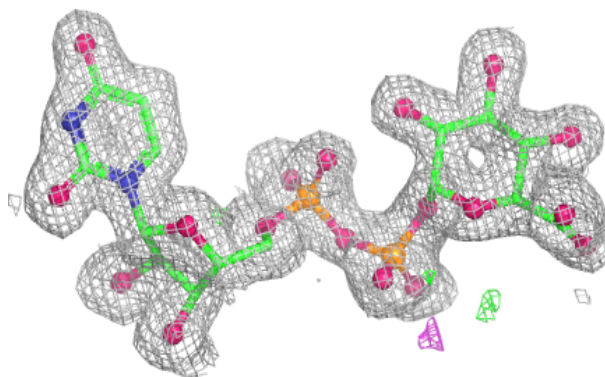


Electron density around UGA C 3000:

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

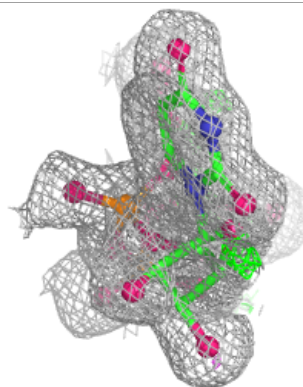
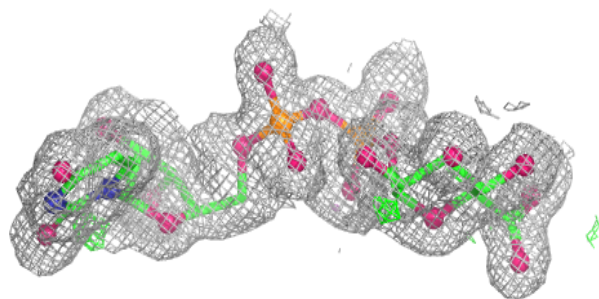
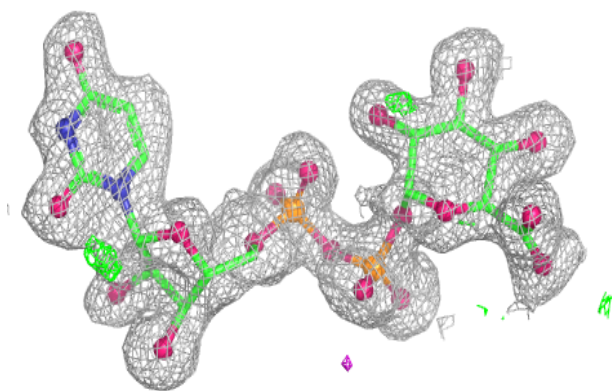
**Electron density around UGA B 2000:**

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

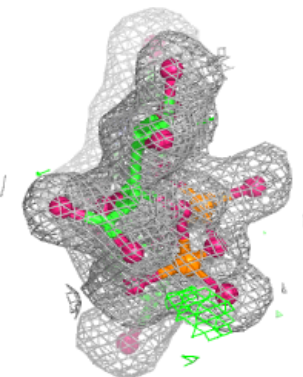
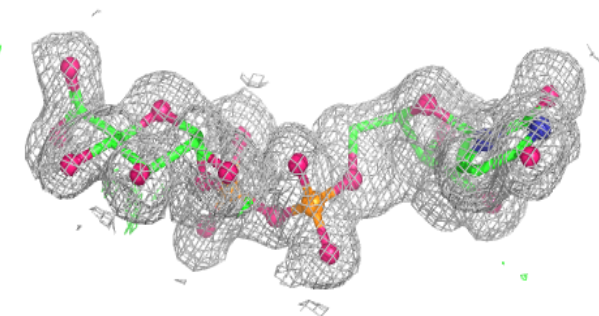
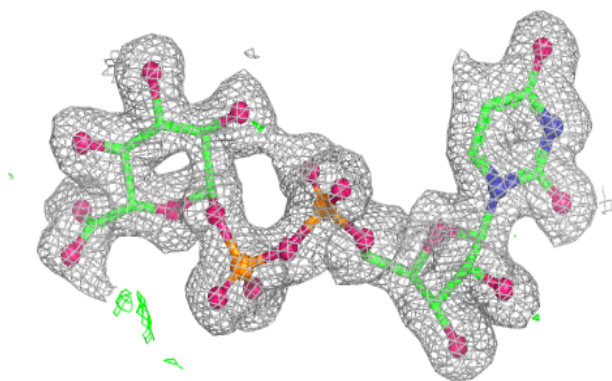


Electron density around UGA D 4000:

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

**Electron density around UGA A 1000:**

$2mF_o-DF_c$ (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.