Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:19 am BST

PDB ID	:	3UKF
Title	:	CRYSTAL STRUCTURE OF UDP-galactopyranose mutase from Aspergillus fumigatus in complex with UDPgalp (reduced)
Authors	:	Van Straaten, K.E.; Sanders, D.A.R.
Deposited on	:	2011-11-09
Resolution	:	2.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

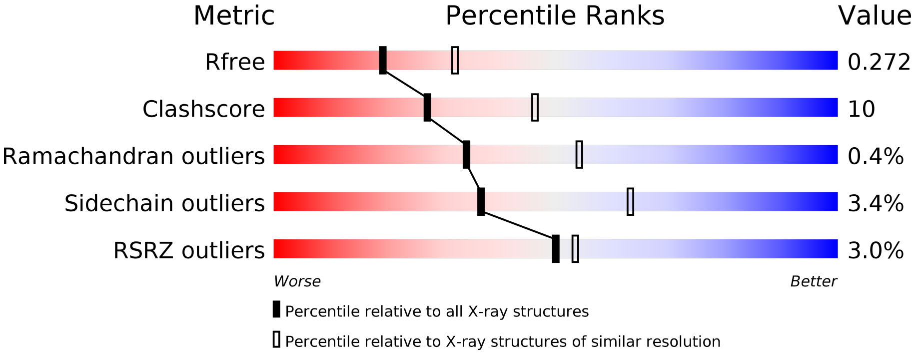
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

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

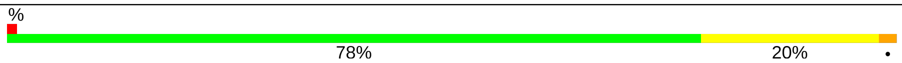
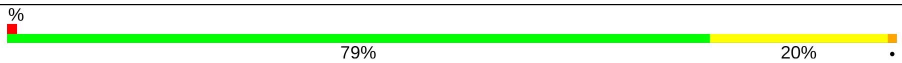
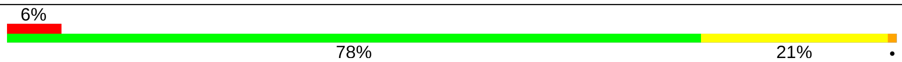
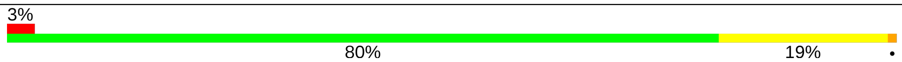
The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	509	
1	B	509	
1	C	509	
1	D	509	
1	E	509	
1	F	509	

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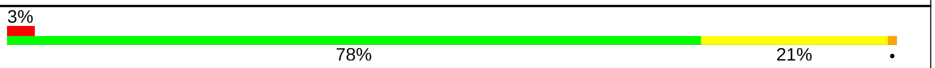
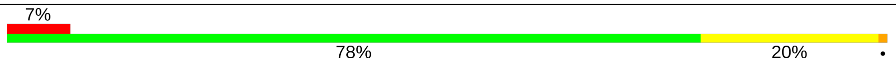
Mol	Chain	Length	Quality of chain
1	G	509	
1	H	509	

2 Entry composition

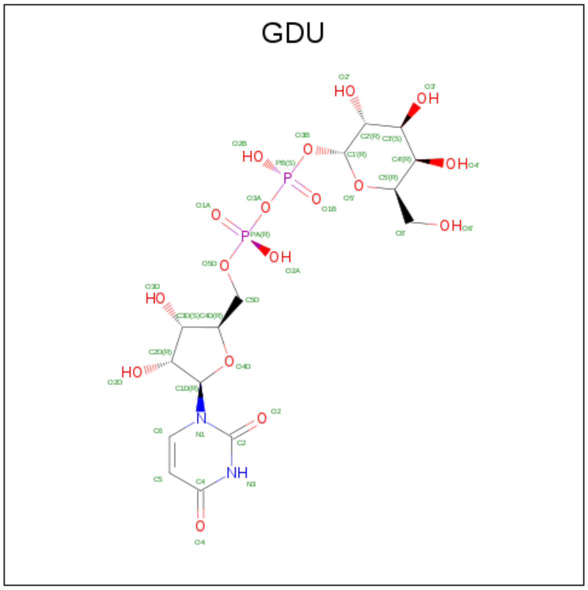
There are 5 unique types of molecules in this entry. The entry contains 33444 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-galactopyranose mutase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	509	3996	2534	686	755	7	14	0	0	0
1	B	509	3996	2534	686	755	7	14	0	0	0
1	C	509	3996	2534	686	755	7	14	0	0	0
1	D	509	3996	2534	686	755	7	14	0	0	0
1	E	509	3996	2534	686	755	7	14	0	0	0
1	F	509	3996	2534	686	755	7	14	0	0	0
1	G	509	3996	2534	686	755	7	14	0	0	0
1	H	509	3996	2534	686	755	7	14	0	0	0

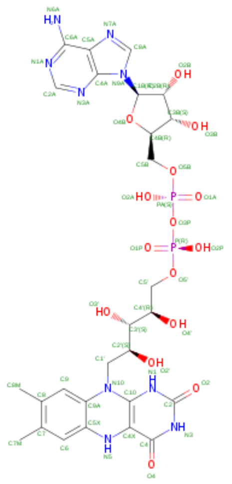
- Molecule 2 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (three-letter code: GDU) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	36	15	2	17	2	0	0
2	B	1	36	15	2	17	2	0	0
2	C	1	36	15	2	17	2	0	0
2	D	1	36	15	2	17	2	0	0
2	E	1	36	15	2	17	2	0	0
2	F	1	36	15	2	17	2	0	0
2	G	1	36	15	2	17	2	0	0
2	H	1	36	15	2	17	2	0	0

- Molecule 3 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).

FDA



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 53 27 9 15 2	0	0
3	B	1	Total C N O P 53 27 9 15 2	0	0
3	C	1	Total C N O P 53 27 9 15 2	0	0
3	D	1	Total C N O P 53 27 9 15 2	0	0
3	E	1	Total C N O P 53 27 9 15 2	0	0
3	F	1	Total C N O P 53 27 9 15 2	0	0
3	G	1	Total C N O P 53 27 9 15 2	0	0
3	H	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0
4	B	2	Total Cl 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Cl 2	0	0
4	F	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

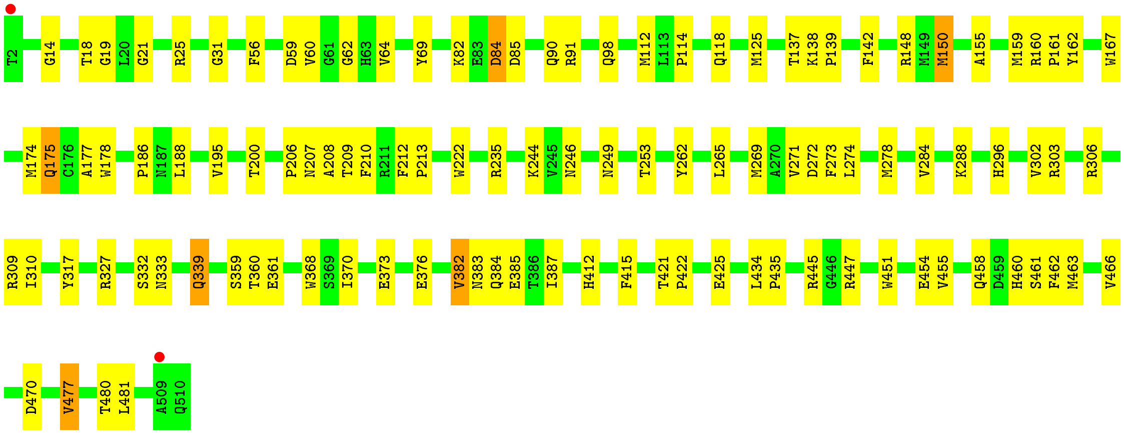
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	109	Total 109	O 109	0	0
5	B	122	Total 122	O 122	0	0
5	C	71	Total 71	O 71	0	0
5	D	104	Total 104	O 104	0	0
5	E	90	Total 90	O 90	0	0
5	F	78	Total 78	O 78	0	0
5	G	97	Total 97	O 97	0	0
5	H	85	Total 85	O 85	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.

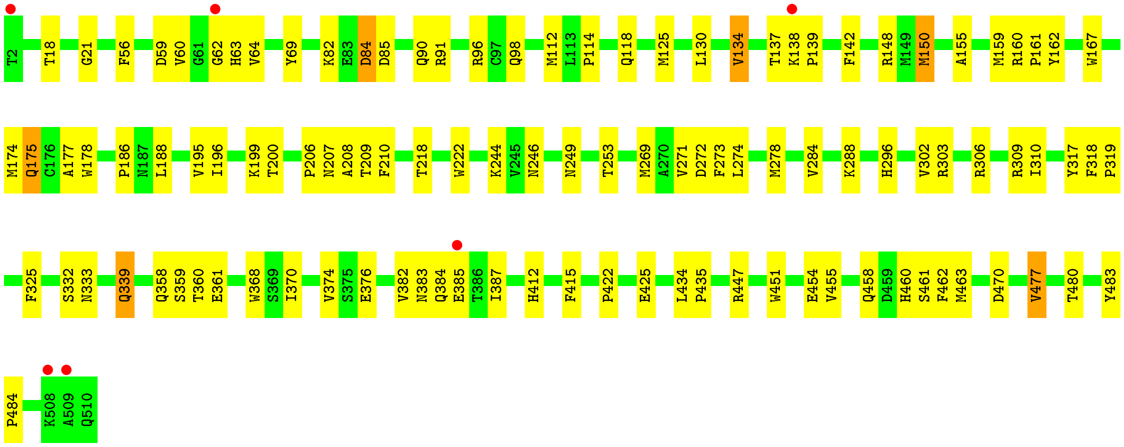
- Molecule 1: UDP-galactopyranose mutase

Chain A:



- Molecule 1: UDP-galactopyranose mutase

Chain B:

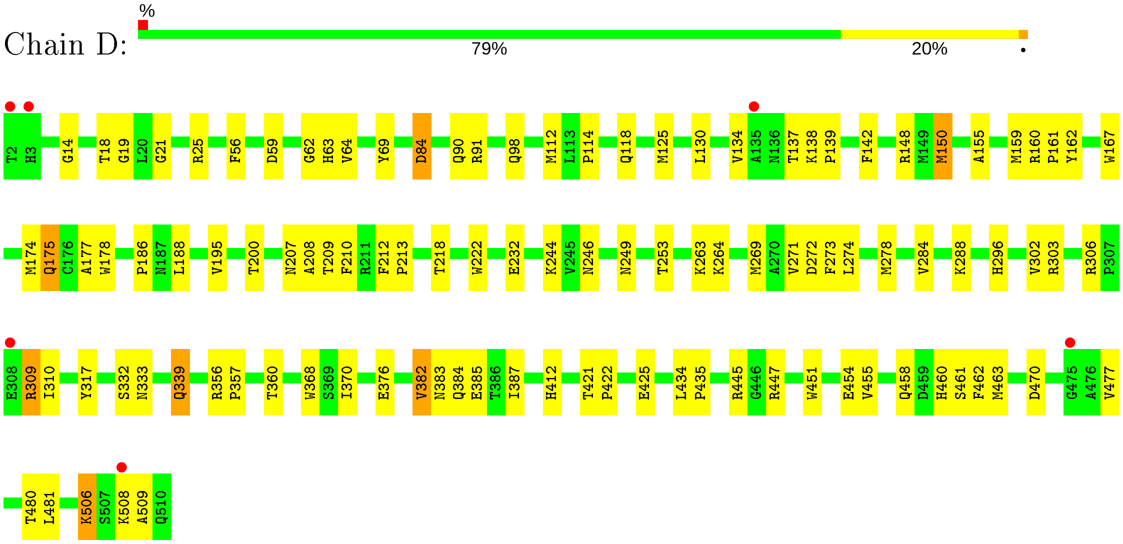


- Molecule 1: UDP-galactopyranose mutase

Chain C:

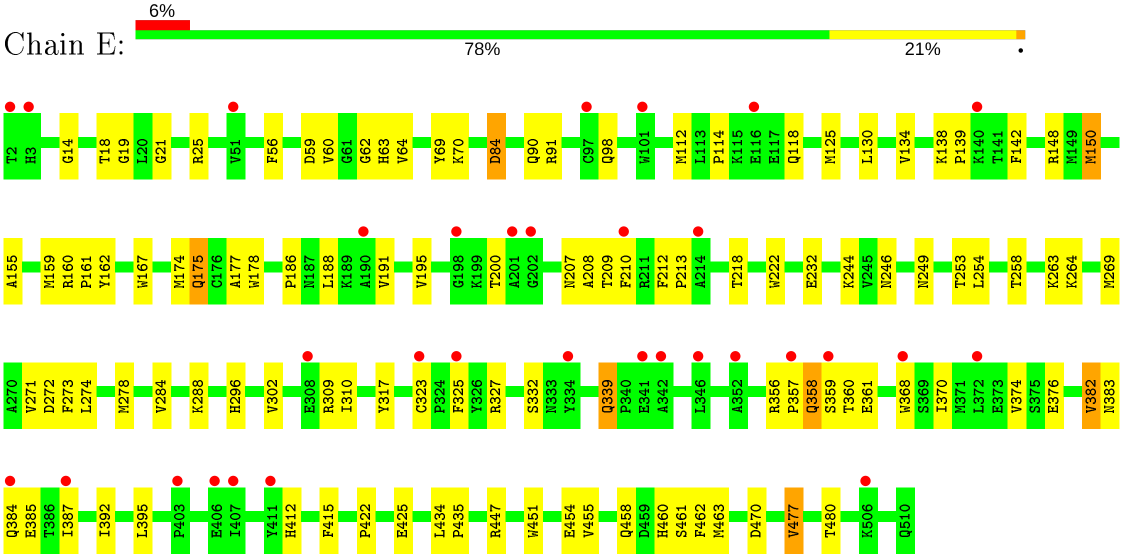
- Molecule 1: UDP-galactopyranose mutase

Chain D:



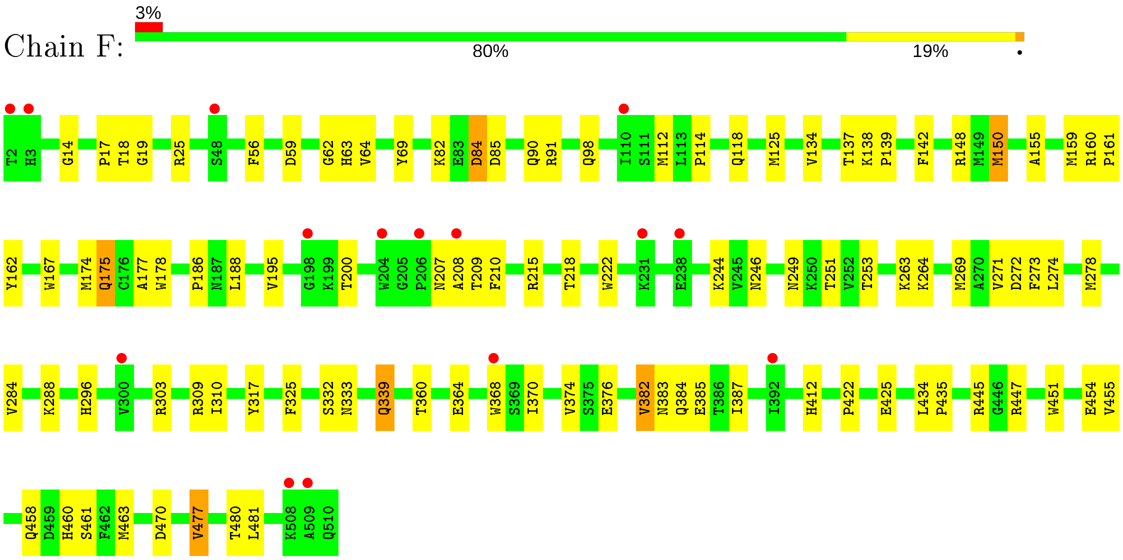
- Molecule 1: UDP-galactopyranose mutase

Chain E:



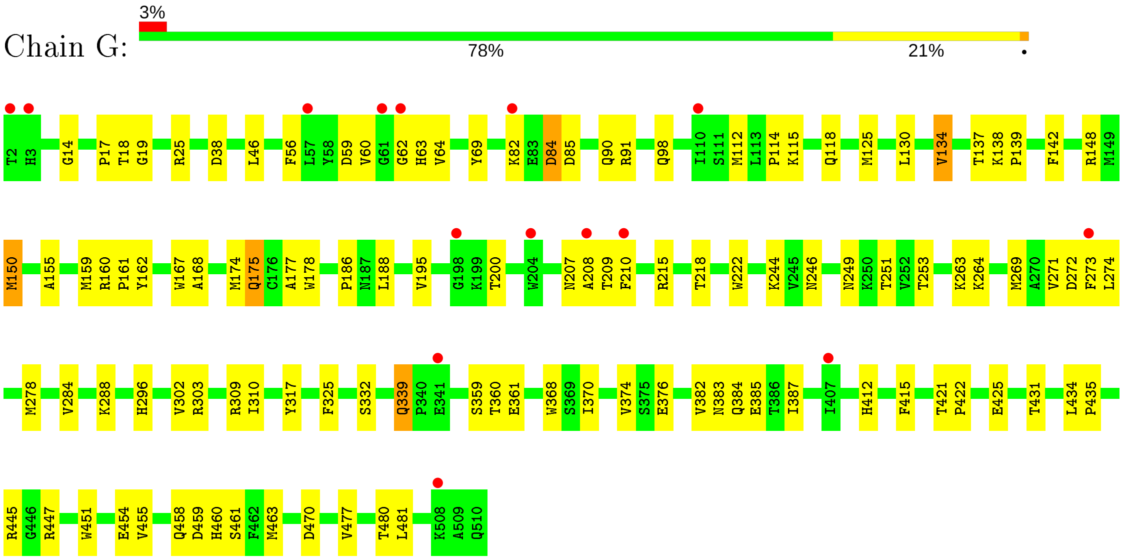
- Molecule 1: UDP-galactopyranose mutase

Chain F:



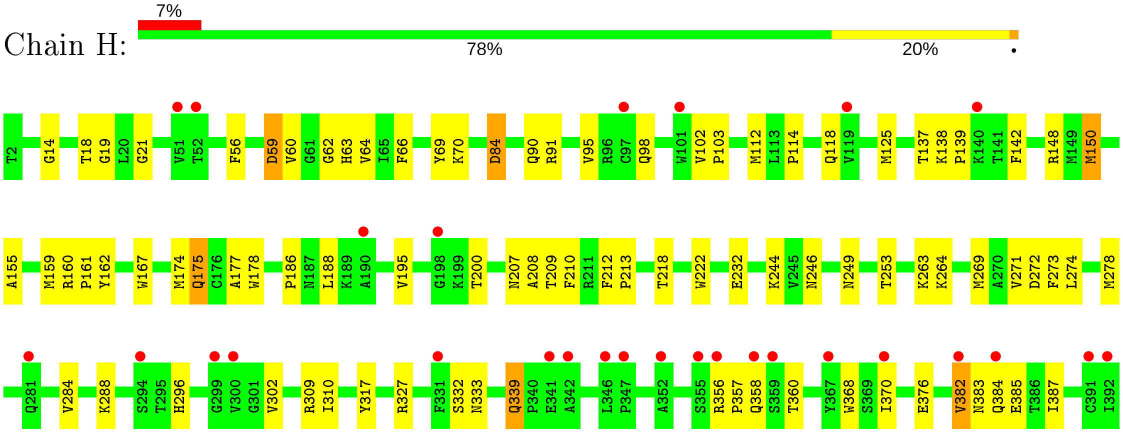
- Molecule 1: UDP-galactopyranose mutase

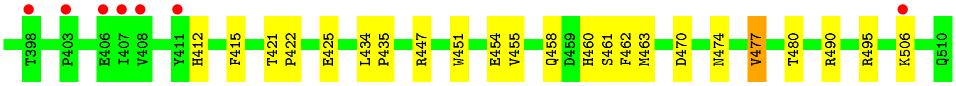
Chain G:



- Molecule 1: UDP-galactopyranose mutase

Chain H:




T398
P403
E406
I407
V408
Y411
H412
F415
T421
P422
E425
L434
P435
R447
W451
E454
V455
Q458
D459
H460
S461
F462
M463
D470
N474
V477
T480
R490
R495
K506
Q510

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.08Å 129.34Å 175.08Å 89.97° 103.61° 90.14°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-2.50) 96.5 (20.00-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.41Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.250 , 0.293 0.226 , 0.272	Depositor DCC
R_{free} test set	11653 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.4	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.8	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.50, $< L^2 >$ = 0.33	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l 0.399 for -h,k,-l 0.000 for -h,-k,h+l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	33444	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FDA, GDU, CL

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	0.22	0/4081	0.41	0/5523
1	B	0.23	0/4081	0.41	0/5523
1	C	0.22	0/4081	0.40	0/5523
1	D	0.22	0/4081	0.40	0/5523
1	E	0.22	0/4081	0.40	0/5523
1	F	0.22	0/4081	0.41	0/5523
1	G	0.22	0/4081	0.41	0/5523
1	H	0.22	0/4081	0.40	0/5523
All	All	0.22	0/32648	0.40	0/44184

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3996	0	3914	81	0
1	B	3996	0	3914	81	0
1	C	3996	0	3914	90	0
1	D	3996	0	3914	79	0
1	E	3996	0	3914	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3996	0	3914	70	0
1	G	3996	0	3914	88	0
1	H	3996	0	3914	87	0
2	A	36	0	22	2	0
2	B	36	0	22	1	0
2	C	36	0	22	2	0
2	D	36	0	22	2	0
2	E	36	0	22	1	0
2	F	36	0	22	0	0
2	G	36	0	22	2	0
2	H	36	0	22	3	0
3	A	53	0	32	1	0
3	B	53	0	32	1	0
3	C	53	0	32	1	0
3	D	53	0	32	1	0
3	E	53	0	32	1	0
3	F	53	0	32	2	0
3	G	53	0	32	6	0
3	H	53	0	32	1	0
4	A	2	0	0	1	0
4	B	2	0	0	2	0
4	E	1	0	0	1	0
4	F	1	0	0	1	0
4	G	1	0	0	0	0
4	H	1	0	0	1	0
5	A	109	0	0	7	0
5	B	122	0	0	5	0
5	C	71	0	0	5	0
5	D	104	0	0	5	0
5	E	90	0	0	4	0
5	F	78	0	0	3	0
5	G	97	0	0	8	0
5	H	85	0	0	7	0
All	All	33444	0	31744	650	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 10.

All (650) 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:E:323:CYS:SG	5:E:542:HOH:O	2.26	0.94
1:G:69:TYR:HE2	5:G:729:HOH:O	1.55	0.87
1:F:125:MSE:HE2	1:F:188:LEU:HA	1.58	0.84
1:D:125:MSE:HE2	1:D:188:LEU:HA	1.59	0.84
1:G:125:MSE:HE2	1:G:188:LEU:HA	1.59	0.83
1:H:125:MSE:HE2	1:H:188:LEU:HA	1.60	0.82
1:A:125:MSE:HE2	1:A:188:LEU:HA	1.60	0.82
1:C:125:MSE:HE2	1:C:188:LEU:HA	1.60	0.82
1:B:125:MSE:HE2	1:B:188:LEU:HA	1.60	0.82
1:E:125:MSE:HE2	1:E:188:LEU:HA	1.61	0.81
1:G:360:THR:HG22	1:G:360:THR:O	1.83	0.77
1:G:125:MSE:HB2	5:G:553:HOH:O	1.85	0.75
1:B:477:VAL:HG12	4:B:511:CL:CL	2.25	0.73
1:D:134:VAL:HG22	1:E:134:VAL:HG22	1.70	0.73
1:C:508:LYS:HG2	1:C:509:ALA:N	2.04	0.72
1:D:112:MSE:HE3	1:D:200:THR:HG23	1.72	0.71
1:D:91:ARG:HH11	1:D:207:ASN:HB2	1.55	0.71
1:B:91:ARG:HH11	1:B:207:ASN:HB2	1.56	0.71
1:C:112:MSE:HE3	1:C:200:THR:HG23	1.73	0.71
1:G:112:MSE:HE3	1:G:200:THR:HG23	1.73	0.71
1:G:91:ARG:HH11	1:G:207:ASN:HB2	1.56	0.71
1:A:91:ARG:HH11	1:A:207:ASN:HB2	1.56	0.70
1:A:327:ARG:N	5:A:660:HOH:O	2.20	0.70
1:E:112:MSE:HE3	1:E:200:THR:HG23	1.74	0.70
1:F:112:MSE:HE3	1:F:200:THR:HG23	1.72	0.70
1:A:455:VAL:HG21	1:A:480:THR:HG23	1.74	0.69
1:C:296:HIS:HD2	1:C:412:HIS:HE1	1.40	0.69
1:F:91:ARG:HH11	1:F:207:ASN:HB2	1.56	0.69
1:C:358:GLN:CD	1:C:358:GLN:H	1.95	0.69
1:E:274:LEU:HD11	1:E:278:MSE:HE3	1.75	0.69
1:H:477:VAL:HG12	4:H:511:CL:CL	2.30	0.69
1:D:138:LYS:HG3	1:D:139:PRO:HD2	1.75	0.69
1:H:112:MSE:HE3	1:H:200:THR:HG23	1.75	0.69
1:E:138:LYS:HG3	1:E:139:PRO:HD2	1.76	0.68
1:C:91:ARG:HH11	1:C:207:ASN:HB2	1.59	0.68
1:C:138:LYS:HG3	1:C:139:PRO:HD2	1.76	0.68
1:H:91:ARG:HH11	1:H:207:ASN:HB2	1.58	0.68
1:D:455:VAL:HG21	1:D:480:THR:HG23	1.75	0.67
1:C:455:VAL:HG21	1:C:480:THR:HG23	1.75	0.67
1:A:159:MSE:HE1	2:A:802:GDU:O2	1.94	0.67
1:B:112:MSE:HE3	1:B:200:THR:HG23	1.77	0.67
1:D:296:HIS:HD2	1:D:412:HIS:HE1	1.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:LYS:HG3	1:G:139:PRO:HD2	1.77	0.67
1:E:91:ARG:HH11	1:E:207:ASN:HB2	1.60	0.67
1:H:274:LEU:HD11	1:H:278:MSE:HE3	1.76	0.67
1:H:138:LYS:HG3	1:H:139:PRO:HD2	1.77	0.67
1:E:455:VAL:HG21	1:E:480:THR:HG23	1.77	0.66
1:F:138:LYS:HG3	1:F:139:PRO:HD2	1.76	0.66
1:G:296:HIS:HD2	1:G:412:HIS:HE1	1.44	0.66
1:C:455:VAL:HG22	1:C:460:HIS:HB3	1.78	0.66
1:E:455:VAL:HG22	1:E:460:HIS:HB3	1.78	0.66
1:H:296:HIS:HD2	1:H:412:HIS:HE1	1.43	0.66
1:F:360:THR:HG22	1:F:360:THR:O	1.94	0.66
1:B:274:LEU:HD11	1:B:278:MSE:HE3	1.78	0.66
1:A:477:VAL:HG12	4:A:511:CL:CL	2.33	0.65
1:E:296:HIS:HD2	1:E:412:HIS:HE1	1.45	0.65
1:F:455:VAL:HG21	1:F:480:THR:HG23	1.78	0.65
1:G:455:VAL:HG21	1:G:480:THR:HG23	1.78	0.65
1:F:455:VAL:HG22	1:F:460:HIS:HB3	1.77	0.65
1:A:138:LYS:HG3	1:A:139:PRO:HD2	1.77	0.65
1:A:296:HIS:HD2	1:A:412:HIS:HE1	1.43	0.65
1:D:137:THR:HG23	5:D:724:HOH:O	1.97	0.64
1:H:455:VAL:HG22	1:H:460:HIS:HB3	1.78	0.64
1:E:477:VAL:HG12	4:E:511:CL:CL	2.34	0.64
1:A:112:MSE:HE3	1:A:200:THR:HG23	1.78	0.64
1:A:274:LEU:HD11	1:A:278:MSE:HE3	1.79	0.64
1:D:455:VAL:HG22	1:D:460:HIS:HB3	1.78	0.64
1:G:455:VAL:HG22	1:G:460:HIS:HB3	1.77	0.64
1:B:138:LYS:HG3	1:B:139:PRO:HD2	1.79	0.64
1:C:232:GLU:HG3	1:H:232:GLU:CG	2.28	0.63
1:B:359:SER:OG	1:B:361:GLU:HG2	1.98	0.63
1:F:296:HIS:HD2	1:F:412:HIS:HE1	1.44	0.63
1:B:455:VAL:HG21	1:B:480:THR:HG23	1.80	0.62
1:E:359:SER:HB3	1:E:361:GLU:HG2	1.79	0.62
1:G:17:PRO:HD2	3:G:600:FDA:O5'	1.99	0.62
1:B:178:TRP:CB	1:B:454:GLU:HG3	2.28	0.62
1:H:455:VAL:HG21	1:H:480:THR:HG23	1.80	0.62
1:A:178:TRP:CB	1:A:454:GLU:HG3	2.30	0.62
1:B:296:HIS:HD2	1:B:412:HIS:HE1	1.45	0.62
1:C:232:GLU:CG	1:H:232:GLU:HG3	2.30	0.62
1:C:232:GLU:HG3	1:H:232:GLU:HG2	1.80	0.62
1:B:159:MSE:HE1	2:B:802:GDU:O2	2.00	0.61
1:F:178:TRP:CB	1:F:454:GLU:HG3	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:VAL:HG22	1:B:460:HIS:HB3	1.82	0.60
1:G:178:TRP:CB	1:G:454:GLU:HG3	2.30	0.60
1:A:455:VAL:HG22	1:A:460:HIS:HB3	1.82	0.60
1:G:460:HIS:CD2	5:G:729:HOH:O	2.53	0.60
1:A:175:GLN:NE2	1:A:177:ALA:H	2.00	0.60
1:B:178:TRP:HB2	1:B:454:GLU:HG3	1.83	0.60
1:H:178:TRP:HB2	1:H:454:GLU:HG3	1.84	0.60
1:H:178:TRP:CB	1:H:454:GLU:HG3	2.31	0.60
1:E:178:TRP:CB	1:E:454:GLU:HG3	2.32	0.60
1:F:178:TRP:HB2	1:F:454:GLU:HG3	1.84	0.59
1:F:17:PRO:HD2	3:F:600:FDA:O5’	2.01	0.59
1:G:91:ARG:NH1	1:G:207:ASN:HB2	2.17	0.59
1:H:125:MSE:HG2	1:H:188:LEU:HD13	1.84	0.59
1:G:207:ASN:ND2	5:G:563:HOH:O	2.35	0.59
1:D:178:TRP:CB	1:D:454:GLU:HG3	2.33	0.59
1:F:91:ARG:NH1	1:F:207:ASN:HB2	2.17	0.59
1:E:18:THR:OG1	1:E:461:SER:HB3	2.03	0.59
1:C:137:THR:HG23	5:C:543:HOH:O	2.01	0.58
1:C:232:GLU:HG2	1:H:232:GLU:HG3	1.83	0.58
1:D:274:LEU:HD11	1:D:278:MSE:HE3	1.84	0.58
1:G:178:TRP:HB2	1:G:454:GLU:HG3	1.84	0.58
1:A:178:TRP:HB2	1:A:454:GLU:HG3	1.85	0.58
1:A:303:ARG:NH1	5:A:567:HOH:O	2.23	0.58
1:A:91:ARG:NH1	1:A:207:ASN:HB2	2.18	0.58
1:F:18:THR:OG1	1:F:461:SER:HB3	2.04	0.58
1:H:18:THR:OG1	1:H:461:SER:HB3	2.04	0.58
1:B:222:TRP:HE1	1:B:458:GLN:NE2	2.02	0.57
1:E:274:LEU:CD1	1:E:278:MSE:HE3	2.33	0.57
1:H:274:LEU:CD1	1:H:278:MSE:HE3	2.33	0.57
1:E:178:TRP:HB2	1:E:454:GLU:HG3	1.86	0.57
1:D:91:ARG:NH1	1:D:207:ASN:HB2	2.17	0.57
1:C:178:TRP:CB	1:C:454:GLU:HG3	2.34	0.57
1:F:125:MSE:HG2	1:F:188:LEU:HD13	1.86	0.57
1:F:222:TRP:HE1	1:F:458:GLN:NE2	2.02	0.57
1:G:274:LEU:HD11	1:G:278:MSE:HE3	1.87	0.57
1:H:91:ARG:NH1	1:H:207:ASN:HB2	2.19	0.57
1:C:159:MSE:HE1	2:C:802:GDU:O2	2.04	0.56
1:B:358:GLN:NE2	1:C:84:ASP:HA	2.20	0.56
1:E:317:TYR:N	5:E:530:HOH:O	2.38	0.56
1:A:18:THR:OG1	1:A:461:SER:HB3	2.05	0.56
1:B:91:ARG:NH1	1:B:207:ASN:HB2	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:LEU:HB2	1:B:435:PRO:HD3	1.88	0.56
1:F:477:VAL:HG12	4:F:511:CL:CL	2.42	0.56
1:B:425:GLU:OE2	1:B:425:GLU:N	2.39	0.56
1:B:125:MSE:HG2	1:B:188:LEU:HD13	1.87	0.56
1:E:91:ARG:NH1	1:E:207:ASN:HB2	2.20	0.56
1:F:274:LEU:HD11	1:F:278:MSE:HE3	1.88	0.56
1:B:18:THR:OG1	1:B:461:SER:HB3	2.06	0.55
1:D:175:GLN:NE2	1:D:177:ALA:H	2.04	0.55
1:D:125:MSE:HG2	1:D:188:LEU:HD13	1.88	0.55
1:D:178:TRP:HB2	1:D:454:GLU:HG3	1.87	0.55
1:D:222:TRP:HE1	1:D:458:GLN:NE2	2.04	0.55
1:C:499:ASP:O	1:C:503:VAL:HG12	2.07	0.55
1:C:178:TRP:HB2	1:C:454:GLU:HG3	1.89	0.55
1:D:506:LYS:N	1:D:506:LYS:HE3	2.22	0.55
1:E:222:TRP:HE1	1:E:458:GLN:NE2	2.05	0.55
1:G:159:MSE:HE1	2:G:802:GDU:O2	2.07	0.55
1:H:159:MSE:HE1	2:H:802:GDU:O2	2.07	0.55
1:B:274:LEU:CD1	1:B:278:MSE:HE3	2.37	0.55
1:B:360:THR:O	1:B:360:THR:HG22	2.06	0.55
1:C:125:MSE:HG2	1:C:188:LEU:HD13	1.88	0.55
1:G:459:ASP:CG	5:G:729:HOH:O	2.45	0.55
1:C:222:TRP:HE1	1:C:458:GLN:NE2	2.03	0.55
1:E:383:ASN:OD1	1:E:385:GLU:HG2	2.07	0.55
1:G:434:LEU:HB2	1:G:435:PRO:HD3	1.89	0.55
1:A:222:TRP:HE1	1:A:458:GLN:NE2	2.04	0.54
1:D:508:LYS:HG2	1:D:509:ALA:N	2.21	0.54
1:E:434:LEU:HB2	1:E:435:PRO:HD3	1.88	0.54
1:G:18:THR:OG1	1:G:461:SER:HB3	2.07	0.54
1:H:383:ASN:OD1	1:H:385:GLU:HG2	2.07	0.54
1:A:359:SER:OG	1:A:361:GLU:HG2	2.07	0.54
1:G:222:TRP:HE1	1:G:458:GLN:NE2	2.05	0.54
1:A:425:GLU:OE2	1:A:425:GLU:N	2.39	0.54
1:C:91:ARG:NH1	1:C:207:ASN:HB2	2.21	0.54
1:D:162:TYR:HH	1:D:317:TYR:HD1	1.53	0.54
1:G:118:GLN:NE2	1:G:195:VAL:HG13	2.22	0.54
1:D:18:THR:OG1	1:D:461:SER:HB3	2.08	0.54
1:H:222:TRP:HE1	1:H:458:GLN:NE2	2.06	0.54
1:G:460:HIS:N	5:G:729:HOH:O	2.41	0.54
1:E:125:MSE:HG2	1:E:188:LEU:HD13	1.88	0.54
1:G:125:MSE:HG2	1:G:188:LEU:HD13	1.88	0.54
1:H:118:GLN:NE2	1:H:195:VAL:HG13	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ASN:ND2	1:A:249:ASN:HD21	2.06	0.53
1:B:56:PHE:CE1	1:B:339:GLN:HB3	2.43	0.53
1:G:84:ASP:OD1	1:G:84:ASP:N	2.40	0.53
1:C:248:ASN:ND2	5:C:528:HOH:O	2.40	0.53
1:F:118:GLN:NE2	1:F:195:VAL:HG13	2.23	0.53
1:B:269:MSE:HE2	1:B:273:PHE:HB3	1.90	0.53
1:A:125:MSE:HG2	1:A:188:LEU:HD13	1.91	0.53
1:A:434:LEU:HB2	1:A:435:PRO:HD3	1.89	0.53
1:C:274:LEU:HD11	1:C:278:MSE:HE3	1.90	0.53
1:H:246:ASN:ND2	1:H:249:ASN:HD21	2.07	0.53
1:A:274:LEU:CD1	1:A:278:MSE:HE3	2.37	0.53
1:D:383:ASN:OD1	1:D:385:GLU:HG2	2.07	0.53
1:D:434:LEU:HB2	1:D:435:PRO:HD3	1.90	0.53
1:C:434:LEU:HB2	1:C:435:PRO:HD3	1.91	0.53
1:C:502:GLN:O	1:C:506:LYS:HE2	2.08	0.53
1:F:174:MSE:HB2	1:F:422:PRO:O	2.09	0.53
1:C:383:ASN:OD1	1:C:385:GLU:HG2	2.09	0.52
1:H:434:LEU:HB2	1:H:435:PRO:HD3	1.92	0.52
1:B:175:GLN:NE2	1:B:177:ALA:H	2.07	0.52
1:D:455:VAL:HG21	1:D:480:THR:CG2	2.40	0.52
1:A:207:ASN:ND2	5:A:559:HOH:O	2.43	0.52
1:B:246:ASN:ND2	1:B:249:ASN:HD21	2.08	0.52
1:C:175:GLN:NE2	1:C:177:ALA:H	2.06	0.52
1:G:162:TYR:HH	1:G:317:TYR:HD1	1.57	0.52
1:C:18:THR:OG1	1:C:461:SER:HB3	2.09	0.52
1:G:175:GLN:NE2	1:G:177:ALA:H	2.07	0.52
1:A:269:MSE:HE2	1:A:273:PHE:HB3	1.90	0.52
1:G:56:PHE:CE1	1:G:339:GLN:HB3	2.44	0.52
1:G:174:MSE:HB2	1:G:422:PRO:O	2.10	0.52
1:H:84:ASP:OD1	1:H:84:ASP:N	2.42	0.52
1:E:455:VAL:HG21	1:E:480:THR:CG2	2.40	0.52
1:F:303:ARG:NH1	5:F:531:HOH:O	2.27	0.52
1:B:96:ARG:NH2	5:B:568:HOH:O	2.22	0.52
1:D:368:TRP:CZ3	1:D:370:ILE:HD11	2.45	0.52
1:F:56:PHE:CE1	1:F:339:GLN:HB3	2.45	0.52
1:H:64:VAL:HG13	1:H:210:PHE:CD1	2.45	0.52
1:C:17:PRO:HD2	3:C:600:FDA:O5’	2.10	0.51
1:D:274:LEU:CD1	1:D:278:MSE:HE3	2.40	0.51
1:F:269:MSE:HE2	1:F:273:PHE:HB3	1.92	0.51
1:A:175:GLN:HE21	1:A:177:ALA:H	1.58	0.51
1:B:383:ASN:OD1	1:B:385:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:GLN:NE2	1:E:195:VAL:HG13	2.25	0.51
1:E:70:LYS:NZ	5:E:561:HOH:O	2.39	0.51
3:B:600:FDA:H9	3:B:600:FDA:O2'	2.11	0.51
1:B:84:ASP:N	1:B:84:ASP:OD1	2.42	0.51
1:F:434:LEU:HB2	1:F:435:PRO:HD3	1.91	0.51
1:H:327:ARG:NH1	2:H:802:GDU:H5'	2.25	0.51
1:H:356:ARG:HB3	1:H:357:PRO:HD2	1.92	0.51
1:H:368:TRP:CZ3	1:H:370:ILE:HD11	2.46	0.51
1:G:360:THR:O	1:G:360:THR:CG2	2.54	0.51
1:H:56:PHE:CE1	1:H:339:GLN:HB3	2.46	0.51
1:A:383:ASN:OD1	1:A:385:GLU:HG2	2.11	0.51
1:C:56:PHE:CE1	1:C:339:GLN:HB3	2.46	0.51
1:D:175:GLN:HE21	1:D:177:ALA:H	1.58	0.51
1:E:162:TYR:HH	1:E:317:TYR:HD1	1.58	0.51
1:F:175:GLN:NE2	1:F:177:ALA:H	2.09	0.51
1:F:246:ASN:ND2	1:F:249:ASN:HD21	2.09	0.51
1:H:269:MSE:HE2	1:H:273:PHE:HB3	1.92	0.51
1:C:246:ASN:ND2	1:C:249:ASN:HD21	2.08	0.51
1:G:368:TRP:CZ3	1:G:370:ILE:HD11	2.46	0.51
1:D:269:MSE:HE2	1:D:273:PHE:HB3	1.92	0.51
1:D:112:MSE:HE3	1:D:200:THR:CG2	2.41	0.51
1:D:56:PHE:CE1	1:D:339:GLN:HB3	2.46	0.51
1:D:425:GLU:OE2	1:D:425:GLU:N	2.44	0.51
1:A:455:VAL:HG21	1:A:480:THR:CG2	2.40	0.50
1:D:455:VAL:O	1:D:455:VAL:HG13	2.11	0.50
1:E:64:VAL:HG13	1:E:210:PHE:CD1	2.45	0.50
1:C:455:VAL:HG21	1:C:480:THR:CG2	2.40	0.50
1:F:162:TYR:HH	1:F:317:TYR:HD1	1.57	0.50
1:A:21:GLY:HA2	1:A:462:PHE:CE1	2.47	0.50
1:C:269:MSE:HE2	1:C:273:PHE:HB3	1.94	0.50
1:A:64:VAL:HG13	1:A:210:PHE:CD1	2.47	0.50
1:C:84:ASP:OD1	1:C:84:ASP:N	2.40	0.50
1:E:246:ASN:ND2	1:E:249:ASN:HD21	2.10	0.50
1:E:356:ARG:HB3	1:E:357:PRO:HD2	1.94	0.50
1:H:382:VAL:HG22	5:H:557:HOH:O	2.11	0.50
1:D:159:MSE:HE1	2:D:802:GDU:O2	2.12	0.50
1:E:327:ARG:NH1	2:E:802:GDU:H5'	2.27	0.50
1:A:56:PHE:CE1	1:A:339:GLN:HB3	2.47	0.50
1:B:118:GLN:NE2	1:B:195:VAL:HG13	2.27	0.50
1:B:303:ARG:NH1	5:B:549:HOH:O	2.22	0.50
1:C:64:VAL:HG13	1:C:210:PHE:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:TRP:CZ3	1:E:370:ILE:HD11	2.46	0.50
1:F:167:TRP:HB3	1:F:174:MSE:HE1	1.93	0.50
1:A:150:MSE:HG3	1:A:186:PRO:HG3	1.93	0.50
1:B:368:TRP:CZ3	1:B:370:ILE:HD11	2.47	0.49
1:D:167:TRP:HB3	1:D:174:MSE:HE1	1.93	0.49
1:E:167:TRP:HB3	1:E:174:MSE:HE1	1.93	0.49
1:H:317:TYR:N	5:H:524:HOH:O	2.45	0.49
1:H:384:GLN:O	1:H:387:ILE:HG22	2.12	0.49
1:A:162:TYR:HH	1:A:317:TYR:HD1	1.59	0.49
1:F:425:GLU:OE2	1:F:425:GLU:N	2.44	0.49
1:A:155:ALA:HA	1:A:159:MSE:HB2	1.94	0.49
1:C:495:ARG:HB2	5:F:544:HOH:O	2.12	0.49
1:E:56:PHE:CE1	1:E:339:GLN:HB3	2.47	0.49
1:H:69:TYR:CG	1:H:463:MSE:HG3	2.47	0.49
1:D:84:ASP:N	1:D:84:ASP:OD1	2.41	0.49
1:G:269:MSE:HE2	1:G:273:PHE:HB3	1.94	0.49
1:G:296:HIS:CE1	1:G:382:VAL:HG21	2.48	0.49
1:B:359:SER:HB3	4:B:512:CL:CL	2.50	0.49
1:B:296:HIS:CE1	1:B:382:VAL:HG21	2.48	0.49
1:G:246:ASN:ND2	1:G:249:ASN:HD21	2.11	0.49
1:A:303:ARG:NH2	5:A:567:HOH:O	2.39	0.49
1:E:332:SER:HA	1:E:339:GLN:HE21	1.78	0.49
1:E:425:GLU:OE2	1:E:425:GLU:N	2.46	0.49
1:E:84:ASP:N	1:E:84:ASP:OD1	2.41	0.49
1:F:64:VAL:HG13	1:F:210:PHE:CD1	2.48	0.49
1:B:134:VAL:HG22	1:G:134:VAL:HG22	1.93	0.49
1:F:69:TYR:CG	1:F:463:MSE:HG3	2.47	0.49
1:G:112:MSE:HE3	1:G:200:THR:CG2	2.42	0.49
1:F:383:ASN:OD1	1:F:385:GLU:HG2	2.13	0.49
1:G:175:GLN:HE21	1:G:177:ALA:H	1.61	0.49
1:H:91:ARG:HD3	1:H:207:ASN:HB3	1.94	0.49
1:A:142:PHE:HB2	1:A:174:MSE:HG3	1.95	0.49
1:C:160:ARG:N	1:C:161:PRO:HD2	2.28	0.49
1:C:167:TRP:HB3	1:C:174:MSE:HE1	1.94	0.49
1:G:425:GLU:OE2	1:G:425:GLU:N	2.45	0.49
1:E:160:ARG:N	1:E:161:PRO:HD2	2.27	0.48
1:F:84:ASP:OD1	1:F:84:ASP:N	2.40	0.48
1:C:232:GLU:CG	1:H:232:GLU:CG	2.90	0.48
1:A:91:ARG:HD3	1:A:207:ASN:HB3	1.95	0.48
1:C:118:GLN:NE2	1:C:195:VAL:HG13	2.28	0.48
1:E:175:GLN:NE2	1:E:177:ALA:H	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:495:ARG:HB2	5:H:533:HOH:O	2.12	0.48
1:F:455:VAL:HG21	1:F:480:THR:CG2	2.43	0.48
1:G:274:LEU:CD1	1:G:278:MSE:HE3	2.43	0.48
1:G:284:VAL:HG12	1:G:288:LYS:HE2	1.95	0.48
1:G:69:TYR:CG	1:G:463:MSE:HG3	2.48	0.48
1:A:118:GLN:NE2	1:A:195:VAL:HG13	2.29	0.48
1:C:332:SER:HA	1:C:339:GLN:HE21	1.79	0.48
1:D:118:GLN:NE2	1:D:195:VAL:HG13	2.28	0.48
1:H:455:VAL:HG21	1:H:480:THR:CG2	2.43	0.48
1:B:56:PHE:CD1	1:B:339:GLN:HB3	2.48	0.48
1:B:358:GLN:HE22	1:C:84:ASP:HA	1.78	0.48
1:E:112:MSE:HE3	1:E:200:THR:CG2	2.42	0.48
1:E:91:ARG:HD3	1:E:207:ASN:HB3	1.95	0.48
1:E:269:MSE:HE2	1:E:273:PHE:HB3	1.95	0.48
1:E:69:TYR:CG	1:E:463:MSE:HG3	2.48	0.48
1:H:274:LEU:CG	1:H:278:MSE:HE3	2.43	0.48
3:H:600:FDA:H9	3:H:600:FDA:H1'1	1.56	0.48
1:C:112:MSE:HE3	1:C:200:THR:CG2	2.42	0.48
1:C:425:GLU:N	1:C:425:GLU:OE2	2.44	0.48
1:F:274:LEU:CD1	1:F:278:MSE:HE3	2.44	0.48
1:B:199:LYS:NZ	5:B:750:HOH:O	2.47	0.48
1:C:510:GLN:HE21	1:H:506:LYS:HB3	1.79	0.48
1:C:368:TRP:CZ3	1:C:370:ILE:HD11	2.49	0.48
1:D:64:VAL:HG13	1:D:210:PHE:CD1	2.47	0.48
1:G:150:MSE:HG3	1:G:186:PRO:HG3	1.96	0.48
1:H:160:ARG:N	1:H:161:PRO:HD2	2.28	0.48
1:H:174:MSE:HB2	1:H:422:PRO:O	2.14	0.48
1:B:64:VAL:HG13	1:B:210:PHE:CD1	2.48	0.48
1:C:175:GLN:HE21	1:C:177:ALA:H	1.62	0.48
1:D:91:ARG:HD3	1:D:207:ASN:HB3	1.96	0.48
1:B:91:ARG:HD3	1:B:207:ASN:HB3	1.94	0.48
1:E:296:HIS:HE1	1:E:376:GLU:OE2	1.97	0.48
1:E:384:GLN:O	1:E:387:ILE:HG22	2.12	0.48
1:A:447:ARG:O	1:A:451:TRP:HA	2.14	0.47
1:D:356:ARG:HB3	1:D:357:PRO:HD2	1.96	0.47
1:G:64:VAL:HG13	1:G:210:PHE:CD1	2.49	0.47
1:C:69:TYR:CG	1:C:463:MSE:HG3	2.49	0.47
1:D:272:ASP:N	1:D:272:ASP:OD1	2.47	0.47
1:D:309:ARG:HB3	5:D:642:HOH:O	2.13	0.47
1:F:332:SER:HA	1:F:339:GLN:HE21	1.79	0.47
1:F:455:VAL:O	1:F:455:VAL:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASP:OD1	1:A:84:ASP:N	2.42	0.47
1:B:455:VAL:HG21	1:B:480:THR:CG2	2.44	0.47
1:H:70:LYS:NZ	5:H:553:HOH:O	2.47	0.47
1:E:274:LEU:CG	1:E:278:MSE:HE3	2.45	0.47
1:G:167:TRP:HB3	1:G:174:MSE:HE1	1.96	0.47
1:D:160:ARG:N	1:D:161:PRO:HD2	2.29	0.47
1:D:246:ASN:ND2	1:D:249:ASN:HD21	2.11	0.47
1:F:91:ARG:HD3	1:F:207:ASN:HB3	1.96	0.47
1:A:384:GLN:O	1:A:387:ILE:HG22	2.14	0.47
1:A:69:TYR:CG	1:A:463:MSE:HG3	2.49	0.47
1:D:69:TYR:CG	1:D:463:MSE:HG3	2.49	0.47
1:G:455:VAL:HG21	1:G:480:THR:CG2	2.44	0.47
1:A:368:TRP:CZ3	1:A:370:ILE:HD11	2.50	0.47
1:B:162:TYR:HH	1:B:317:TYR:HD1	1.61	0.47
1:B:69:TYR:CG	1:B:463:MSE:HG3	2.50	0.47
1:C:303:ARG:NH1	5:C:524:HOH:O	2.28	0.47
1:C:91:ARG:HD3	1:C:207:ASN:HB3	1.96	0.47
1:F:303:ARG:NH2	5:F:531:HOH:O	2.44	0.47
1:F:447:ARG:O	1:F:451:TRP:HA	2.15	0.47
1:G:160:ARG:N	1:G:161:PRO:HD2	2.30	0.47
1:G:91:ARG:HD3	1:G:207:ASN:HB3	1.97	0.47
1:H:425:GLU:OE2	1:H:425:GLU:N	2.47	0.47
1:B:174:MSE:HB2	1:B:422:PRO:O	2.14	0.47
1:B:384:GLN:O	1:B:387:ILE:HG22	2.14	0.47
1:H:167:TRP:HB3	1:H:174:MSE:HE1	1.97	0.47
1:A:160:ARG:N	1:A:161:PRO:HD2	2.30	0.47
1:C:426:ARG:NH2	1:C:454:GLU:OE1	2.39	0.47
1:D:302:VAL:HG11	1:D:368:TRP:CE2	2.49	0.47
1:D:384:GLN:O	1:D:387:ILE:HG22	2.15	0.47
1:D:458:GLN:HG3	3:D:600:FDA:HN1	1.80	0.47
1:F:150:MSE:HG3	1:F:186:PRO:HG3	1.97	0.47
1:B:160:ARG:N	1:B:161:PRO:HD2	2.30	0.47
1:C:455:VAL:O	1:C:455:VAL:HG13	2.15	0.47
1:H:284:VAL:HG12	1:H:288:LYS:HE2	1.97	0.47
1:C:272:ASP:OD1	1:C:272:ASP:N	2.48	0.47
1:A:69:TYR:CD2	1:A:463:MSE:HG3	2.50	0.46
1:F:175:GLN:HE21	1:F:177:ALA:H	1.63	0.46
1:C:504:PHE:HE1	1:F:263:LYS:HD2	1.81	0.46
1:A:296:HIS:HE1	1:A:376:GLU:OE2	1.98	0.46
1:A:98:GLN:NE2	1:A:114:PRO:HG2	2.31	0.46
1:B:360:THR:HG21	5:C:519:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:384:GLN:O	1:G:387:ILE:HG22	2.15	0.46
1:H:332:SER:HA	1:H:339:GLN:HE21	1.79	0.46
1:B:155:ALA:HA	1:B:159:MSE:HB2	1.97	0.46
1:C:274:LEU:HG	1:C:278:MSE:HE3	1.97	0.46
1:A:296:HIS:CE1	1:A:382:VAL:HG21	2.51	0.46
1:B:142:PHE:HB2	1:B:174:MSE:HG3	1.98	0.46
1:C:274:LEU:CD1	1:C:278:MSE:HE3	2.45	0.46
1:D:284:VAL:HG12	1:D:288:LYS:HE2	1.97	0.46
1:E:14:GLY:O	1:E:19:GLY:HA3	2.16	0.46
1:F:160:ARG:N	1:F:161:PRO:HD2	2.30	0.46
1:F:368:TRP:CZ3	1:F:370:ILE:HD11	2.51	0.46
1:A:274:LEU:CG	1:A:278:MSE:HE3	2.46	0.46
1:F:284:VAL:HG12	1:F:288:LYS:HE2	1.97	0.46
1:E:130:LEU:HD23	1:G:130:LEU:HD23	1.97	0.46
1:B:455:VAL:HG13	1:B:455:VAL:O	2.16	0.46
1:B:21:GLY:HA2	1:B:462:PHE:CE1	2.50	0.46
1:C:284:VAL:HG12	1:C:288:LYS:HE2	1.98	0.46
1:F:263:LYS:O	1:F:264:LYS:HD3	2.16	0.46
1:F:274:LEU:CG	1:F:278:MSE:HE3	2.45	0.46
1:G:383:ASN:OD1	1:G:385:GLU:HG2	2.15	0.46
1:A:272:ASP:OD1	1:A:272:ASP:N	2.45	0.46
1:D:447:ARG:O	1:D:451:TRP:HA	2.15	0.46
1:F:112:MSE:HE3	1:F:200:THR:CG2	2.41	0.46
1:C:384:GLN:O	1:C:387:ILE:HG22	2.16	0.46
1:C:296:HIS:CE1	1:C:382:VAL:HG21	2.51	0.46
1:H:272:ASP:N	1:H:272:ASP:OD1	2.46	0.46
1:H:490:ARG:NH2	5:H:530:HOH:O	2.47	0.46
1:B:274:LEU:CG	1:B:278:MSE:HE3	2.46	0.46
1:D:303:ARG:NH1	5:D:539:HOH:O	2.31	0.46
1:G:142:PHE:HB2	1:G:174:MSE:HG3	1.98	0.46
1:G:274:LEU:HG	1:G:278:MSE:HE3	1.98	0.46
1:H:14:GLY:O	1:H:19:GLY:HA3	2.16	0.46
1:H:296:HIS:HE1	1:H:376:GLU:OE2	1.99	0.46
1:C:175:GLN:HE22	1:C:177:ALA:HB3	1.81	0.45
1:D:332:SER:HA	1:D:339:GLN:HE21	1.80	0.45
1:F:384:GLN:O	1:F:387:ILE:HG22	2.16	0.45
1:G:274:LEU:CG	1:G:278:MSE:HE3	2.46	0.45
1:G:332:SER:HA	1:G:339:GLN:HE21	1.81	0.45
1:B:112:MSE:HE3	1:B:200:THR:CG2	2.44	0.45
1:B:447:ARG:O	1:B:451:TRP:HA	2.15	0.45
1:E:244:LYS:HB3	1:E:253:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:HIS:CE1	1:F:382:VAL:HG21	2.50	0.45
1:H:142:PHE:HB2	1:H:174:MSE:HG3	1.99	0.45
1:C:274:LEU:CG	1:C:278:MSE:HE3	2.46	0.45
1:E:155:ALA:HA	1:E:159:MSE:HB2	1.99	0.45
1:E:383:ASN:HA	5:E:552:HOH:O	2.15	0.45
1:H:175:GLN:NE2	1:H:177:ALA:H	2.13	0.45
1:D:445:ARG:NE	1:D:481:LEU:HD22	2.32	0.45
1:G:272:ASP:N	1:G:272:ASP:OD1	2.45	0.45
1:G:455:VAL:HG13	1:G:455:VAL:O	2.17	0.45
1:C:155:ALA:HA	1:C:159:MSE:HB2	1.97	0.45
1:C:150:MSE:SE	1:C:159:MSE:HE3	2.66	0.45
1:D:274:LEU:CG	1:D:278:MSE:HE3	2.46	0.45
1:D:360:THR:O	1:D:360:THR:HG22	2.16	0.45
2:D:802:GDU:O2B	2:D:802:GDU:O2’	2.29	0.45
1:E:212:PHE:CG	1:E:213:PRO:HD2	2.51	0.45
1:F:142:PHE:HB2	1:F:174:MSE:HG3	1.97	0.45
1:G:115:LYS:HD2	5:G:558:HOH:O	2.15	0.45
1:C:281:GLN:HG2	5:C:552:HOH:O	2.15	0.45
1:G:38:ASP:OD1	3:G:600:FDA:O3B	2.31	0.45
1:G:447:ARG:O	1:G:451:TRP:HA	2.17	0.45
1:G:56:PHE:CD1	1:G:339:GLN:HB3	2.52	0.45
1:G:46:LEU:HB2	3:G:600:FDA:O4’	2.16	0.45
1:A:112:MSE:HE3	1:A:200:THR:CG2	2.45	0.45
1:B:150:MSE:HG3	1:B:186:PRO:HG3	1.97	0.45
1:B:284:VAL:HG12	1:B:288:LYS:HE2	1.98	0.45
1:C:244:LYS:HB3	1:C:253:THR:HB	1.98	0.45
1:H:455:VAL:O	1:H:455:VAL:HG13	2.16	0.45
1:C:138:LYS:HG3	1:C:139:PRO:CD	2.45	0.45
1:F:155:ALA:HA	1:F:159:MSE:HB2	1.97	0.45
1:A:174:MSE:HB2	1:A:422:PRO:O	2.17	0.45
1:A:175:GLN:HE22	1:A:177:ALA:HB3	1.82	0.45
1:C:447:ARG:O	1:C:451:TRP:HA	2.17	0.45
1:E:310:ILE:HD13	1:E:368:TRP:CZ3	2.52	0.45
1:F:138:LYS:HG3	1:F:139:PRO:CD	2.46	0.45
1:H:112:MSE:HE3	1:H:200:THR:CG2	2.43	0.45
1:H:212:PHE:CG	1:H:213:PRO:HD2	2.52	0.45
1:D:296:HIS:CE1	1:D:382:VAL:HG21	2.52	0.44
1:H:274:LEU:HG	1:H:278:MSE:HE3	2.00	0.44
1:H:69:TYR:CD2	1:H:463:MSE:HG3	2.51	0.44
1:D:69:TYR:CD2	1:D:463:MSE:HG3	2.52	0.44
1:E:263:LYS:O	1:E:264:LYS:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:GLN:NE2	1:E:114:PRO:HG2	2.32	0.44
1:F:274:LEU:HG	1:F:278:MSE:HE3	1.99	0.44
1:C:142:PHE:HB2	1:C:174:MSE:HG3	1.98	0.44
1:C:302:VAL:HG11	1:C:368:TRP:CE2	2.50	0.44
1:C:500:GLY:HA2	1:C:503:VAL:HG13	1.99	0.44
1:D:175:GLN:HE22	1:D:177:ALA:HB3	1.81	0.44
1:E:138:LYS:HG3	1:E:139:PRO:CD	2.46	0.44
1:E:284:VAL:HG12	1:E:288:LYS:HE2	1.99	0.44
1:A:302:VAL:HG11	1:A:368:TRP:CE2	2.52	0.44
1:G:263:LYS:O	1:G:264:LYS:HD3	2.17	0.44
1:B:310:ILE:HD13	1:B:368:TRP:CZ3	2.52	0.44
1:C:21:GLY:HA2	1:C:462:PHE:CE1	2.52	0.44
1:B:332:SER:HA	1:B:339:GLN:HE21	1.82	0.44
1:B:302:VAL:HG11	1:B:368:TRP:CE2	2.53	0.44
1:C:150:MSE:HG3	1:C:186:PRO:HG3	1.99	0.44
1:C:69:TYR:CD2	1:C:463:MSE:HG3	2.53	0.44
1:D:56:PHE:CD1	1:D:339:GLN:HB3	2.52	0.44
1:F:244:LYS:HB3	1:F:253:THR:HB	1.99	0.44
1:B:167:TRP:HB3	1:B:174:MSE:HE1	2.00	0.44
1:D:263:LYS:O	1:D:264:LYS:HD3	2.17	0.44
1:D:421:THR:HA	1:D:422:PRO:HD3	1.86	0.44
1:G:155:ALA:HA	1:G:159:MSE:HB2	1.99	0.44
1:C:296:HIS:HE1	1:C:376:GLU:OE2	2.01	0.44
1:D:142:PHE:HB2	1:D:174:MSE:HG3	1.99	0.44
1:E:272:ASP:OD1	1:E:272:ASP:N	2.46	0.44
1:G:244:LYS:HB3	1:G:253:THR:HB	1.98	0.44
1:B:82:LYS:HB2	1:B:85:ASP:OD1	2.18	0.44
1:E:174:MSE:HB2	1:E:422:PRO:O	2.17	0.44
1:E:207:ASN:O	1:E:208:ALA:C	2.57	0.44
1:A:25:ARG:HD2	1:A:466:VAL:HG13	2.00	0.43
1:B:296:HIS:HE1	1:B:376:GLU:OE2	2.01	0.43
1:D:274:LEU:HG	1:D:278:MSE:HE3	2.00	0.43
1:E:150:MSE:SE	1:E:159:MSE:HE3	2.68	0.43
1:A:332:SER:HA	1:A:339:GLN:HE21	1.82	0.43
1:A:310:ILE:HD13	1:A:368:TRP:CZ3	2.54	0.43
1:B:60:VAL:HG13	1:B:415:PHE:CE2	2.53	0.43
1:C:98:GLN:NE2	1:C:114:PRO:HG2	2.33	0.43
1:E:69:TYR:CD2	1:E:463:MSE:HG3	2.53	0.43
1:F:445:ARG:NE	1:F:481:LEU:HD22	2.34	0.43
1:F:98:GLN:NE2	1:F:114:PRO:HG2	2.34	0.43
1:F:63:HIS:HB2	1:F:218:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:359:SER:OG	1:G:361:GLU:HB3	2.19	0.43
1:A:167:TRP:HB3	1:A:174:MSE:HE1	2.01	0.43
1:B:207:ASN:O	1:B:208:ALA:C	2.57	0.43
1:F:207:ASN:O	1:F:208:ALA:C	2.57	0.43
1:G:167:TRP:O	1:G:168:ALA:HB3	2.18	0.43
1:H:162:TYR:HH	1:H:317:TYR:HD1	1.65	0.43
1:H:98:GLN:NE2	1:H:114:PRO:HG2	2.32	0.43
1:A:244:LYS:HB3	1:A:253:THR:HB	2.00	0.43
1:A:60:VAL:HG13	1:A:415:PHE:CE2	2.53	0.43
1:D:150:MSE:HG3	1:D:186:PRO:HG3	2.00	0.43
1:H:310:ILE:HD13	1:H:368:TRP:CZ3	2.54	0.43
1:E:63:HIS:HB2	1:E:218:THR:HG21	2.00	0.43
1:G:63:HIS:HB2	1:G:218:THR:HG21	2.01	0.43
1:H:360:THR:O	1:H:360:THR:HG22	2.19	0.43
1:B:175:GLN:HE21	1:B:177:ALA:H	1.65	0.43
1:E:150:MSE:HG3	1:E:186:PRO:HG3	1.99	0.43
1:F:296:HIS:HE1	1:F:376:GLU:OE2	2.01	0.43
1:A:284:VAL:HG12	1:A:288:LYS:HE2	1.99	0.43
1:B:303:ARG:NH2	5:B:549:HOH:O	2.45	0.43
1:E:60:VAL:HG13	1:E:415:PHE:CE2	2.53	0.43
1:F:249:ASN:O	1:F:251:THR:HG23	2.19	0.43
1:G:207:ASN:O	1:G:208:ALA:C	2.57	0.43
1:H:155:ALA:HA	1:H:159:MSE:HB2	2.00	0.43
1:A:207:ASN:O	1:A:208:ALA:C	2.57	0.43
3:A:600:FDA:H9	3:A:600:FDA:O2’	2.19	0.43
1:B:196:ILE:HG21	1:D:118:GLN:HB3	2.00	0.43
1:C:56:PHE:CD1	1:C:339:GLN:HB3	2.53	0.43
1:H:60:VAL:HG13	1:H:415:PHE:CE2	2.54	0.43
1:C:207:ASN:O	1:C:208:ALA:C	2.57	0.42
1:E:21:GLY:HA2	1:E:462:PHE:CE1	2.54	0.42
1:H:56:PHE:CD1	1:H:339:GLN:HB3	2.54	0.42
1:B:272:ASP:OD1	1:B:272:ASP:N	2.45	0.42
1:C:212:PHE:CG	1:C:213:PRO:HD2	2.54	0.42
1:G:421:THR:HA	1:G:422:PRO:HD3	1.87	0.42
1:H:447:ARG:O	1:H:451:TRP:HA	2.19	0.42
1:B:98:GLN:NE2	1:B:114:PRO:HG2	2.34	0.42
1:C:310:ILE:HD13	1:C:368:TRP:CZ3	2.53	0.42
1:D:98:GLN:NE2	1:D:114:PRO:HG2	2.34	0.42
1:D:296:HIS:HE1	1:D:376:GLU:OE2	2.01	0.42
1:E:56:PHE:CD1	1:E:339:GLN:HB3	2.54	0.42
1:F:333:ASN:HA	1:F:333:ASN:HD22	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:PHE:CD1	1:F:339:GLN:HB3	2.54	0.42
1:G:249:ASN:O	1:G:251:THR:HG23	2.19	0.42
1:H:63:HIS:HB2	1:H:218:THR:HG21	2.01	0.42
1:H:333:ASN:HA	1:H:333:ASN:HD22	1.71	0.42
1:H:66:PHE:CD2	1:H:66:PHE:N	2.88	0.42
1:A:82:LYS:HB2	1:A:85:ASP:OD1	2.19	0.42
2:C:802:GDU:O2’	2:C:802:GDU:O2B	2.29	0.42
1:D:244:LYS:HB3	1:D:253:THR:HB	2.01	0.42
1:H:207:ASN:O	1:H:208:ALA:C	2.57	0.42
1:A:150:MSE:SE	1:A:159:MSE:HE3	2.69	0.42
1:A:373:GLU:HB2	5:A:660:HOH:O	2.19	0.42
1:G:303:ARG:NH1	5:G:519:HOH:O	2.40	0.42
1:B:325:PHE:HA	1:B:374:VAL:HG22	2.02	0.42
1:D:155:ALA:HA	1:D:159:MSE:HB2	2.02	0.42
1:E:358:GLN:H	1:E:358:GLN:CD	2.23	0.42
1:E:296:HIS:CE1	1:E:382:VAL:HG21	2.54	0.42
1:F:69:TYR:CD2	1:F:463:MSE:HG3	2.54	0.42
1:H:474:ASN:ND2	5:H:523:HOH:O	2.52	0.42
1:A:212:PHE:CG	1:A:213:PRO:HD2	2.54	0.42
1:B:63:HIS:HB2	1:B:218:THR:HG21	2.01	0.42
1:A:360:THR:HG21	5:D:512:HOH:O	2.19	0.42
1:A:421:THR:HA	1:A:422:PRO:HD3	1.87	0.42
1:D:138:LYS:HG3	1:D:139:PRO:CD	2.45	0.42
1:D:232:GLU:H	1:D:232:GLU:CD	2.22	0.42
1:F:14:GLY:O	1:F:19:GLY:HA3	2.20	0.42
1:H:150:MSE:SE	1:H:159:MSE:HE3	2.70	0.42
1:H:244:LYS:HB3	1:H:253:THR:HB	2.02	0.42
1:B:138:LYS:HG3	1:B:139:PRO:CD	2.48	0.42
1:E:302:VAL:HG11	1:E:368:TRP:CE2	2.55	0.42
1:G:296:HIS:HE1	1:G:376:GLU:OE2	2.02	0.42
1:H:296:HIS:CE1	1:H:382:VAL:HG21	2.55	0.42
1:A:445:ARG:NE	1:A:481:LEU:HD22	2.34	0.42
1:A:455:VAL:HG13	1:A:455:VAL:O	2.18	0.42
1:B:244:LYS:HB3	1:B:253:THR:HB	2.02	0.42
1:E:447:ARG:O	1:E:451:TRP:HA	2.19	0.42
1:G:14:GLY:O	1:G:19:GLY:HA3	2.20	0.42
1:A:235:ARG:NH1	5:A:550:HOH:O	2.52	0.41
1:E:360:THR:O	1:E:360:THR:HG22	2.20	0.41
1:G:60:VAL:HG13	1:G:415:PHE:CE2	2.54	0.41
1:D:382:VAL:HG22	5:D:658:HOH:O	2.19	0.41
1:H:150:MSE:HG3	1:H:186:PRO:HG3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:GLY:O	1:C:19:GLY:HA3	2.20	0.41
1:D:207:ASN:O	1:D:208:ALA:C	2.58	0.41
1:E:455:VAL:O	1:E:455:VAL:HG13	2.20	0.41
1:G:455:VAL:HG23	1:G:460:HIS:CD2	2.54	0.41
1:G:98:GLN:NE2	1:G:114:PRO:HG2	2.36	0.41
1:C:162:TYR:HH	1:C:317:TYR:HD1	1.66	0.41
1:C:263:LYS:O	1:C:264:LYS:HD3	2.20	0.41
1:D:21:GLY:HA2	1:D:462:PHE:CE1	2.55	0.41
1:F:310:ILE:HD13	1:F:368:TRP:CZ3	2.55	0.41
1:H:21:GLY:HA2	1:H:462:PHE:CE1	2.55	0.41
1:A:31:GLY:N	5:A:513:HOH:O	2.35	0.41
1:A:327:ARG:NH1	2:A:802:GDU:H5’	2.36	0.41
1:A:360:THR:HG22	1:A:360:THR:O	2.20	0.41
1:B:175:GLN:HE22	1:B:177:ALA:HB3	1.85	0.41
1:E:125:MSE:HE1	1:E:191:VAL:HG21	2.02	0.41
1:A:306:ARG:HH11	1:A:333:ASN:HD21	1.67	0.41
1:B:130:LEU:HD23	1:D:130:LEU:HD23	2.03	0.41
1:C:174:MSE:HB2	1:C:422:PRO:O	2.21	0.41
1:D:63:HIS:HB2	1:D:218:THR:HG21	2.01	0.41
1:D:310:ILE:HD13	1:D:368:TRP:CZ3	2.55	0.41
3:E:600:FDA:H9	3:E:600:FDA:H1’1	1.72	0.41
1:A:262:TYR:CE1	1:A:265:LEU:HB2	2.55	0.41
1:A:274:LEU:HG	1:A:278:MSE:HE3	2.02	0.41
1:C:421:THR:HA	1:C:422:PRO:HD3	1.85	0.41
1:D:174:MSE:HB2	1:D:422:PRO:O	2.20	0.41
1:F:332:SER:HA	1:F:339:GLN:NE2	2.36	0.41
1:G:302:VAL:HG11	1:G:368:TRP:CE2	2.56	0.41
3:G:600:FDA:O2’	3:G:600:FDA:H9	2.21	0.41
1:B:361:GLU:O	5:B:536:HOH:O	2.22	0.41
1:E:274:LEU:HG	1:E:278:MSE:HE3	2.02	0.41
1:F:325:PHE:HA	1:F:374:VAL:HG22	2.02	0.41
1:G:69:TYR:CD2	1:G:463:MSE:HG3	2.55	0.41
2:G:802:GDU:O2B	2:G:802:GDU:O2’	2.31	0.41
1:G:82:LYS:HB2	1:G:85:ASP:OD1	2.20	0.41
1:C:63:HIS:HB2	1:C:218:THR:HG21	2.03	0.41
1:E:325:PHE:HA	1:E:374:VAL:HG22	2.02	0.41
1:H:59:ASP:HB3	1:H:60:VAL:H	1.78	0.41
1:G:431:THR:O	1:G:435:PRO:HG2	2.21	0.41
1:H:327:ARG:HH12	2:H:802:GDU:H5’	1.84	0.41
1:B:318:PHE:HA	1:B:319:PRO:HD2	1.93	0.41
1:C:333:ASN:HD22	1:C:333:ASN:HA	1.69	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:E:392:ILE:HA	1:E:395:LEU:HD12	2.02	0.41
1:F:82:LYS:HB2	1:F:85:ASP:OD1	2.20	0.41
1:G:138:LYS:HG3	1:G:139:PRO:CD	2.47	0.41
1:G:310:ILE:HD13	1:G:368:TRP:CZ3	2.56	0.41
1:G:46:LEU:HB2	3:G:600:FDA:HO4'	1.86	0.41
1:H:302:VAL:HG11	1:H:368:TRP:CE2	2.55	0.41
1:B:69:TYR:CD2	1:B:463:MSE:HG3	2.56	0.40
1:E:232:GLU:H	1:E:232:GLU:CD	2.22	0.40
1:G:325:PHE:HA	1:G:374:VAL:HG22	2.03	0.40
1:H:263:LYS:O	1:H:264:LYS:HD3	2.21	0.40
1:A:138:LYS:HG3	1:A:139:PRO:CD	2.47	0.40
1:D:306:ARG:HH11	1:D:333:ASN:HD21	1.70	0.40
1:F:272:ASP:N	1:F:272:ASP:OD1	2.44	0.40
1:G:458:GLN:HG3	3:G:600:FDA:HN1	1.85	0.40
1:A:14:GLY:O	1:A:19:GLY:HA3	2.20	0.40
1:C:510:GLN:NE2	1:H:506:LYS:HB3	2.36	0.40
1:A:56:PHE:CD1	1:A:339:GLN:HB3	2.55	0.40
1:B:222:TRP:HE1	1:B:458:GLN:HE21	1.70	0.40
1:B:306:ARG:HH11	1:B:333:ASN:HD21	1.68	0.40
1:B:483:TYR:N	1:B:484:PRO:HD3	2.37	0.40
1:C:332:SER:HA	1:C:339:GLN:NE2	2.36	0.40
1:D:212:PHE:CG	1:D:213:PRO:HD2	2.57	0.40
1:E:142:PHE:HB2	1:E:174:MSE:HG3	2.04	0.40
1:E:332:SER:HA	1:E:339:GLN:NE2	2.36	0.40
1:H:102:VAL:HA	1:H:103:PRO:HD3	1.95	0.40
1:C:232:GLU:CD	1:C:232:GLU:H	2.23	0.40
1:D:14:GLY:O	1:D:19:GLY:HA3	2.22	0.40
1:E:254:LEU:HD12	1:E:258:THR:HB	2.02	0.40
3:F:600:FDA:H1'1	3:F:600:FDA:H9	1.78	0.40
1:G:296:HIS:HD2	1:G:412:HIS:CE1	2.32	0.40
1:G:445:ARG:NE	1:G:481:LEU:HD22	2.37	0.40
1:H:421:THR:HA	1:H:422:PRO:HD3	1.88	0.40
1:H:64:VAL:HG13	1:H:210:PHE:CG	2.57	0.40
1:H:95:VAL:HA	5:H:524:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/509 (100%)	488 (96%)	17 (3%)	2 (0%)	34	54
1	B	507/509 (100%)	489 (96%)	16 (3%)	2 (0%)	34	54
1	C	507/509 (100%)	486 (96%)	19 (4%)	2 (0%)	34	54
1	D	507/509 (100%)	489 (96%)	16 (3%)	2 (0%)	34	54
1	E	507/509 (100%)	487 (96%)	18 (4%)	2 (0%)	34	54
1	F	507/509 (100%)	488 (96%)	16 (3%)	3 (1%)	25	43
1	G	507/509 (100%)	483 (95%)	22 (4%)	2 (0%)	34	54
1	H	507/509 (100%)	486 (96%)	19 (4%)	2 (0%)	34	54
All	All	4056/4072 (100%)	3896 (96%)	143 (4%)	17 (0%)	34	54

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	59	ASP
1	A	59	ASP
1	B	59	ASP
1	C	59	ASP
1	D	59	ASP
1	E	59	ASP
1	G	59	ASP
1	H	59	ASP
1	F	364	GLU
1	E	62	GLY
1	H	62	GLY
1	B	62	GLY
1	C	62	GLY
1	D	62	GLY
1	F	62	GLY
1	A	62	GLY
1	G	62	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/417 (103%)	417 (97%)	14 (3%)	39	65
1	B	431/417 (103%)	417 (97%)	14 (3%)	39	65
1	C	431/417 (103%)	414 (96%)	17 (4%)	32	57
1	D	431/417 (103%)	417 (97%)	14 (3%)	39	65
1	E	431/417 (103%)	417 (97%)	14 (3%)	39	65
1	F	431/417 (103%)	415 (96%)	16 (4%)	34	60
1	G	431/417 (103%)	416 (96%)	15 (4%)	36	62
1	H	431/417 (103%)	417 (97%)	14 (3%)	39	65
All	All	3448/3336 (103%)	3330 (97%)	118 (3%)	37	63

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASP
1	A	90	GLN
1	A	137	THR
1	A	148	ARG
1	A	150	MSE
1	A	175	GLN
1	A	206	PRO
1	A	209	THR
1	A	271	VAL
1	A	309	ARG
1	A	339	GLN
1	A	382	VAL
1	A	470	ASP
1	A	477	VAL
1	B	84	ASP
1	B	90	GLN
1	B	134	VAL
1	B	137	THR
1	B	148	ARG

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Mol	Chain	Res	Type
1	B	150	MSE
1	B	175	GLN
1	B	206	PRO
1	B	209	THR
1	B	271	VAL
1	B	309	ARG
1	B	339	GLN
1	B	470	ASP
1	B	477	VAL
1	C	25	ARG
1	C	84	ASP
1	C	90	GLN
1	C	148	ARG
1	C	150	MSE
1	C	175	GLN
1	C	209	THR
1	C	271	VAL
1	C	309	ARG
1	C	339	GLN
1	C	358	GLN
1	C	382	VAL
1	C	470	ASP
1	C	477	VAL
1	C	503	VAL
1	C	506	LYS
1	C	508	LYS
1	D	25	ARG
1	D	84	ASP
1	D	90	GLN
1	D	148	ARG
1	D	150	MSE
1	D	175	GLN
1	D	209	THR
1	D	271	VAL
1	D	309	ARG
1	D	339	GLN
1	D	382	VAL
1	D	470	ASP
1	D	477	VAL
1	D	506	LYS
1	E	25	ARG
1	E	84	ASP

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Mol	Chain	Res	Type
1	E	90	GLN
1	E	148	ARG
1	E	150	MSE
1	E	175	GLN
1	E	209	THR
1	E	271	VAL
1	E	309	ARG
1	E	339	GLN
1	E	358	GLN
1	E	382	VAL
1	E	470	ASP
1	E	477	VAL
1	F	25	ARG
1	F	84	ASP
1	F	90	GLN
1	F	134	VAL
1	F	137	THR
1	F	148	ARG
1	F	150	MSE
1	F	175	GLN
1	F	209	THR
1	F	215	ARG
1	F	271	VAL
1	F	309	ARG
1	F	339	GLN
1	F	382	VAL
1	F	470	ASP
1	F	477	VAL
1	G	25	ARG
1	G	84	ASP
1	G	90	GLN
1	G	134	VAL
1	G	137	THR
1	G	148	ARG
1	G	150	MSE
1	G	175	GLN
1	G	209	THR
1	G	215	ARG
1	G	271	VAL
1	G	309	ARG
1	G	339	GLN
1	G	470	ASP

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Mol	Chain	Res	Type
1	G	477	VAL
1	H	84	ASP
1	H	90	GLN
1	H	137	THR
1	H	148	ARG
1	H	150	MSE
1	H	175	GLN
1	H	209	THR
1	H	271	VAL
1	H	309	ARG
1	H	339	GLN
1	H	358	GLN
1	H	382	VAL
1	H	470	ASP
1	H	477	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	98	GLN
1	A	175	GLN
1	A	248	ASN
1	A	249	ASN
1	A	255	GLN
1	A	296	HIS
1	A	333	ASN
1	A	339	GLN
1	A	397	ASN
1	A	412	HIS
1	A	417	HIS
1	A	458	GLN
1	A	474	ASN
1	B	28	GLN
1	B	98	GLN
1	B	175	GLN
1	B	248	ASN
1	B	249	ASN
1	B	255	GLN
1	B	296	HIS
1	B	333	ASN
1	B	339	GLN

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Mol	Chain	Res	Type
1	B	358	GLN
1	B	397	ASN
1	B	417	HIS
1	B	458	GLN
1	B	474	ASN
1	C	28	GLN
1	C	90	GLN
1	C	98	GLN
1	C	175	GLN
1	C	248	ASN
1	C	249	ASN
1	C	255	GLN
1	C	296	HIS
1	C	333	ASN
1	C	339	GLN
1	C	397	ASN
1	C	412	HIS
1	C	417	HIS
1	C	458	GLN
1	C	474	ASN
1	C	510	GLN
1	D	28	GLN
1	D	90	GLN
1	D	98	GLN
1	D	175	GLN
1	D	248	ASN
1	D	249	ASN
1	D	255	GLN
1	D	296	HIS
1	D	333	ASN
1	D	339	GLN
1	D	397	ASN
1	D	412	HIS
1	D	417	HIS
1	D	458	GLN
1	D	474	ASN
1	E	28	GLN
1	E	98	GLN
1	E	175	GLN
1	E	248	ASN
1	E	249	ASN
1	E	255	GLN

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Mol	Chain	Res	Type
1	E	296	HIS
1	E	333	ASN
1	E	339	GLN
1	E	397	ASN
1	E	417	HIS
1	E	458	GLN
1	E	474	ASN
1	F	28	GLN
1	F	98	GLN
1	F	175	GLN
1	F	248	ASN
1	F	249	ASN
1	F	296	HIS
1	F	333	ASN
1	F	339	GLN
1	F	397	ASN
1	F	417	HIS
1	F	458	GLN
1	F	474	ASN
1	G	28	GLN
1	G	98	GLN
1	G	175	GLN
1	G	248	ASN
1	G	249	ASN
1	G	296	HIS
1	G	333	ASN
1	G	339	GLN
1	G	397	ASN
1	G	417	HIS
1	G	458	GLN
1	G	474	ASN
1	H	28	GLN
1	H	98	GLN
1	H	175	GLN
1	H	248	ASN
1	H	249	ASN
1	H	255	GLN
1	H	296	HIS
1	H	333	ASN
1	H	339	GLN
1	H	397	ASN
1	H	417	HIS

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Mol	Chain	Res	Type
1	H	458	GLN
1	H	474	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
2	GDU	E	802	-	31,38,38	1.79	9 (29%)	41,58,58	1.55	7 (17%)
3	FDA	F	600	-	51,58,58	2.49	15 (29%)	60,89,89	1.84	15 (25%)
3	FDA	G	600	-	51,58,58	2.48	14 (27%)	60,89,89	1.83	16 (26%)
3	FDA	D	600	-	51,58,58	2.47	14 (27%)	60,89,89	1.86	16 (26%)
3	FDA	E	600	-	51,58,58	2.43	13 (25%)	60,89,89	1.85	16 (26%)
3	FDA	B	600	-	51,58,58	2.45	15 (29%)	60,89,89	1.86	15 (25%)
3	FDA	C	600	-	51,58,58	2.46	13 (25%)	60,89,89	1.84	17 (28%)
3	FDA	A	600	-	51,58,58	2.47	13 (25%)	60,89,89	1.87	16 (26%)
2	GDU	H	802	-	31,38,38	1.80	9 (29%)	41,58,58	1.58	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	FDA	H	600	-	51,58,58	2.44	13 (25%)	60,89,89	1.85	16 (26%)
2	GDU	F	802	-	31,38,38	1.77	9 (29%)	41,58,58	1.53	7 (17%)
2	GDU	A	802	-	31,38,38	1.76	9 (29%)	41,58,58	1.45	7 (17%)
2	GDU	D	802	-	31,38,38	1.80	9 (29%)	41,58,58	1.50	7 (17%)
2	GDU	G	802	-	31,38,38	1.78	9 (29%)	41,58,58	1.47	7 (17%)
2	GDU	B	802	-	31,38,38	1.77	9 (29%)	41,58,58	1.47	7 (17%)
2	GDU	C	802	-	31,38,38	1.80	9 (29%)	41,58,58	1.53	7 (17%)

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	GDU	E	802	-	-	8/21/59/59	0/3/3/3
3	FDA	F	600	-	-	4/30/50/50	0/6/6/6
3	FDA	G	600	-	-	6/30/50/50	0/6/6/6
3	FDA	D	600	-	-	2/30/50/50	0/6/6/6
3	FDA	E	600	-	-	4/30/50/50	0/6/6/6
3	FDA	B	600	-	-	3/30/50/50	0/6/6/6
3	FDA	C	600	-	-	3/30/50/50	0/6/6/6
3	FDA	A	600	-	-	1/30/50/50	0/6/6/6
2	GDU	H	802	-	-	13/21/59/59	0/3/3/3
3	FDA	H	600	-	-	5/30/50/50	0/6/6/6
2	GDU	F	802	-	-	8/21/59/59	0/3/3/3
2	GDU	A	802	-	-	6/21/59/59	0/3/3/3
2	GDU	D	802	-	-	8/21/59/59	0/3/3/3
2	GDU	G	802	-	-	8/21/59/59	0/3/3/3
2	GDU	B	802	-	-	5/21/59/59	0/3/3/3
2	GDU	C	802	-	-	13/21/59/59	0/3/3/3

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	600	FDA	C10-N1	8.29	1.43	1.33
3	D	600	FDA	C10-N1	8.27	1.43	1.33
3	G	600	FDA	C1'-N10	-8.25	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	600	FDA	C10-N1	8.22	1.43	1.33
3	H	600	FDA	C10-N1	8.20	1.43	1.33
3	A	600	FDA	C10-N1	8.14	1.43	1.33
3	G	600	FDA	C10-N1	8.12	1.43	1.33
3	D	600	FDA	C1'-N10	-8.05	1.39	1.48
3	E	600	FDA	C10-N1	8.04	1.43	1.33
3	F	600	FDA	C1'-N10	-8.02	1.40	1.48
3	B	600	FDA	C10-N1	8.01	1.43	1.33
3	C	600	FDA	C1'-N10	-7.89	1.40	1.48
3	B	600	FDA	C1'-N10	-7.83	1.40	1.48
3	A	600	FDA	C1'-N10	-7.78	1.40	1.48
3	E	600	FDA	C1'-N10	-7.63	1.40	1.48
3	H	600	FDA	C1'-N10	-7.60	1.40	1.48
3	A	600	FDA	C2B-C3B	-5.43	1.38	1.53
3	G	600	FDA	C2B-C3B	-5.40	1.38	1.53
3	F	600	FDA	C2B-C3B	-5.35	1.38	1.53
3	C	600	FDA	C2B-C3B	-5.34	1.38	1.53
3	B	600	FDA	C2B-C3B	-5.33	1.38	1.53
3	H	600	FDA	C2B-C3B	-5.23	1.39	1.53
3	E	600	FDA	C2B-C3B	-5.22	1.39	1.53
3	D	600	FDA	C2B-C3B	-5.21	1.39	1.53
3	A	600	FDA	C4-N3	4.20	1.40	1.33
3	G	600	FDA	C4-N3	4.15	1.40	1.33
3	F	600	FDA	C4-N3	4.14	1.40	1.33
3	D	600	FDA	C4-N3	4.08	1.40	1.33
3	H	600	FDA	C4-N3	4.08	1.40	1.33
3	E	600	FDA	C4-N3	4.07	1.40	1.33
3	B	600	FDA	C4-N3	4.06	1.40	1.33
3	C	600	FDA	C4-N3	4.03	1.40	1.33
3	A	600	FDA	C9A-C5X	-3.92	1.34	1.42
3	C	600	FDA	C9A-C5X	-3.91	1.34	1.42
3	B	600	FDA	C9A-C5X	-3.90	1.34	1.42
3	H	600	FDA	C9A-C5X	-3.89	1.34	1.42
3	F	600	FDA	C9A-C5X	-3.88	1.34	1.42
3	D	600	FDA	C9A-C5X	-3.83	1.34	1.42
3	G	600	FDA	C9A-C5X	-3.83	1.34	1.42
2	G	802	GDU	PB-O3B	-3.83	1.50	1.60
2	F	802	GDU	PB-O3B	-3.82	1.50	1.60
3	E	600	FDA	C9A-C5X	-3.82	1.35	1.42
2	A	802	GDU	PB-O3B	-3.78	1.50	1.60
2	H	802	GDU	PB-O3B	-3.78	1.50	1.60
2	B	802	GDU	PB-O3B	-3.76	1.50	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	FDA	C7M-C7	3.75	1.58	1.51
3	F	600	FDA	C7M-C7	3.75	1.58	1.51
2	D	802	GDU	PB-O3B	-3.74	1.50	1.60
3	B	600	FDA	C7M-C7	3.73	1.58	1.51
3	E	600	FDA	C7M-C7	3.71	1.58	1.51
2	C	802	GDU	PB-O3B	-3.71	1.50	1.60
3	C	600	FDA	C7M-C7	3.71	1.58	1.51
2	E	802	GDU	PB-O3B	-3.71	1.50	1.60
3	H	600	FDA	C7M-C7	3.69	1.58	1.51
2	H	802	GDU	O4-C4	3.69	1.33	1.24
3	D	600	FDA	C7M-C7	3.67	1.58	1.51
3	G	600	FDA	C7M-C7	3.67	1.58	1.51
2	C	802	GDU	O4-C4	3.66	1.33	1.24
2	E	802	GDU	O4-C4	3.63	1.33	1.24
3	F	600	FDA	O3'-C3'	-3.63	1.34	1.43
2	D	802	GDU	O4-C4	3.62	1.33	1.24
2	F	802	GDU	O4-C4	3.59	1.33	1.24
3	D	600	FDA	O3'-C3'	-3.58	1.34	1.43
3	H	600	FDA	O3'-C3'	-3.56	1.34	1.43
3	E	600	FDA	O3'-C3'	-3.55	1.34	1.43
2	G	802	GDU	O4-C4	3.55	1.33	1.24
3	C	600	FDA	O3'-C3'	-3.54	1.34	1.43
3	G	600	FDA	O3'-C3'	-3.52	1.34	1.43
3	B	600	FDA	O3'-C3'	-3.50	1.34	1.43
2	B	802	GDU	O4-C4	3.50	1.33	1.24
2	A	802	GDU	O4-C4	3.49	1.33	1.24
3	A	600	FDA	O3'-C3'	-3.44	1.34	1.43
3	A	600	FDA	C4-C4X	3.39	1.47	1.41
2	E	802	GDU	C3D-C2D	-3.35	1.44	1.53
3	E	600	FDA	C4-C4X	3.33	1.47	1.41
2	D	802	GDU	C3D-C2D	-3.33	1.44	1.53
3	F	600	FDA	C4'-C3'	-3.29	1.47	1.53
3	C	600	FDA	C4-C4X	3.29	1.47	1.41
3	B	600	FDA	C4-C4X	3.29	1.47	1.41
3	D	600	FDA	C4-C4X	3.27	1.47	1.41
3	H	600	FDA	C4-C4X	3.26	1.47	1.41
2	B	802	GDU	C3D-C2D	-3.26	1.44	1.53
2	H	802	GDU	C3D-C2D	-3.24	1.44	1.53
2	C	802	GDU	C3D-C2D	-3.23	1.44	1.53
3	F	600	FDA	C4-C4X	3.22	1.46	1.41
2	G	802	GDU	C3D-C2D	-3.20	1.44	1.53
3	G	600	FDA	C4-C4X	3.17	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	600	FDA	C4'-C3'	-3.17	1.47	1.53
2	F	802	GDU	C3D-C2D	-3.16	1.44	1.53
3	H	600	FDA	C2-N1	3.16	1.44	1.38
3	B	600	FDA	C4'-C3'	-3.13	1.47	1.53
2	A	802	GDU	C3D-C2D	-3.13	1.44	1.53
3	E	600	FDA	C2-N1	3.08	1.44	1.38
3	A	600	FDA	C4'-C3'	-3.07	1.47	1.53
3	F	600	FDA	C2-N1	3.05	1.44	1.38
2	G	802	GDU	C4'-C3'	-3.05	1.44	1.52
2	A	802	GDU	C4'-C3'	-3.04	1.44	1.52
2	H	802	GDU	C2D-C1D	-3.04	1.49	1.53
2	H	802	GDU	C4'-C3'	-3.04	1.44	1.52
2	C	802	GDU	C4'-C3'	-3.04	1.44	1.52
2	D	802	GDU	C4'-C3'	-3.03	1.44	1.52
3	E	600	FDA	C4'-C3'	-3.02	1.47	1.53
2	B	802	GDU	C4'-C3'	-3.01	1.44	1.52
2	E	802	GDU	C4'-C3'	-3.01	1.44	1.52
3	C	600	FDA	C4'-C3'	-3.00	1.47	1.53
2	F	802	GDU	C4'-C3'	-3.00	1.44	1.52
3	D	600	FDA	C2-N1	3.00	1.44	1.38
3	C	600	FDA	C2-N1	2.99	1.44	1.38
3	F	600	FDA	C9A-N10	-2.98	1.34	1.38
3	H	600	FDA	C4'-C3'	-2.98	1.47	1.53
3	A	600	FDA	C9A-N10	-2.95	1.34	1.38
3	B	600	FDA	C9A-N10	-2.95	1.34	1.38
3	B	600	FDA	C2-N1	2.95	1.44	1.38
3	G	600	FDA	C2-N1	2.94	1.44	1.38
3	D	600	FDA	C9A-N10	-2.91	1.34	1.38
3	G	600	FDA	C9A-N10	-2.90	1.34	1.38
3	A	600	FDA	C2-N1	2.88	1.43	1.38
2	C	802	GDU	C3D-C4D	-2.87	1.45	1.53
3	D	600	FDA	C4'-C3'	-2.87	1.48	1.53
3	C	600	FDA	C9A-N10	-2.85	1.34	1.38
2	G	802	GDU	C3D-C4D	-2.85	1.45	1.53
2	E	802	GDU	C2D-C1D	-2.84	1.49	1.53
2	D	802	GDU	C3D-C4D	-2.84	1.45	1.53
2	D	802	GDU	C2D-C1D	-2.83	1.49	1.53
3	H	600	FDA	C9A-N10	-2.83	1.34	1.38
2	B	802	GDU	C3D-C4D	-2.80	1.45	1.53
2	F	802	GDU	C2D-C1D	-2.80	1.49	1.53
2	C	802	GDU	C2D-C1D	-2.78	1.49	1.53
2	A	802	GDU	C3D-C4D	-2.78	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	802	GDU	C3D-C4D	-2.78	1.45	1.53
3	E	600	FDA	C9A-N10	-2.78	1.34	1.38
2	B	802	GDU	C2D-C1D	-2.76	1.49	1.53
2	F	802	GDU	C3D-C4D	-2.75	1.46	1.53
2	A	802	GDU	C2D-C1D	-2.74	1.49	1.53
2	H	802	GDU	C3D-C4D	-2.70	1.46	1.53
2	G	802	GDU	C2D-C1D	-2.70	1.49	1.53
3	G	600	FDA	O4'-C4'	2.53	1.48	1.43
3	D	600	FDA	O4'-C4'	2.50	1.48	1.43
3	F	600	FDA	O4'-C4'	2.46	1.48	1.43
3	E	600	FDA	O4'-C4'	2.44	1.48	1.43
3	C	600	FDA	O4'-C4'	2.43	1.48	1.43
2	C	802	GDU	O4D-C1D	-2.39	1.37	1.41
2	C	802	GDU	C3'-C2'	-2.38	1.46	1.52
3	H	600	FDA	O4'-C4'	2.37	1.48	1.43
3	A	600	FDA	O3B-C3B	-2.33	1.37	1.43
2	D	802	GDU	C3'-C2'	-2.33	1.46	1.52
2	A	802	GDU	C3'-C2'	-2.33	1.46	1.52
2	E	802	GDU	C3'-C2'	-2.32	1.46	1.52
2	B	802	GDU	C3'-C2'	-2.31	1.46	1.52
2	F	802	GDU	C3'-C2'	-2.29	1.46	1.52
2	H	802	GDU	C3'-C2'	-2.28	1.46	1.52
3	B	600	FDA	O4'-C4'	2.28	1.48	1.43
2	C	802	GDU	O5'-C5'	2.27	1.49	1.44
2	E	802	GDU	O5'-C5'	2.27	1.49	1.44
2	G	802	GDU	C3'-C2'	-2.27	1.46	1.52
2	D	802	GDU	O4D-C1D	-2.27	1.37	1.41
2	F	802	GDU	O4D-C1D	-2.23	1.38	1.41
2	H	802	GDU	O5'-C5'	2.22	1.49	1.44
2	A	802	GDU	O5'-C5'	2.21	1.49	1.44
2	G	802	GDU	O4D-C1D	-2.21	1.38	1.41
3	B	600	FDA	O3B-C3B	-2.20	1.37	1.43
2	B	802	GDU	O5'-C5'	2.19	1.49	1.44
2	D	802	GDU	O5'-C5'	2.19	1.49	1.44
3	A	600	FDA	O4'-C4'	2.14	1.47	1.43
2	A	802	GDU	O4D-C1D	-2.14	1.38	1.41
2	F	802	GDU	O5'-C5'	2.11	1.49	1.44
3	E	600	FDA	O3B-C3B	-2.11	1.38	1.43
3	D	600	FDA	O4B-C1B	-2.10	1.38	1.41
3	B	600	FDA	O4B-C1B	-2.10	1.38	1.41
2	H	802	GDU	O4D-C1D	-2.10	1.38	1.41
3	H	600	FDA	O3B-C3B	-2.09	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	600	FDA	O4B-C1B	-2.09	1.38	1.41
2	B	802	GDU	O4D-C1D	-2.08	1.38	1.41
2	G	802	GDU	O5'-C5'	2.07	1.49	1.44
3	G	600	FDA	O3B-C3B	-2.06	1.38	1.43
3	C	600	FDA	O3B-C3B	-2.05	1.38	1.43
2	E	802	GDU	O4D-C1D	-2.03	1.38	1.41
3	F	600	FDA	O3B-C3B	-2.02	1.38	1.43
3	D	600	FDA	O5B-C5B	-2.02	1.37	1.44
3	F	600	FDA	O5B-C5B	-2.01	1.37	1.44
3	B	600	FDA	P-O5'	-2.01	1.51	1.59
3	G	600	FDA	O5B-C5B	-2.00	1.37	1.44

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	600	FDA	C4-N3-C2	5.47	119.76	115.14
3	E	600	FDA	C4-N3-C2	5.42	119.72	115.14
3	A	600	FDA	C4-N3-C2	5.35	119.66	115.14
3	B	600	FDA	C4-N3-C2	5.27	119.59	115.14
3	H	600	FDA	C4-N3-C2	5.25	119.57	115.14
3	G	600	FDA	C4-N3-C2	5.22	119.55	115.14
3	C	600	FDA	C4-N3-C2	4.94	119.31	115.14
3	B	600	FDA	O5B-PA-O1A	-4.86	90.07	109.07
3	A	600	FDA	O5B-PA-O1A	-4.70	90.70	109.07
3	D	600	FDA	O5B-PA-O1A	-4.62	91.01	109.07
3	G	600	FDA	O5B-PA-O1A	-4.58	91.16	109.07
3	F	600	FDA	O5B-PA-O1A	-4.48	91.56	109.07
3	H	600	FDA	C1'-N10-C10	4.47	122.41	118.41
3	C	600	FDA	O5B-PA-O1A	-4.43	91.75	109.07
3	B	600	FDA	O5'-P-O1P	-4.38	91.94	109.07
3	F	600	FDA	C1'-N10-C10	4.34	122.30	118.41
3	D	600	FDA	C4-N3-C2	4.33	118.80	115.14
3	H	600	FDA	O5B-PA-O1A	-4.29	92.29	109.07
3	C	600	FDA	C1'-N10-C10	4.29	122.25	118.41
3	G	600	FDA	N3A-C2A-N1A	-4.29	121.97	128.68
3	B	600	FDA	C1'-N10-C10	4.27	122.24	118.41
3	E	600	FDA	O5B-PA-O1A	-4.27	92.37	109.07
3	A	600	FDA	O5'-P-O1P	-4.26	92.44	109.07
3	F	600	FDA	N3A-C2A-N1A	-4.25	122.04	128.68
3	C	600	FDA	N3A-C2A-N1A	-4.19	122.14	128.68
3	D	600	FDA	N3A-C2A-N1A	-4.16	122.18	128.68
3	B	600	FDA	N3A-C2A-N1A	-4.13	122.22	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	600	FDA	N3A-C2A-N1A	-4.11	122.26	128.68
3	A	600	FDA	N3A-C2A-N1A	-4.10	122.28	128.68
2	H	802	GDU	C3'-C4'-C5'	4.08	117.51	110.24
2	H	802	GDU	O5'-C5'-C4'	4.07	117.09	109.69
3	A	600	FDA	C1'-N10-C10	4.07	122.05	118.41
3	H	600	FDA	N3A-C2A-N1A	-4.00	122.43	128.68
3	D	600	FDA	C1'-N10-C10	3.99	121.98	118.41
2	E	802	GDU	O5'-C5'-C4'	3.96	116.89	109.69
2	E	802	GDU	C3'-C4'-C5'	3.95	117.28	110.24
2	F	802	GDU	C3'-C4'-C5'	3.88	117.17	110.24
2	D	802	GDU	O5'-C5'-C4'	3.81	116.61	109.69
3	G	600	FDA	C1'-N10-C10	3.79	121.80	118.41
2	D	802	GDU	C3'-C4'-C5'	3.75	116.93	110.24
3	E	600	FDA	C1'-N10-C10	3.75	121.77	118.41
3	E	600	FDA	O5'-P-O1P	-3.74	94.46	109.07
2	B	802	GDU	C3'-C4'-C5'	3.73	116.89	110.24
2	C	802	GDU	C3'-C4'-C5'	3.72	116.88	110.24
2	C	802	GDU	O5'-C5'-C4'	3.64	116.31	109.69
3	H	600	FDA	O5'-P-O1P	-3.63	94.88	109.07
2	G	802	GDU	C3'-C4'-C5'	3.63	116.71	110.24
2	H	802	GDU	PB-O3A-PA	-3.62	120.40	132.83
2	A	802	GDU	C3'-C4'-C5'	3.61	116.68	110.24
2	E	802	GDU	PB-O3A-PA	-3.60	120.48	132.83
2	A	802	GDU	O5'-C5'-C4'	3.59	116.22	109.69
2	F	802	GDU	O5'-C5'-C4'	3.59	116.21	109.69
3	D	600	FDA	O5'-P-O1P	-3.58	95.09	109.07
3	C	600	FDA	O5'-P-O1P	-3.57	95.10	109.07
3	F	600	FDA	O5'-P-O1P	-3.54	95.24	109.07
3	D	600	FDA	C4X-C4-N3	-3.53	118.61	123.43
3	G	600	FDA	O4B-C1B-C2B	-3.52	101.79	106.93
2	C	802	GDU	PB-O3A-PA	-3.50	120.83	132.83
2	F	802	GDU	PB-O3A-PA	-3.48	120.89	132.83
2	B	802	GDU	O5'-C5'-C4'	3.48	116.01	109.69
3	G	600	FDA	O5'-P-O1P	-3.47	95.52	109.07
3	E	600	FDA	O5'-C5'-C4'	3.44	118.55	109.36
3	C	600	FDA	O5'-C5'-C4'	3.44	118.54	109.36
2	H	802	GDU	C3D-C2D-C1D	3.40	106.10	100.98
3	H	600	FDA	O5'-C5'-C4'	3.40	118.44	109.36
3	G	600	FDA	C4X-C4-N3	-3.33	118.88	123.43
2	G	802	GDU	O5'-C5'-C4'	3.31	115.70	109.69
2	E	802	GDU	C3D-C2D-C1D	3.30	105.95	100.98
3	D	600	FDA	O5'-C5'-C4'	3.30	118.17	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	802	GDU	C3D-C2D-C1D	3.26	105.88	100.98
2	C	802	GDU	C3D-C2D-C1D	3.25	105.87	100.98
3	F	600	FDA	O5'-C5'-C4'	3.24	118.02	109.36
2	D	802	GDU	C3D-C2D-C1D	3.22	105.83	100.98
3	H	600	FDA	C5X-C9A-N10	3.22	120.05	117.72
2	F	802	GDU	C3D-C2D-C1D	3.21	105.82	100.98
3	B	600	FDA	O4B-C1B-C2B	-3.21	102.24	106.93
3	C	600	FDA	C4X-C4-N3	-3.19	119.07	123.43
3	C	600	FDA	O4B-C1B-C2B	-3.15	102.32	106.93
3	F	600	FDA	C4X-C4-N3	-3.14	119.14	123.43
3	A	600	FDA	C5X-C9A-N10	3.12	119.98	117.72
3	H	600	FDA	C4X-C4-N3	-3.09	119.20	123.43
2	G	802	GDU	PB-O3A-PA	-3.09	122.23	132.83
3	F	600	FDA	O4B-C1B-C2B	-3.07	102.44	106.93
3	E	600	FDA	C4X-C4-N3	-3.06	119.25	123.43
2	B	802	GDU	C3D-C2D-C1D	3.05	105.57	100.98
3	A	600	FDA	O4B-C1B-C2B	-3.04	102.48	106.93
3	G	600	FDA	O5'-C5'-C4'	3.04	117.47	109.36
3	D	600	FDA	O4B-C1B-C2B	-3.03	102.50	106.93
3	A	600	FDA	O5'-C5'-C4'	3.03	117.45	109.36
2	D	802	GDU	PB-O3A-PA	-3.02	122.45	132.83
3	E	600	FDA	C5X-C9A-N10	3.00	119.89	117.72
3	A	600	FDA	C4X-C4-N3	-2.98	119.35	123.43
2	A	802	GDU	PB-O3A-PA	-2.97	122.64	132.83
3	E	600	FDA	O4B-C1B-C2B	-2.94	102.63	106.93
3	B	600	FDA	C4X-C4-N3	-2.93	119.43	123.43
2	F	802	GDU	O5D-C5D-C4D	2.91	119.02	108.99
2	A	802	GDU	C3D-C2D-C1D	2.90	105.34	100.98
3	E	600	FDA	O5B-C5B-C4B	2.90	118.96	108.99
2	B	802	GDU	PB-O3A-PA	-2.89	122.91	132.83
3	G	600	FDA	O2'-C2'-C1'	-2.89	102.64	109.59
2	A	802	GDU	O5D-C5D-C4D	2.88	118.90	108.99
3	D	600	FDA	C4X-N5-C5X	2.87	119.64	116.77
3	F	600	FDA	C5X-C9A-N10	2.85	119.78	117.72
3	H	600	FDA	O5B-C5B-C4B	2.84	118.78	108.99
2	C	802	GDU	O3A-PB-O3B	2.84	108.20	102.48
3	D	600	FDA	C5X-C9A-N10	2.82	119.76	117.72
3	A	600	FDA	O2'-C2'-C1'	-2.81	102.84	109.59
3	B	600	FDA	C5X-C9A-N10	2.80	119.75	117.72
2	B	802	GDU	O5D-C5D-C4D	2.79	118.61	108.99
3	C	600	FDA	O2'-C2'-C1'	-2.79	102.89	109.59
3	H	600	FDA	O4B-C1B-C2B	-2.78	102.86	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	600	FDA	O5B-C5B-C4B	2.74	118.43	108.99
3	D	600	FDA	O2'-C2'-C1'	-2.71	103.08	109.59
2	H	802	GDU	O3A-PB-O3B	2.70	107.93	102.48
2	G	802	GDU	O5D-C5D-C4D	2.68	118.22	108.99
3	G	600	FDA	C5X-C9A-N10	2.57	119.58	117.72
2	D	802	GDU	O5D-C5D-C4D	2.56	117.81	108.99
3	D	600	FDA	C4X-C10-N10	-2.56	117.67	120.30
3	F	600	FDA	O5B-C5B-C4B	2.54	117.72	108.99
2	D	802	GDU	O3A-PB-O3B	2.52	107.57	102.48
3	C	600	FDA	C4X-C10-N10	-2.52	117.71	120.30
2	E	802	GDU	O3A-PB-O3B	2.51	107.55	102.48
3	H	600	FDA	C4X-N5-C5X	2.50	119.27	116.77
3	E	600	FDA	O2'-C2'-C1'	-2.50	103.57	109.59
3	G	600	FDA	O5B-C5B-C4B	2.49	117.56	108.99
3	A	600	FDA	O5B-C5B-C4B	2.47	117.49	108.99
3	B	600	FDA	C4X-N5-C5X	2.46	119.23	116.77
3	C	600	FDA	C5X-C9A-N10	2.40	119.45	117.72
3	F	600	FDA	C4X-C10-N10	-2.39	117.84	120.30
3	B	600	FDA	O5B-C5B-C4B	2.39	117.21	108.99
3	E	600	FDA	C4A-C5A-N7A	-2.39	106.91	109.40
3	B	600	FDA	O5'-C5'-C4'	2.38	115.71	109.36
3	B	600	FDA	O2'-C2'-C1'	-2.37	103.88	109.59
3	C	600	FDA	O5B-C5B-C4B	2.37	117.15	108.99
3	A	600	FDA	C4X-N5-C5X	2.36	119.13	116.77
2	B	802	GDU	O3A-PB-O3B	2.35	107.22	102.48
3	E	600	FDA	C4X-N5-C5X	2.35	119.12	116.77
3	B	600	FDA	O2A-PA-O5B	2.35	118.65	107.75
3	D	600	FDA	O2P-P-O5'	2.34	118.63	107.75
3	H	600	FDA	O2A-PA-O5B	2.33	118.58	107.75
2	D	802	GDU	O3B-C1'-C2'	2.32	112.63	108.38
3	C	600	FDA	O2A-PA-O5B	2.31	118.49	107.75
3	C	600	FDA	C4X-N5-C5X	2.28	119.05	116.77
2	G	802	GDU	O3B-C1'-C2'	2.27	112.54	108.38
2	A	802	GDU	O3A-PB-O3B	2.26	107.05	102.48
3	F	600	FDA	O2'-C2'-C1'	-2.26	104.16	109.59
3	F	600	FDA	C4X-N5-C5X	2.25	119.02	116.77
3	C	600	FDA	O2P-P-O5'	2.24	118.15	107.75
3	E	600	FDA	O2A-PA-O5B	2.23	118.10	107.75
3	G	600	FDA	C4X-C10-N10	-2.22	118.02	120.30
3	H	600	FDA	C4A-C5A-N7A	-2.20	107.10	109.40
3	H	600	FDA	C1'-N10-C9A	-2.18	116.58	118.29
2	C	802	GDU	O3B-C1'-C2'	2.18	112.37	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	FDA	C1'-C2'-C3'	2.17	115.84	109.79
2	F	802	GDU	O3A-PB-O3B	2.16	106.84	102.48
3	B	600	FDA	O2P-P-O5'	2.16	117.76	107.75
3	A	600	FDA	O2P-P-O5'	2.15	117.74	107.75
3	F	600	FDA	O2P-P-O5'	2.13	117.65	107.75
3	E	600	FDA	C1'-C2'-C3'	2.12	115.72	109.79
3	H	600	FDA	O2'-C2'-C1'	-2.12	104.49	109.59
3	G	600	FDA	O2A-PA-O5B	2.11	117.56	107.75
3	C	600	FDA	C4A-C5A-N7A	-2.11	107.20	109.40
3	C	600	FDA	C1'-C2'-C3'	2.11	115.68	109.79
2	F	802	GDU	O3B-C1'-C2'	2.10	112.23	108.38
3	G	600	FDA	C4X-N5-C5X	2.10	118.87	116.77
3	A	600	FDA	C4A-C5A-N7A	-2.09	107.22	109.40
3	H	600	FDA	O2P-P-O5'	2.08	117.41	107.75
3	E	600	FDA	O2P-P-O5'	2.08	117.40	107.75
3	D	600	FDA	O2A-PA-O5B	2.08	117.40	107.75
3	A	600	FDA	O2A-PA-O5B	2.07	117.36	107.75
3	G	600	FDA	O2P-P-O5'	2.06	117.32	107.75
2	C	802	GDU	O5D-C5D-C4D	2.05	116.06	108.99
2	E	802	GDU	O5D-C5D-C4D	2.05	116.04	108.99
2	E	802	GDU	O3B-C1'-C2'	2.04	112.12	108.38
3	A	600	FDA	C1'-C2'-C3'	2.04	115.48	109.79
2	B	802	GDU	O3B-C1'-C2'	2.03	112.11	108.38
2	G	802	GDU	O3A-PB-O3B	2.02	106.56	102.48
3	D	600	FDA	C10-C4X-N5	-2.02	119.86	121.26
2	A	802	GDU	O3B-C1'-C2'	2.01	112.07	108.38
3	F	600	FDA	O2A-PA-O5B	2.01	117.08	107.75
3	G	600	FDA	C4A-C5A-N7A	-2.01	107.31	109.40

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	802	GDU	C2D-C1D-N1-C6
2	H	802	GDU	O4D-C1D-N1-C6
2	H	802	GDU	C5D-O5D-PA-O2A
2	H	802	GDU	C5D-O5D-PA-O3A
2	H	802	GDU	C1'-O3B-PB-O2B
2	H	802	GDU	O5'-C1'-O3B-PB
2	A	802	GDU	C1'-O3B-PB-O2B
2	A	802	GDU	C2'-C1'-O3B-PB
2	A	802	GDU	O5'-C1'-O3B-PB

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Mol	Chain	Res	Type	Atoms
2	D	802	GDU	C2D-C1D-N1-C6
2	D	802	GDU	O4D-C1D-N1-C6
2	D	802	GDU	C1'-O3B-PB-O2B
2	D	802	GDU	C2'-C1'-O3B-PB
2	D	802	GDU	O5'-C1'-O3B-PB
2	E	802	GDU	C2D-C1D-N1-C6
2	E	802	GDU	O4D-C1D-N1-C6
2	E	802	GDU	C1'-O3B-PB-O2B
2	E	802	GDU	O5'-C1'-O3B-PB
3	G	600	FDA	PA-O3P-P-O5'
2	B	802	GDU	C1'-O3B-PB-O2B
2	B	802	GDU	C2'-C1'-O3B-PB
2	B	802	GDU	O5'-C1'-O3B-PB
2	C	802	GDU	O4D-C1D-N1-C6
2	C	802	GDU	C5D-O5D-PA-O3A
2	C	802	GDU	PA-O3A-PB-O3B
2	C	802	GDU	C1'-O3B-PB-O2B
2	C	802	GDU	C2'-C1'-O3B-PB
2	C	802	GDU	O5'-C1'-O3B-PB
3	H	600	FDA	C2'-C1'-N10-C9A
3	H	600	FDA	PA-O3P-P-O5'
2	F	802	GDU	C2D-C1D-N1-C6
2	F	802	GDU	O4D-C1D-N1-C6
2	F	802	GDU	C1'-O3B-PB-O2B
2	F	802	GDU	C2'-C1'-O3B-PB
2	F	802	GDU	O5'-C1'-O3B-PB
2	G	802	GDU	C2D-C1D-N1-C6
2	G	802	GDU	O4D-C1D-N1-C6
2	G	802	GDU	C1'-O3B-PB-O2B
2	G	802	GDU	C2'-C1'-O3B-PB
2	G	802	GDU	O5'-C1'-O3B-PB
2	D	802	GDU	O5'-C5'-C6'-O6'
2	H	802	GDU	O5'-C5'-C6'-O6'
2	A	802	GDU	O5'-C5'-C6'-O6'
2	F	802	GDU	O5'-C5'-C6'-O6'
2	C	802	GDU	O5'-C5'-C6'-O6'
2	G	802	GDU	O5'-C5'-C6'-O6'
2	E	802	GDU	O5'-C5'-C6'-O6'
2	B	802	GDU	O5'-C5'-C6'-O6'
2	H	802	GDU	C2'-C1'-O3B-PB
2	E	802	GDU	C2'-C1'-O3B-PB
2	H	802	GDU	C1'-O3B-PB-O3A

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Mol	Chain	Res	Type	Atoms
2	A	802	GDU	C1'-O3B-PB-O3A
2	D	802	GDU	C1'-O3B-PB-O3A
2	E	802	GDU	C1'-O3B-PB-O3A
2	B	802	GDU	C1'-O3B-PB-O3A
2	C	802	GDU	C1'-O3B-PB-O3A
2	F	802	GDU	C1'-O3B-PB-O3A
2	G	802	GDU	C1'-O3B-PB-O3A
3	G	600	FDA	O4'-C4'-C5'-O5'
3	E	600	FDA	C2'-C3'-C4'-O4'
3	E	600	FDA	PA-O3P-P-O5'
3	F	600	FDA	PA-O3P-P-O5'
3	B	600	FDA	PA-O3P-P-O5'
3	C	600	FDA	C5B-O5B-PA-O3P
3	G	600	FDA	C5'-O5'-P-O3P
3	E	600	FDA	C5B-O5B-PA-O3P
3	F	600	FDA	C5B-O5B-PA-O3P
3	F	600	FDA	C5'-O5'-P-O3P
3	D	600	FDA	C5B-O5B-PA-O3P
2	H	802	GDU	PB-O3A-PA-O1A
2	C	802	GDU	PB-O3A-PA-O1A
2	H	802	GDU	C5D-O5D-PA-O1A
2	C	802	GDU	C5D-O5D-PA-O2A
3	H	600	FDA	C2'-C3'-C4'-O4'
2	D	802	GDU	C4'-C5'-C6'-O6'
3	E	600	FDA	O4B-C4B-C5B-O5B
2	A	802	GDU	C4'-C5'-C6'-O6'
3	C	600	FDA	C2'-C3'-C4'-O4'
2	G	802	GDU	C4'-C5'-C6'-O6'
2	F	802	GDU	C4'-C5'-C6'-O6'
3	G	600	FDA	O4B-C4B-C5B-O5B
3	G	600	FDA	C5B-O5B-PA-O3P
3	H	600	FDA	C5B-O5B-PA-O3P
3	C	600	FDA	O4B-C4B-C5B-O5B
3	F	600	FDA	O4B-C4B-C5B-O5B
3	H	600	FDA	O4B-C4B-C5B-O5B
2	H	802	GDU	C1'-O3B-PB-O1B
2	E	802	GDU	PB-O3A-PA-O1A
2	C	802	GDU	C1'-O3B-PB-O1B
2	H	802	GDU	C4'-C5'-C6'-O6'
3	B	600	FDA	C2'-C3'-C4'-O4'
3	G	600	FDA	C5'-O5'-P-O1P
2	C	802	GDU	C5D-O5D-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	600	FDA	O4B-C4B-C5B-O5B
3	D	600	FDA	O4B-C4B-C5B-O5B
3	B	600	FDA	O4B-C4B-C5B-O5B
2	C	802	GDU	C4'-C5'-C6'-O6'

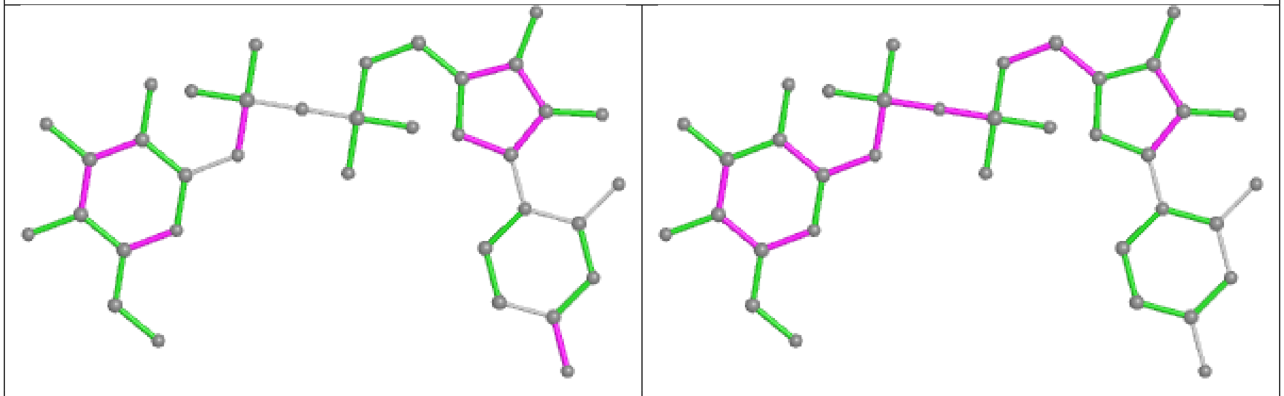
There are no ring outliers.

15 monomers are involved in 27 short contacts:

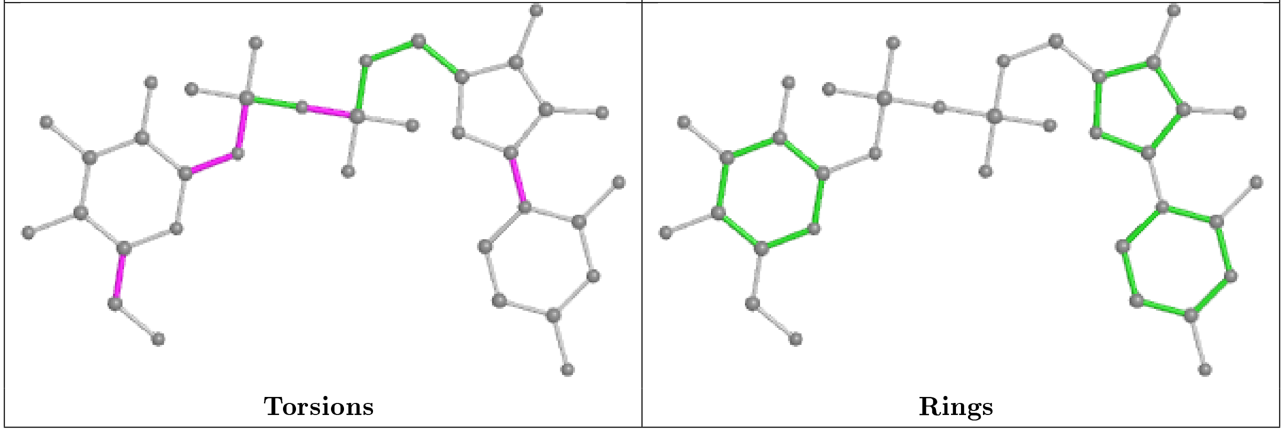
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	802	GDU	1	0
3	F	600	FDA	2	0
3	G	600	FDA	6	0
3	D	600	FDA	1	0
3	E	600	FDA	1	0
3	B	600	FDA	1	0
3	C	600	FDA	1	0
3	A	600	FDA	1	0
2	H	802	GDU	3	0
3	H	600	FDA	1	0
2	A	802	GDU	2	0
2	D	802	GDU	2	0
2	G	802	GDU	2	0
2	B	802	GDU	1	0
2	C	802	GDU	2	0

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 GDU E 802

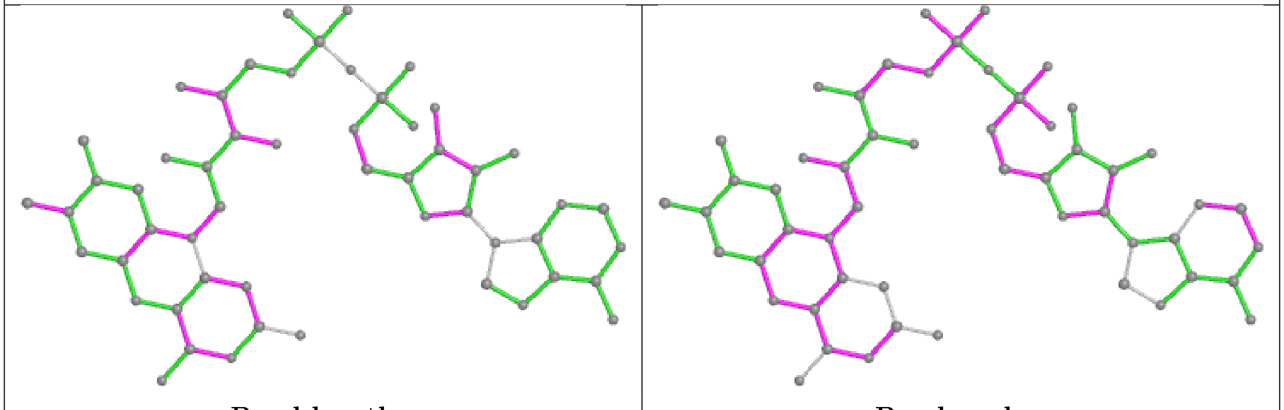


Bond lengths Bond angles

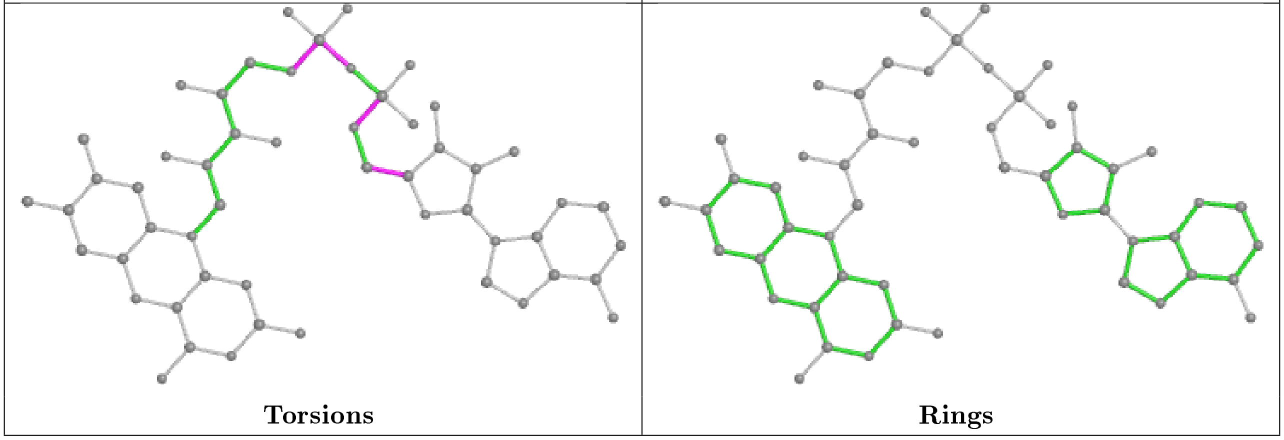


Torsions Rings

Ligand FDA F 600

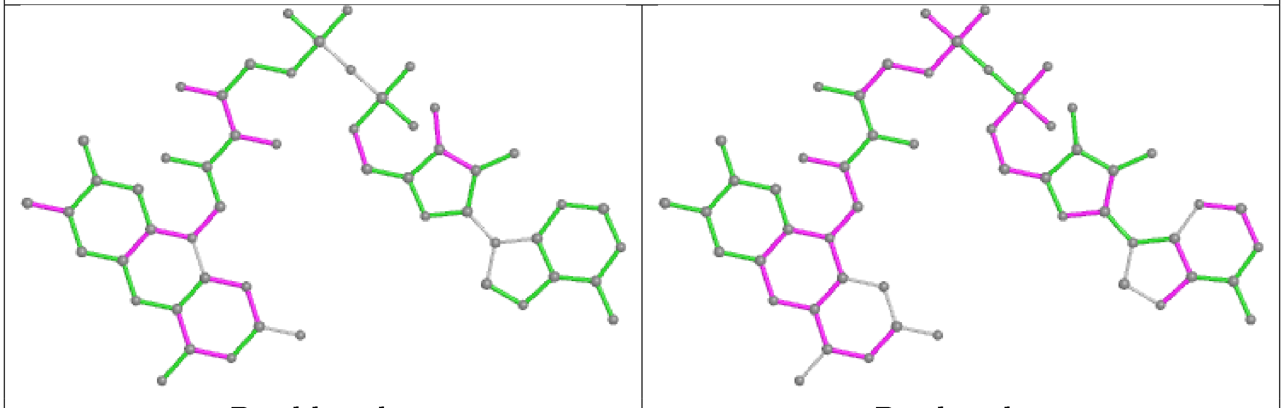


Bond lengths **Bond angles**



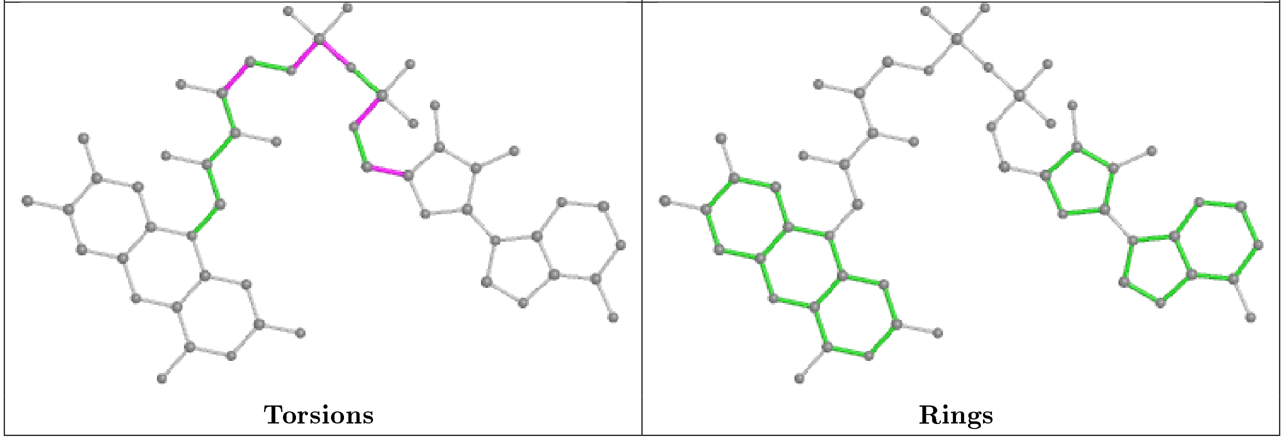
Torsions **Rings**

Ligand FDA G 600



Bond lengths

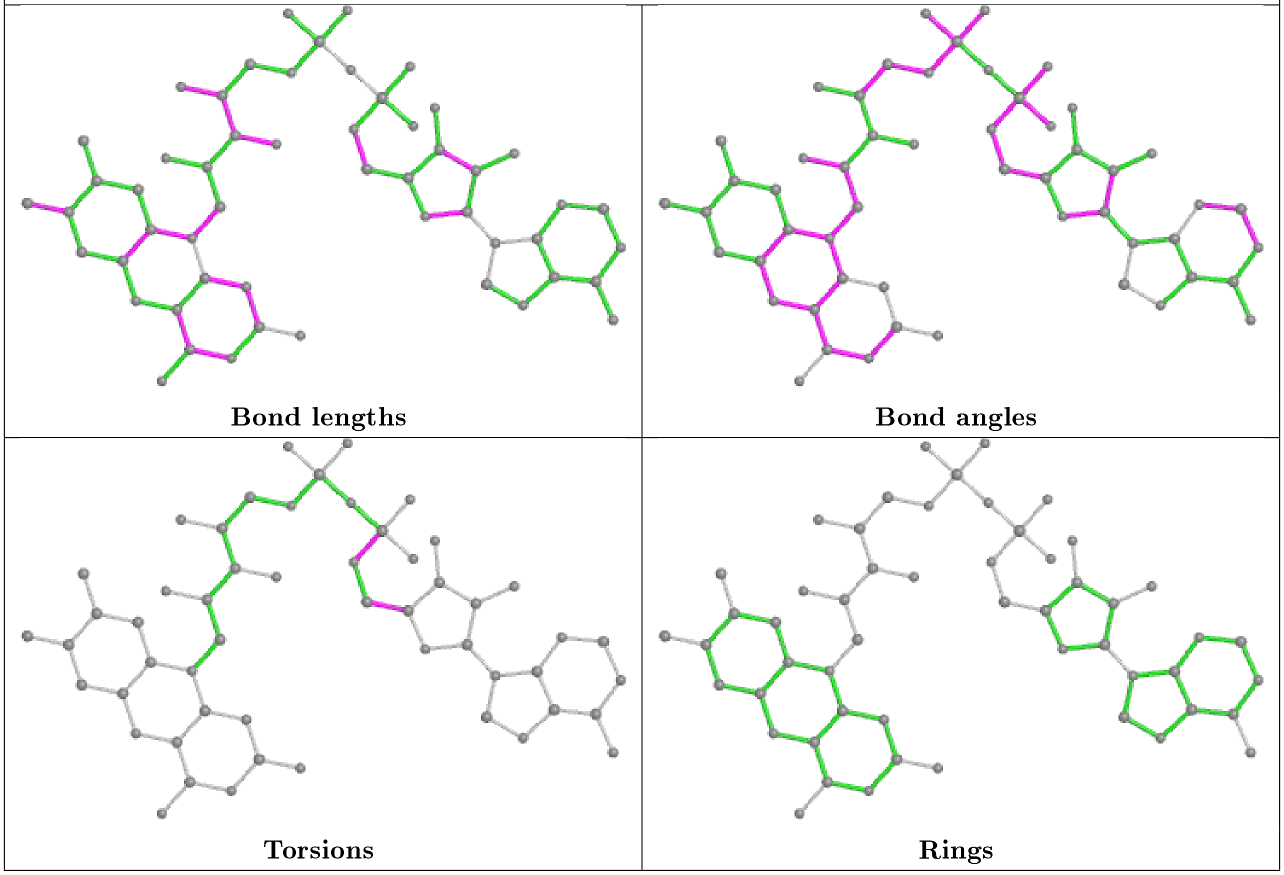
Bond angles



Torsions

Rings

Ligand FDA D 600



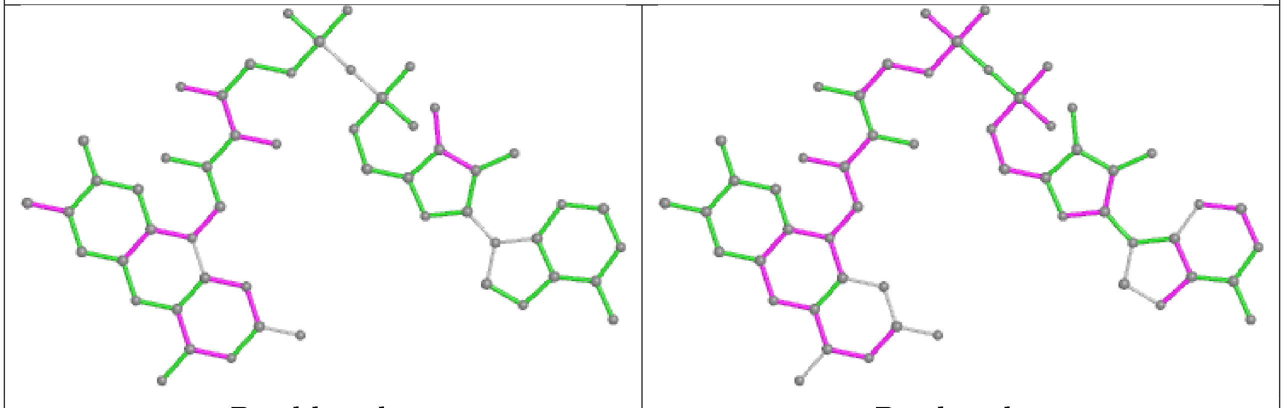
Bond lengths

Bond angles

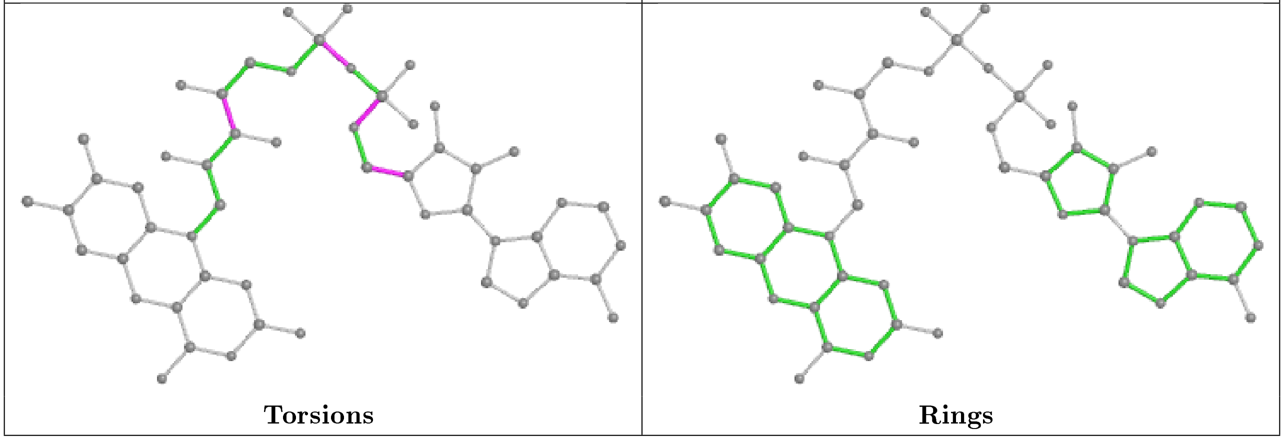
Torsions

Rings

Ligand FDA E 600

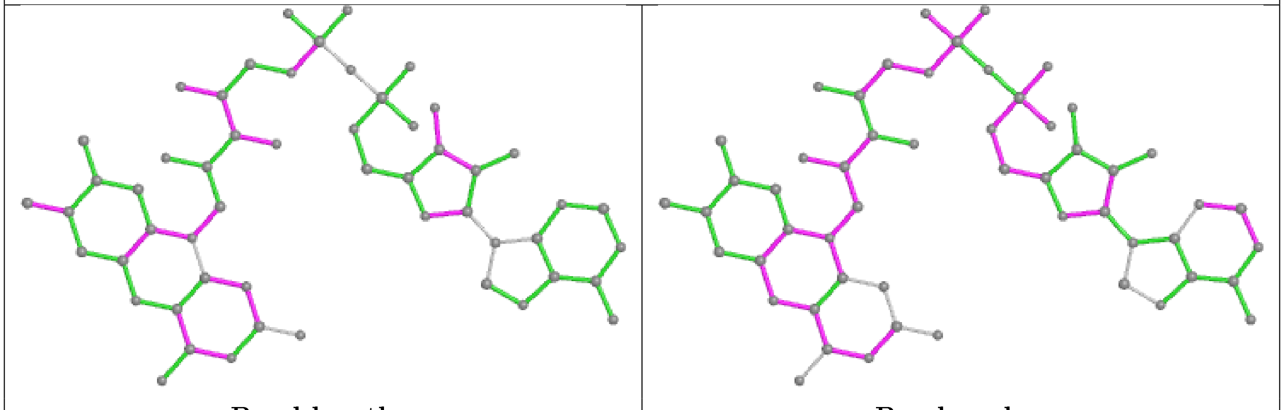


Bond lengths **Bond angles**



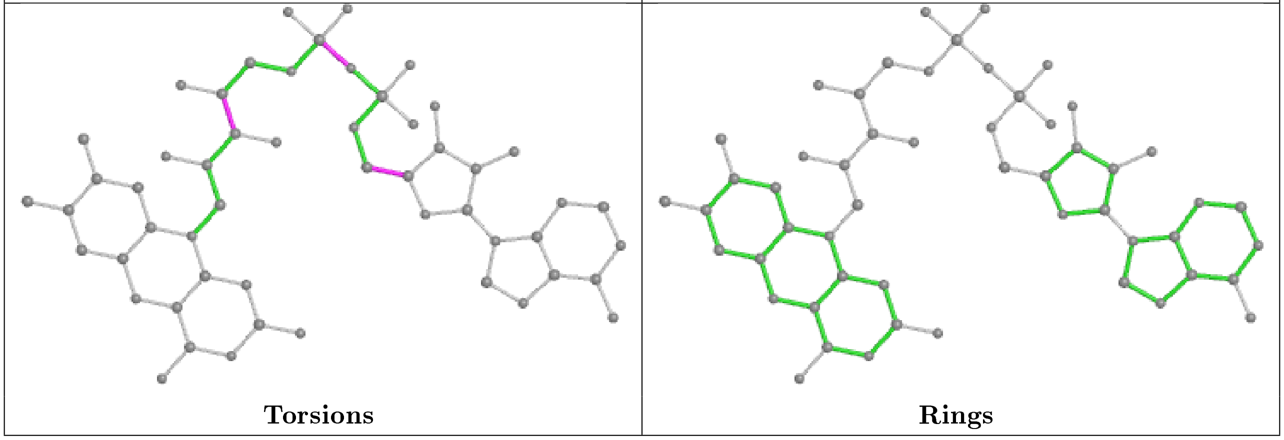
Torsions **Rings**

Ligand FDA B 600



Bond lengths

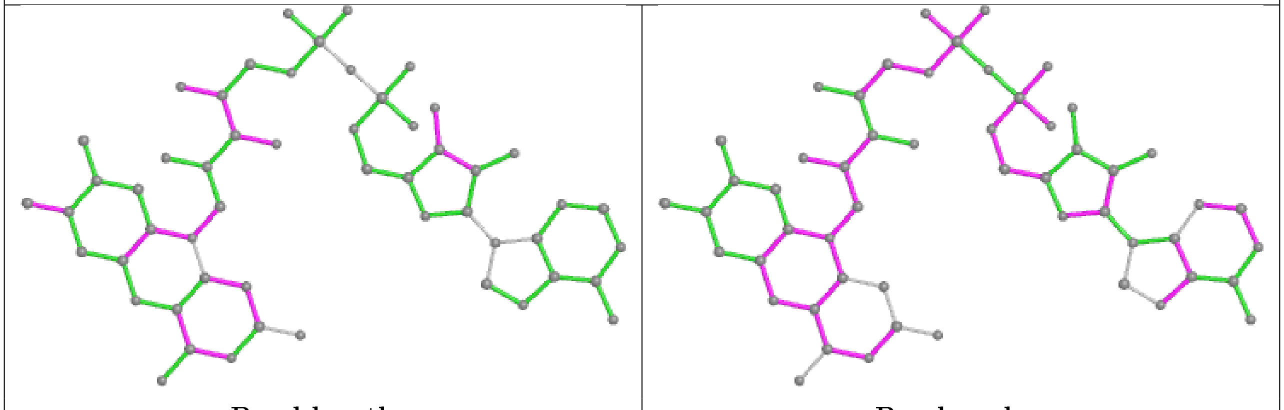
Bond angles



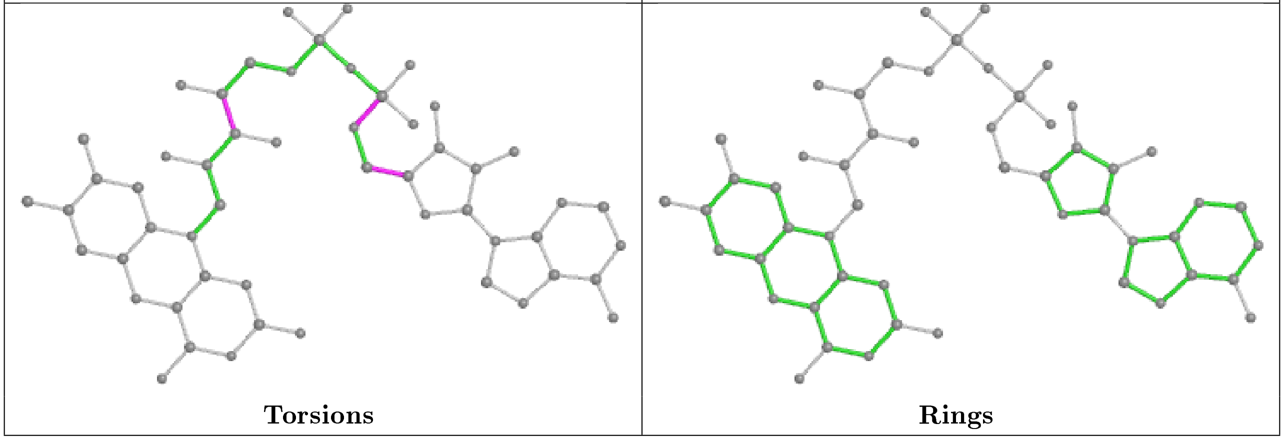
Torsions

Rings

Ligand FDA C 600

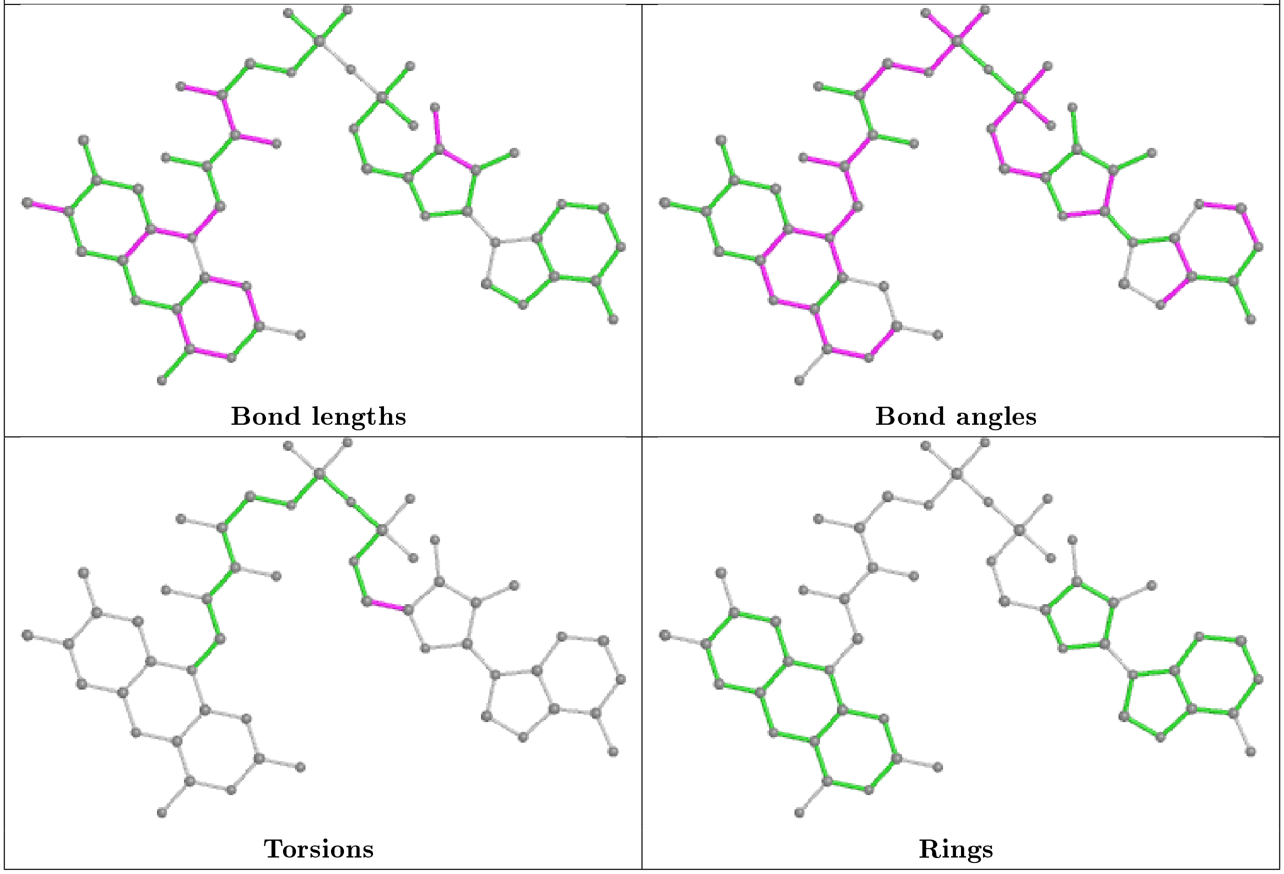


Bond lengths **Bond angles**



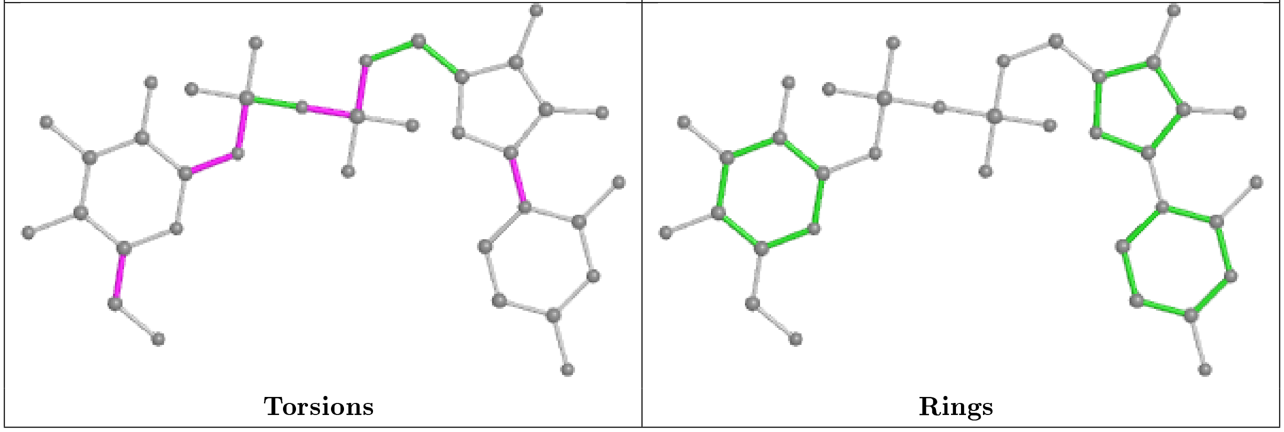
Torsions **Rings**

Ligand FDA A 600



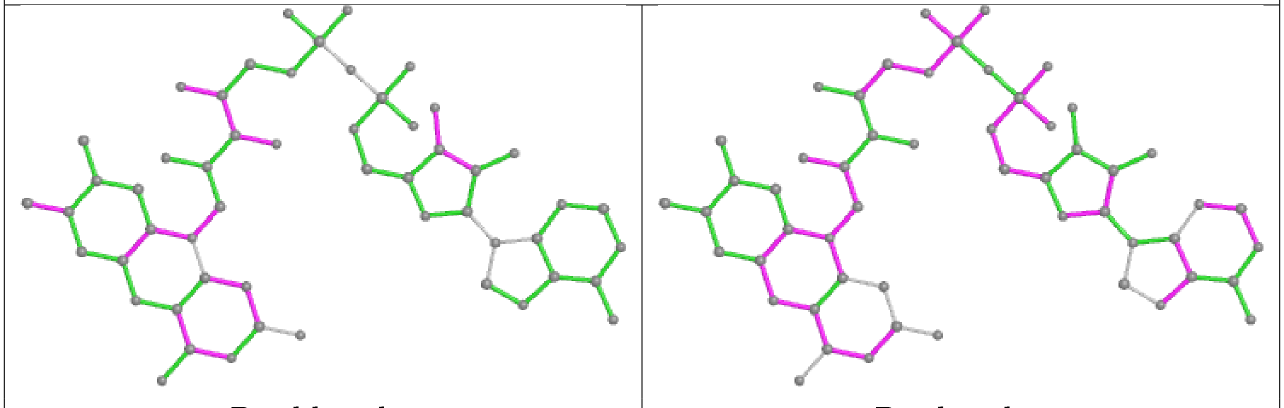
Ligand GDU H 802

Bond lengths **Bond angles**



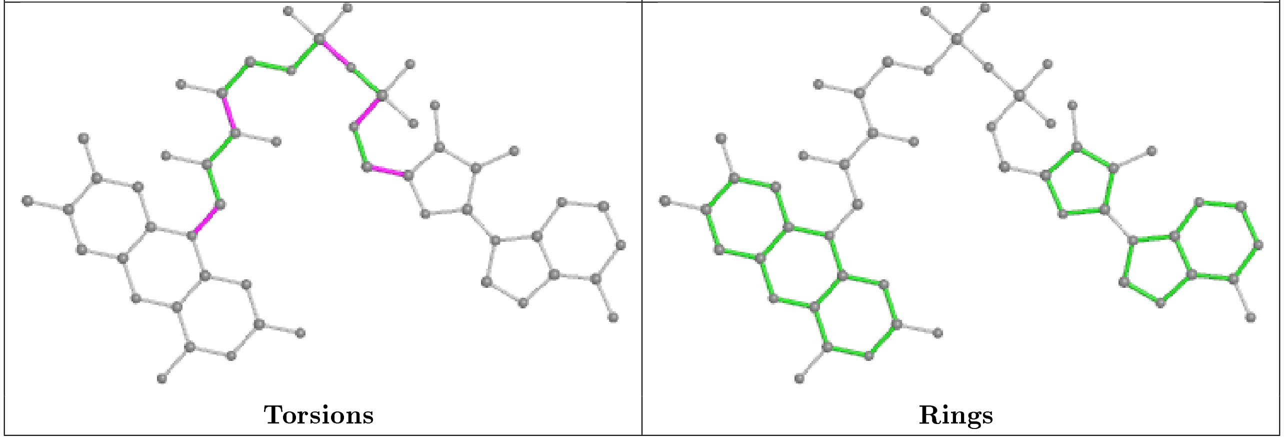
Torsions **Rings**

Ligand FDA H 600



Bond lengths

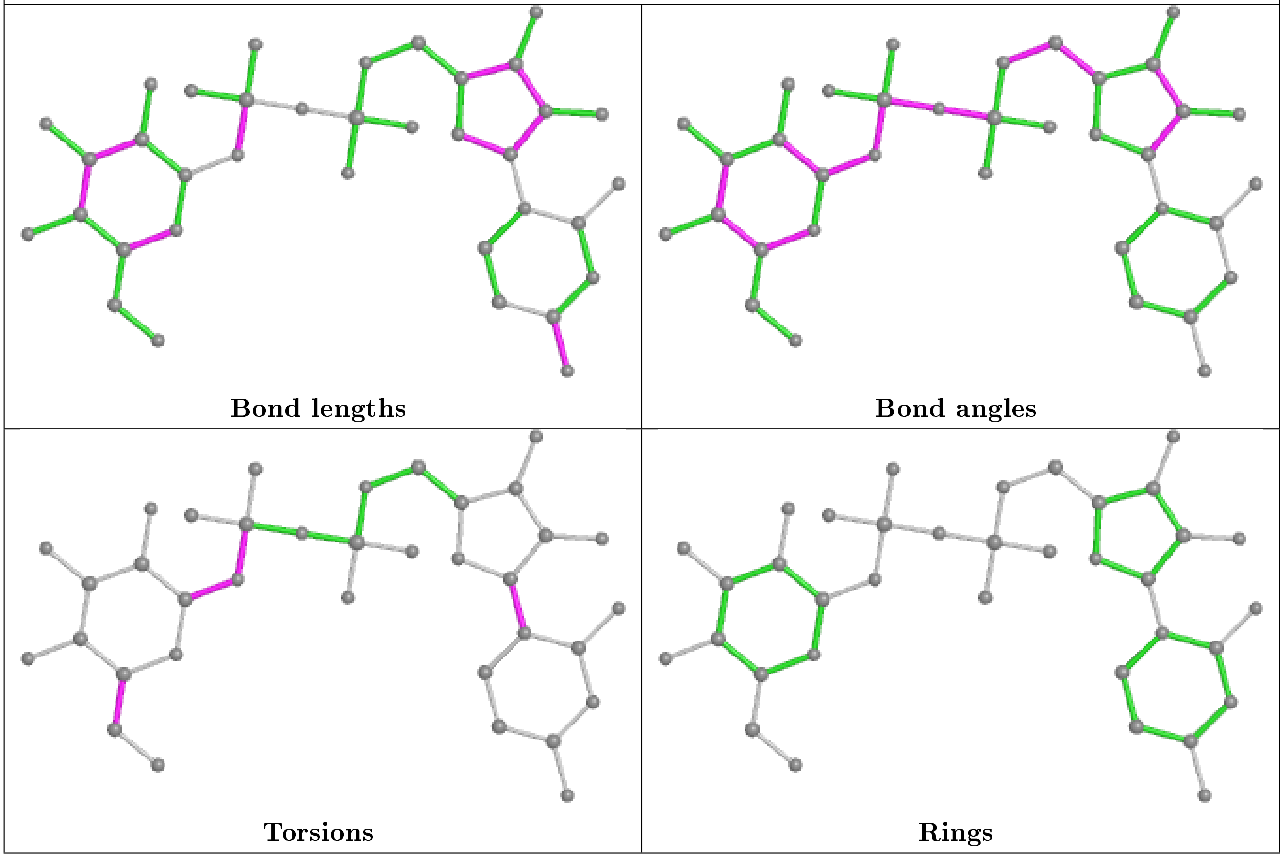
Bond angles



Torsions

Rings

Ligand GDU F 802



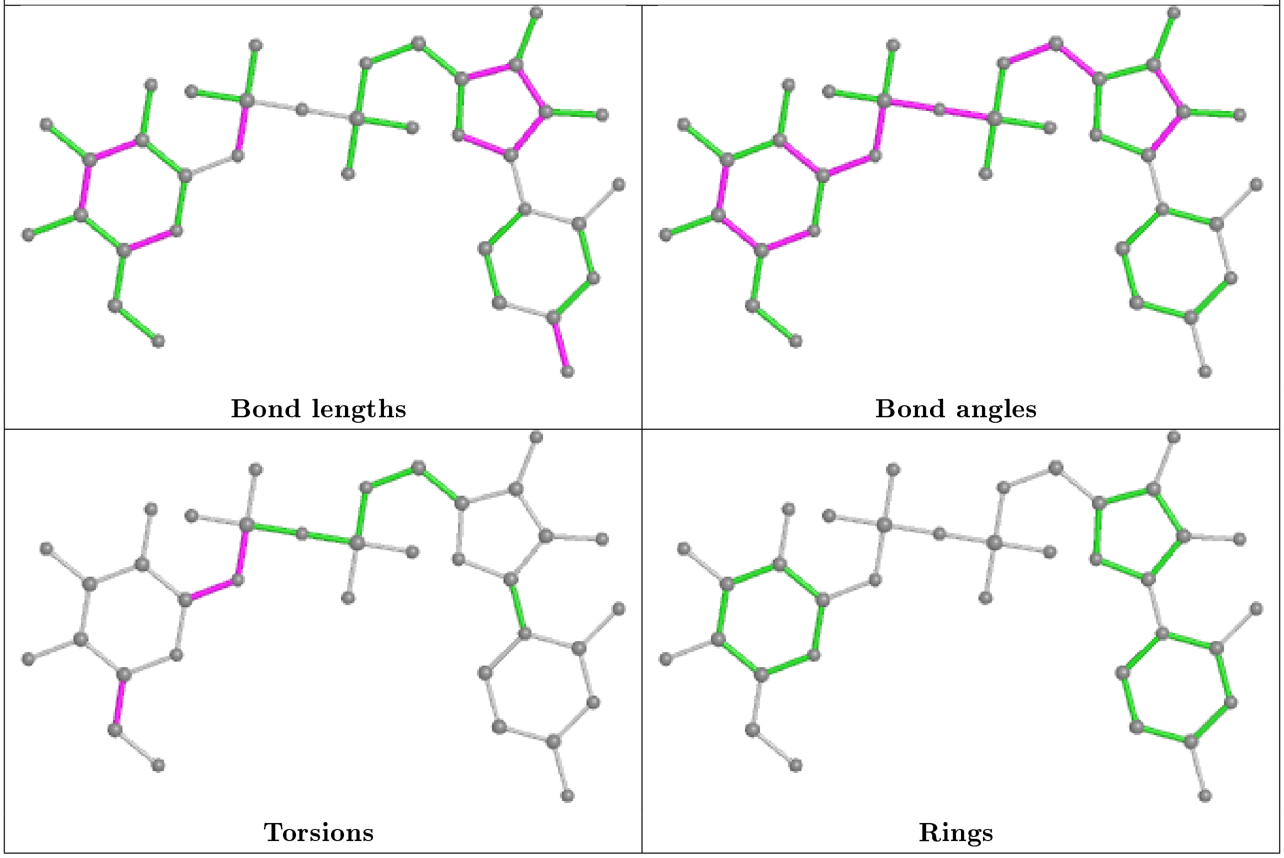
Bond lengths

Bond angles

Torsions

Rings

Ligand GDU A 802



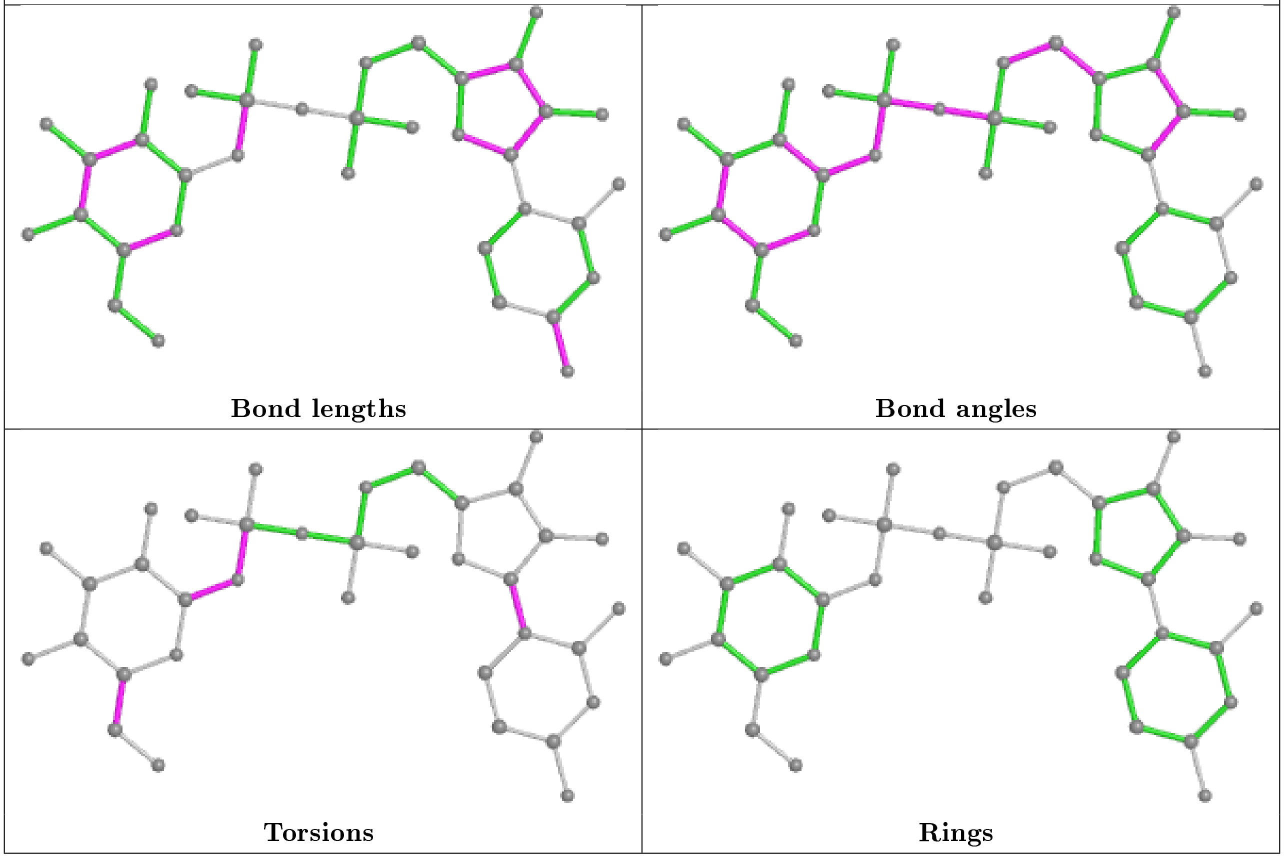
Bond lengths

Bond angles

Torsions

Rings

Ligand GDU D 802



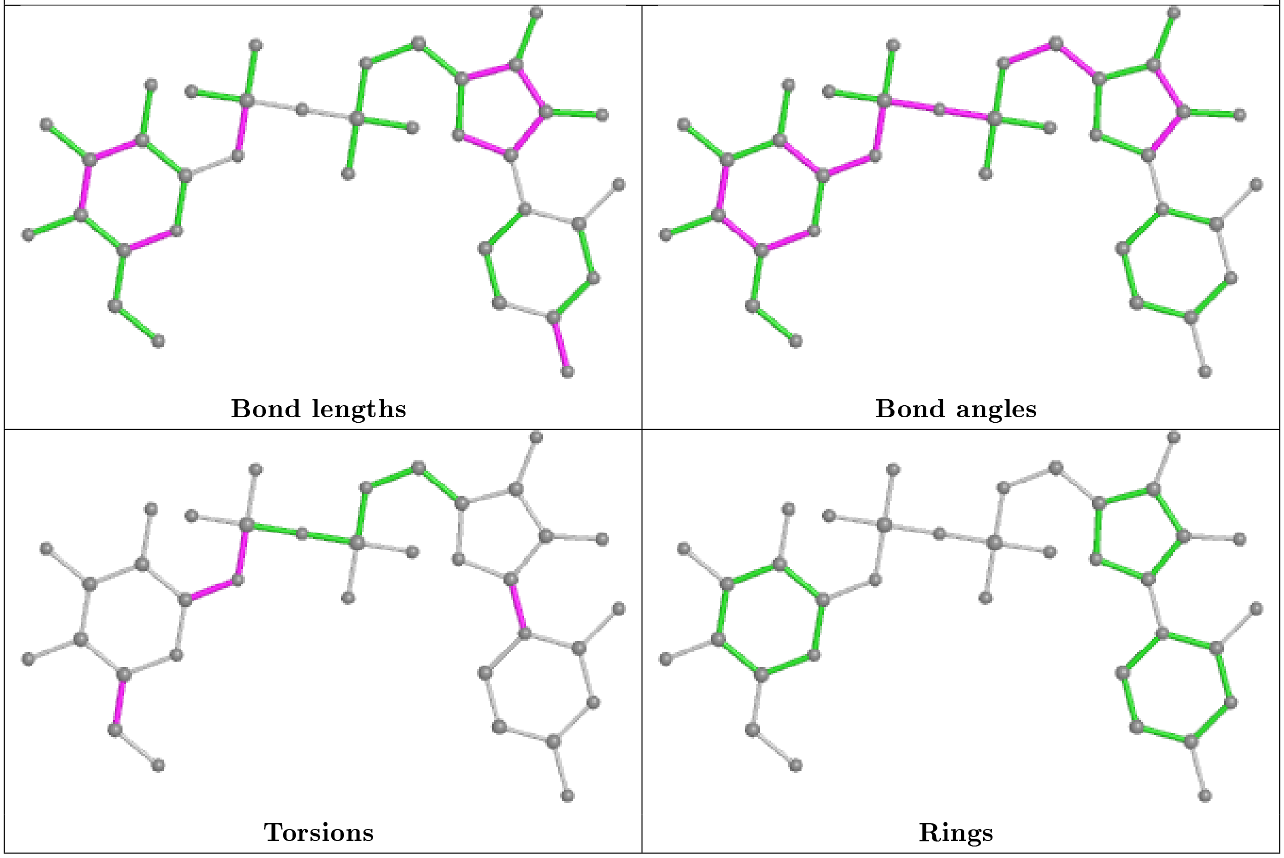
Bond lengths

Bond angles

Torsions

Rings

Ligand GDU G 802



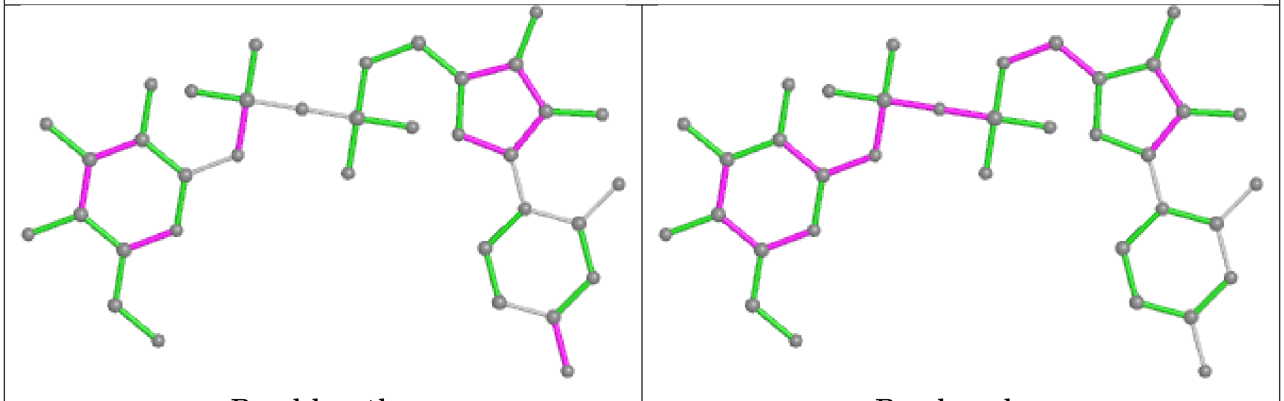
Bond lengths

Bond angles

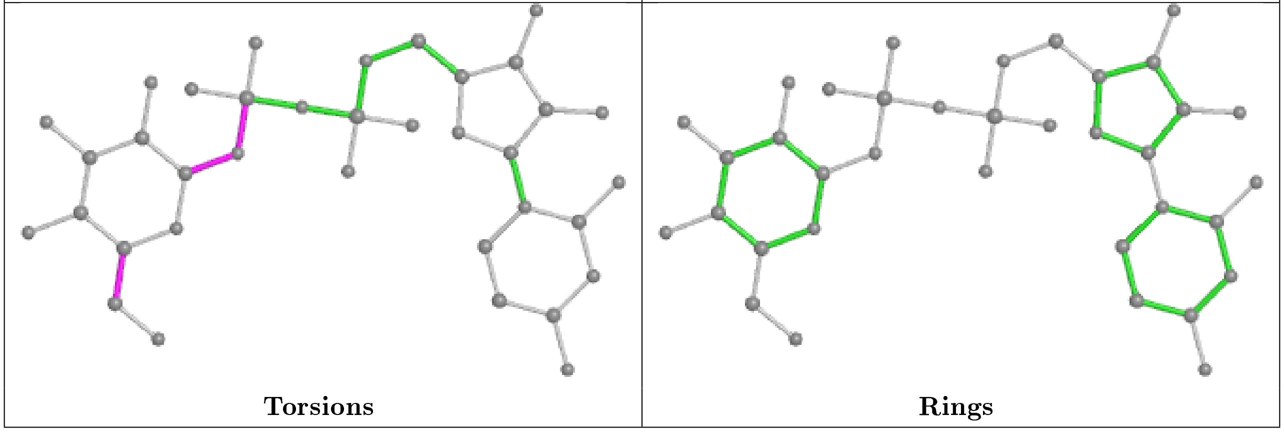
Torsions

Rings

Ligand GDU B 802



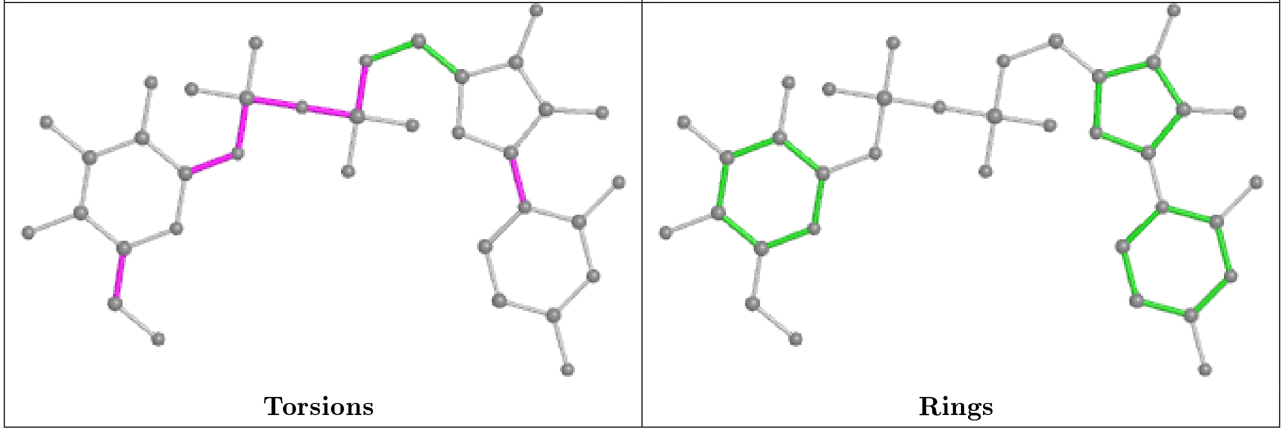
Bond lengths Bond angles



Torsions Rings

Ligand GDU C 802

Bond lengths Bond angles



Torsions Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	495/509 (97%)	0.14	2 (0%)	92	93	35, 62, 94, 155	0
1	B	495/509 (97%)	0.12	6 (1%)	79	80	37, 61, 94, 169	0
1	C	495/509 (97%)	0.13	7 (1%)	75	77	36, 65, 100, 145	0
1	D	495/509 (97%)	0.13	6 (1%)	79	80	39, 65, 98, 145	0
1	E	495/509 (97%)	0.43	32 (6%)	18	19	30, 72, 113, 186	0
1	F	495/509 (97%)	0.21	15 (3%)	50	53	43, 72, 100, 145	0
1	G	495/509 (97%)	0.23	15 (3%)	50	53	45, 72, 101, 149	0
1	H	495/509 (97%)	0.44	35 (7%)	16	16	34, 72, 112, 154	0
All	All	3960/4072 (97%)	0.23	118 (2%)	50	53	30, 68, 104, 186	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	342	ALA	9.3
1	G	2	THR	7.6
1	E	407	ILE	6.2
1	G	110	ILE	6.1
1	A	2	THR	5.8
1	D	2	THR	5.7
1	B	2	THR	5.6
1	E	384	GLN	5.6
1	H	403	PRO	5.3
1	H	51	VAL	5.3
1	G	208	ALA	5.1
1	D	3	HIS	4.9
1	H	407	ILE	4.5
1	G	508	LYS	4.4
1	H	352	ALA	4.1
1	H	392	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	384	GLN	4.0
1	F	48	SER	4.0
1	F	2	THR	4.0
1	G	57	LEU	3.9
1	F	110	ILE	3.8
1	G	3	HIS	3.8
1	C	2	THR	3.7
1	E	201	ALA	3.7
1	E	411	TYR	3.7
1	H	101	TRP	3.6
1	G	62	GLY	3.6
1	B	509	ALA	3.5
1	H	359	SER	3.3
1	F	508	LYS	3.3
1	E	325	PHE	3.3
1	F	509	ALA	3.2
1	C	508	LYS	3.2
1	H	382	VAL	3.2
1	G	341	GLU	3.2
1	C	140	LYS	3.2
1	H	198	GLY	3.1
1	F	3	HIS	3.1
1	H	140	LYS	3.0
1	H	119	VAL	3.0
1	E	352	ALA	3.0
1	H	358	GLN	3.0
1	F	368	TRP	3.0
1	E	190	ALA	2.9
1	C	510	GLN	2.9
1	E	51	VAL	2.9
1	A	509	ALA	2.9
1	E	342	ALA	2.8
1	F	198	GLY	2.8
1	H	97	CYS	2.8
1	C	3	HIS	2.8
1	H	346	LEU	2.8
1	E	341	GLU	2.8
1	G	61	GLY	2.8
1	E	116	GLU	2.7
1	E	202	GLY	2.6
1	G	204	TRP	2.6
1	E	346	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	368	TRP	2.6
1	H	355	SER	2.6
1	E	387	ILE	2.6
1	H	406	GLU	2.6
1	E	372	LEU	2.5
1	E	2	THR	2.5
1	C	190	ALA	2.5
1	H	356	ARG	2.5
1	E	210	PHE	2.5
1	B	508	LYS	2.5
1	H	506	LYS	2.5
1	E	140	LYS	2.5
1	E	403	PRO	2.4
1	C	61	GLY	2.4
1	B	385	GLU	2.4
1	E	323	CYS	2.4
1	F	208	ALA	2.4
1	H	294	SER	2.4
1	H	52	THR	2.4
1	H	190	ALA	2.3
1	H	411	TYR	2.3
1	B	138	LYS	2.3
1	G	407	ILE	2.3
1	F	206	PRO	2.3
1	E	308	GLU	2.3
1	E	334	TYR	2.3
1	G	82	LYS	2.2
1	E	357	PRO	2.2
1	D	508	LYS	2.2
1	F	231	LYS	2.2
1	E	214	ALA	2.2
1	D	308	GLU	2.2
1	E	406	GLU	2.2
1	E	198	GLY	2.2
1	H	331	PHE	2.2
1	H	398	THR	2.2
1	F	204	TRP	2.2
1	F	300	VAL	2.2
1	H	341	GLU	2.2
1	D	475	GLY	2.2
1	H	281	GLN	2.2
1	F	392	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	370	ILE	2.2
1	H	408	VAL	2.1
1	D	135	ALA	2.1
1	H	347	PRO	2.1
1	H	391	CYS	2.1
1	E	506	LYS	2.1
1	E	97	CYS	2.1
1	H	367	TYR	2.1
1	E	101	TRP	2.1
1	H	299	GLY	2.1
1	G	198	GLY	2.1
1	E	3	HIS	2.0
1	B	62	GLY	2.0
1	H	300	VAL	2.0
1	G	210	PHE	2.0
1	E	359	SER	2.0
1	G	273	PHE	2.0
1	F	238	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	F	511	1/1	0.66	0.14	127,127,127,127	0
4	CL	E	511	1/1	0.75	0.17	98,98,98,98	0
4	CL	G	511	1/1	0.84	0.11	91,91,91,91	0
4	CL	H	511	1/1	0.88	0.19	92,92,92,92	0
4	CL	B	511	1/1	0.91	0.13	99,99,99,99	0

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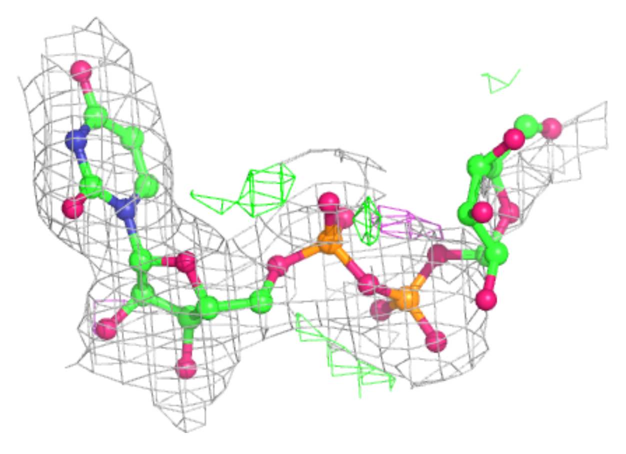
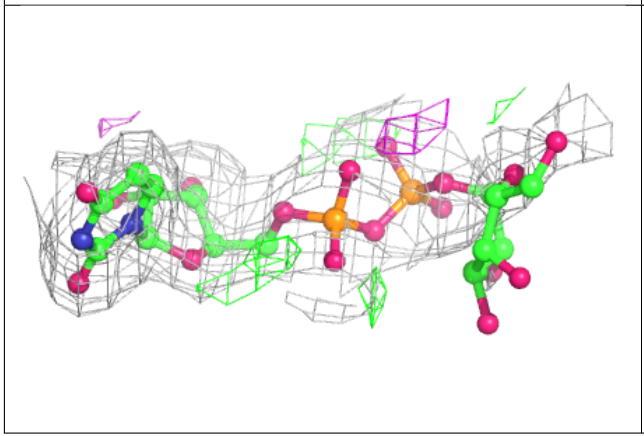
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	A	511	1/1	0.93	0.14	99,99,99,99	0
2	GDU	E	802	36/36	0.93	0.21	36,87,184,204	0
2	GDU	F	802	36/36	0.93	0.16	46,101,172,187	0
2	GDU	H	802	36/36	0.94	0.15	34,83,158,181	0
4	CL	B	512	1/1	0.94	0.15	85,85,85,85	0
2	GDU	G	802	36/36	0.94	0.17	42,96,200,209	0
4	CL	A	1	1/1	0.95	0.25	94,94,94,94	0
2	GDU	B	802	36/36	0.95	0.16	47,68,189,191	0
2	GDU	C	802	36/36	0.95	0.17	34,83,170,193	0
3	FDA	G	600	53/53	0.95	0.12	35,67,86,99	0
2	GDU	D	802	36/36	0.95	0.15	37,80,177,208	0
3	FDA	H	600	53/53	0.96	0.14	28,55,92,130	0
3	FDA	E	600	53/53	0.96	0.15	27,56,102,130	0
3	FDA	F	600	53/53	0.96	0.13	34,62,84,98	0
3	FDA	D	600	53/53	0.97	0.14	26,64,91,108	0
3	FDA	B	600	53/53	0.97	0.13	31,49,72,95	0
2	GDU	A	802	36/36	0.97	0.16	40,66,183,201	0
3	FDA	C	600	53/53	0.97	0.14	34,66,92,99	0
3	FDA	A	600	53/53	0.97	0.13	33,48,67,82	0

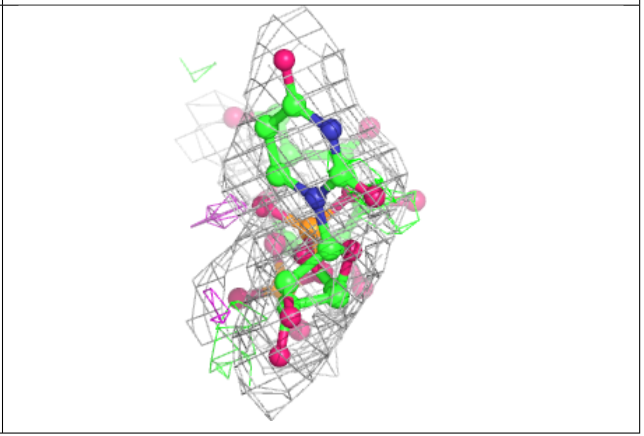
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDU E 802:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

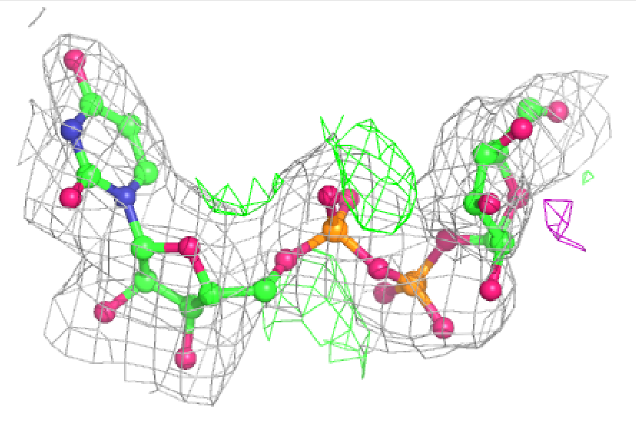


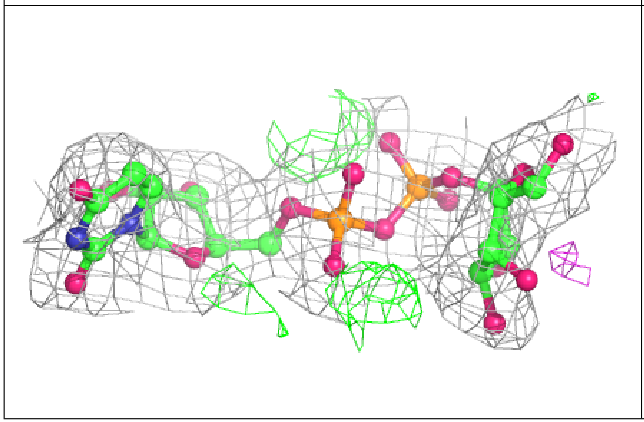


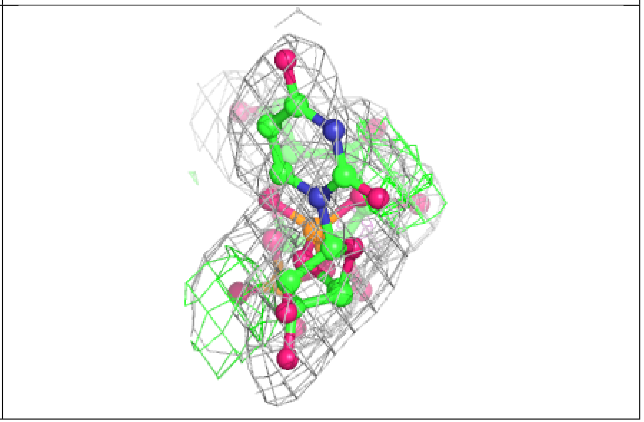


Electron density around GDU F 802:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

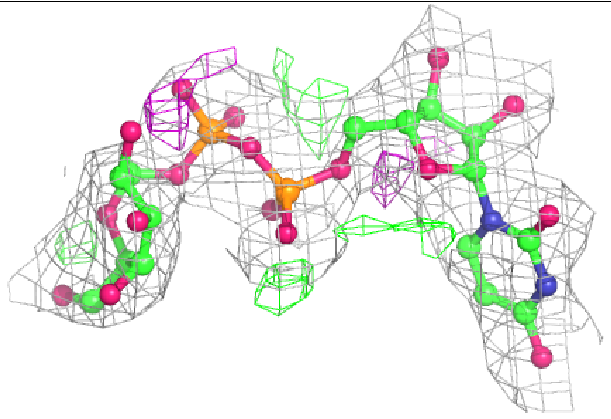


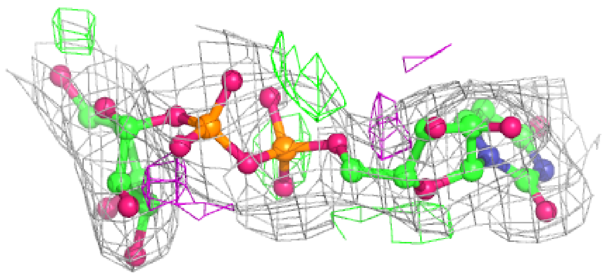


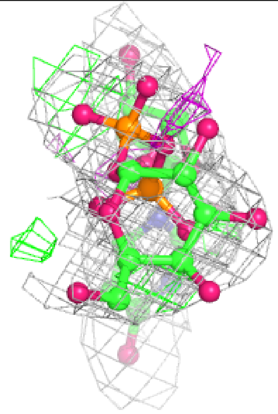


Electron density around GDU H 802:

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 GDU G 802:

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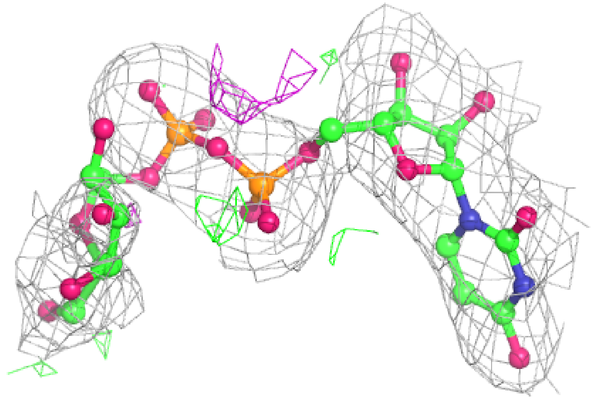
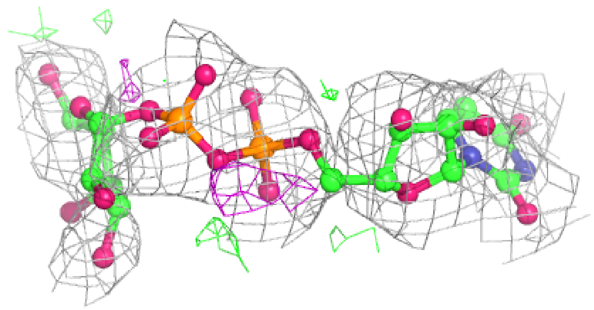
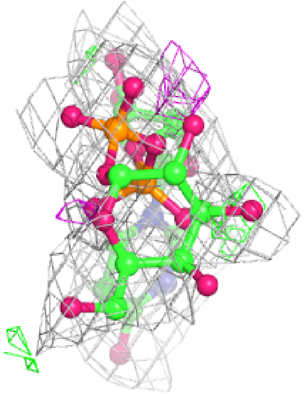
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

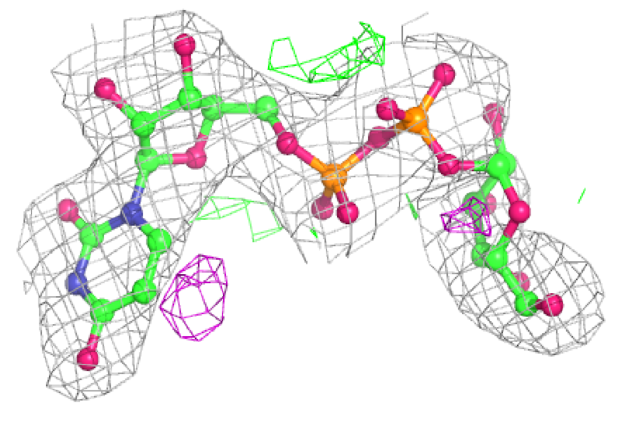


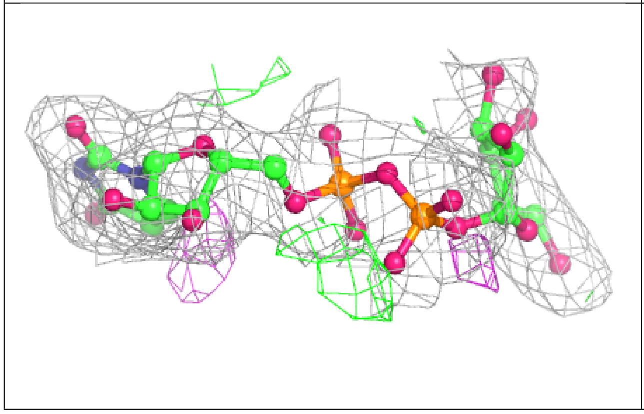


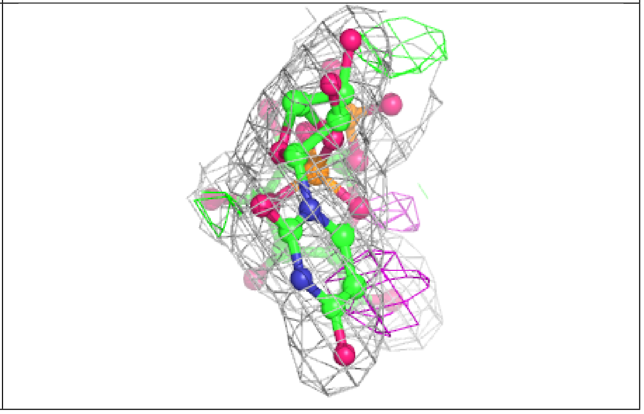


Electron density around GDU B 802:

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

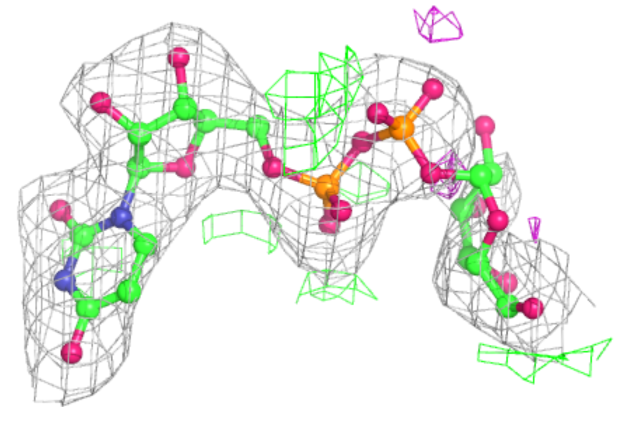


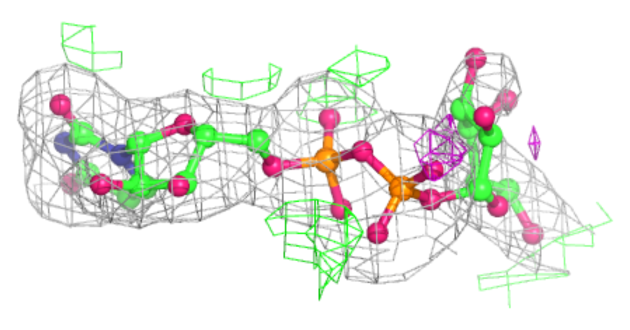


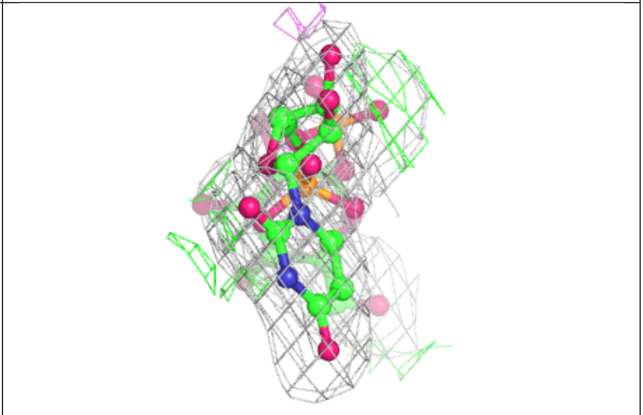


Electron density around GDU C 802:

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







Electron density around FDA G 600:

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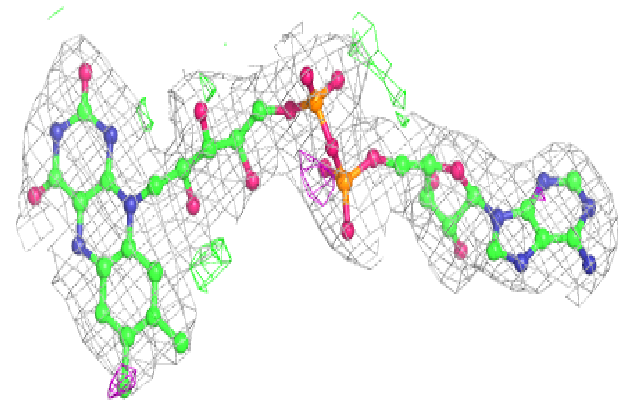
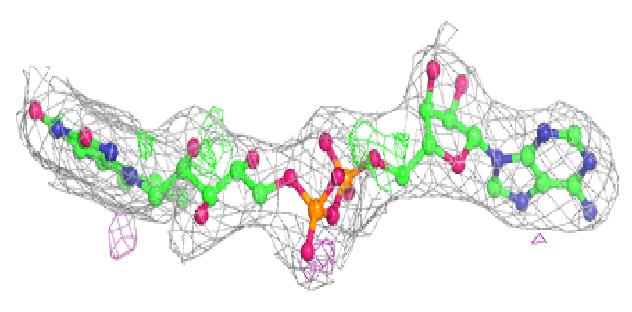
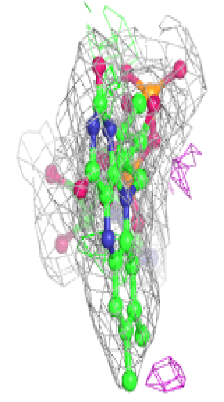
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around GDU D 802:

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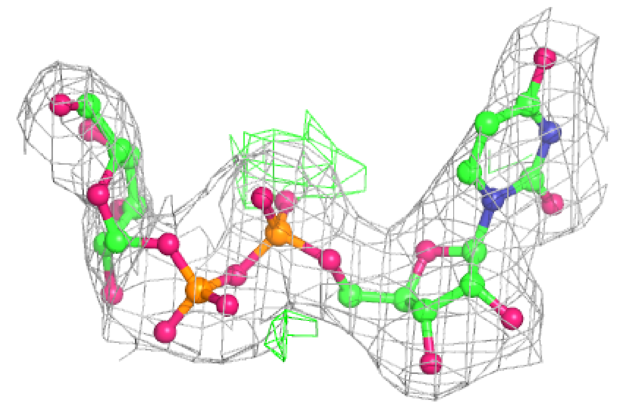
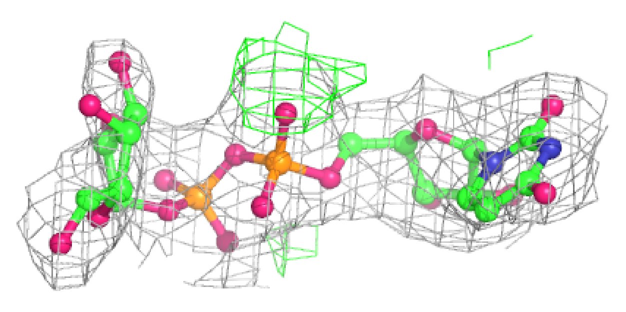
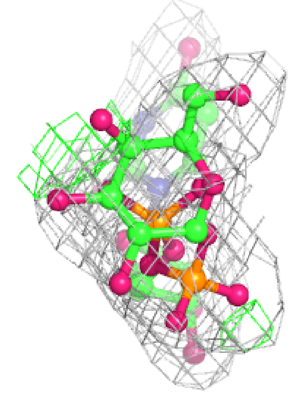
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

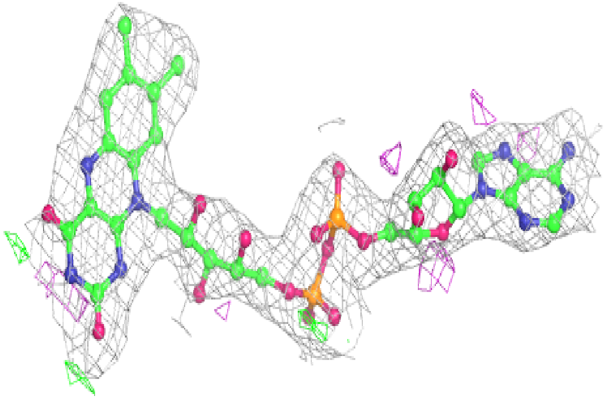


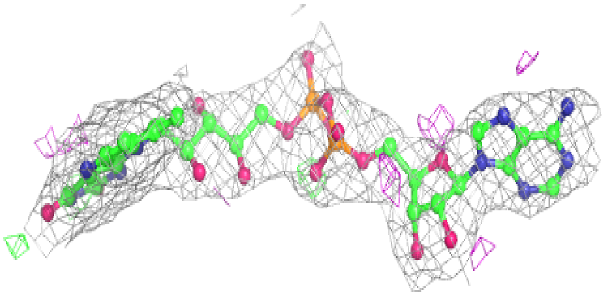


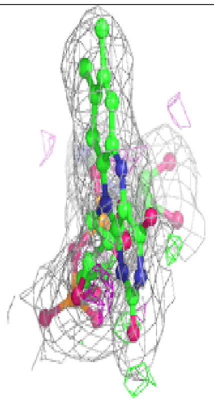


Electron density around FDA H 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

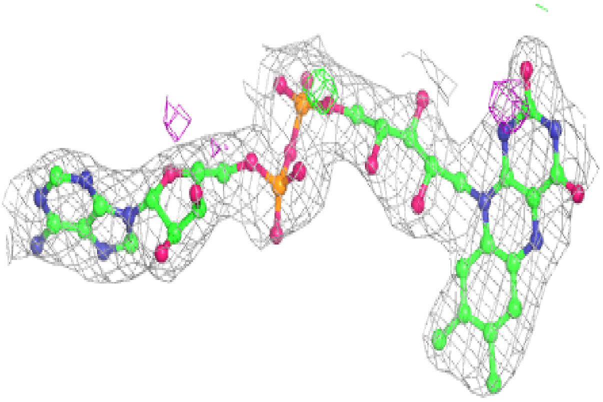


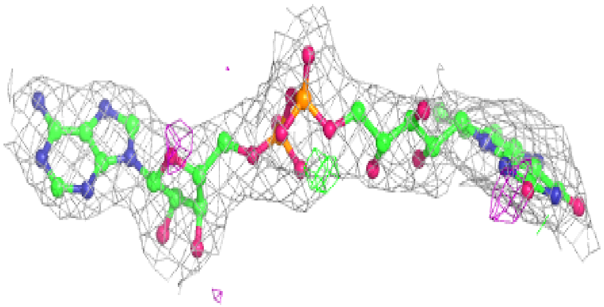


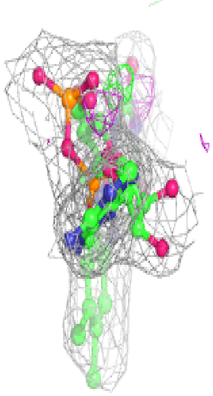


Electron density around FDA E 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

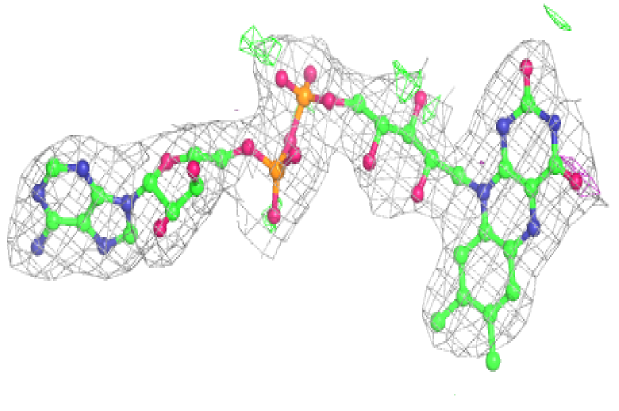


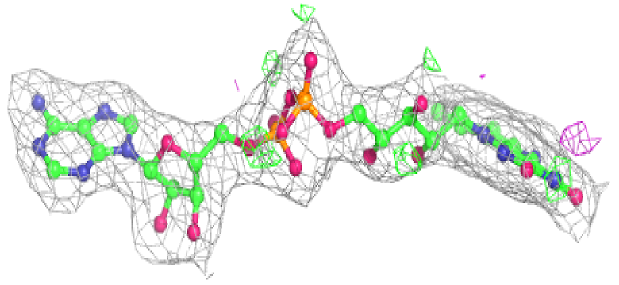


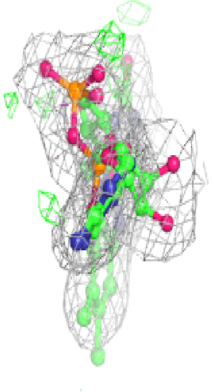


Electron density around FDA F 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

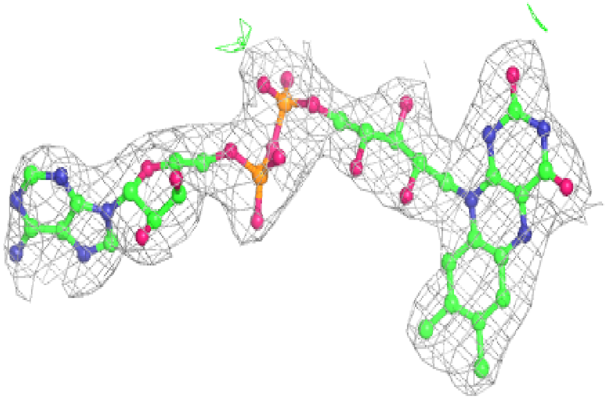


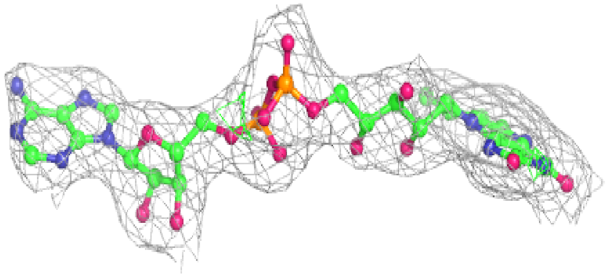


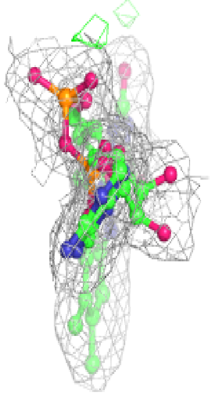


Electron density around FDA D 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

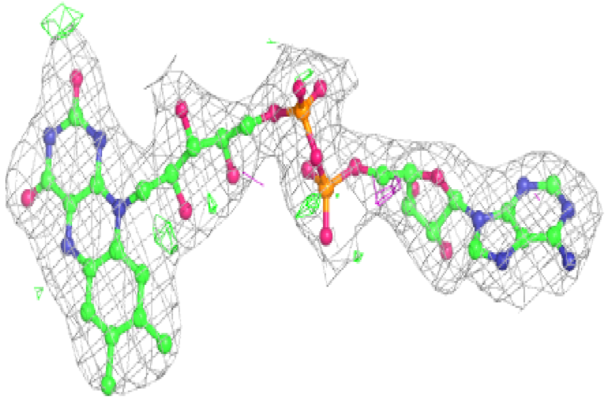


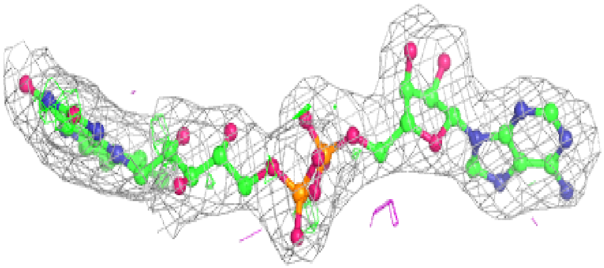


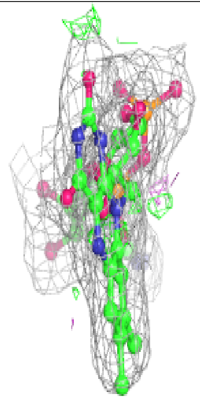


Electron density around FDA B 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

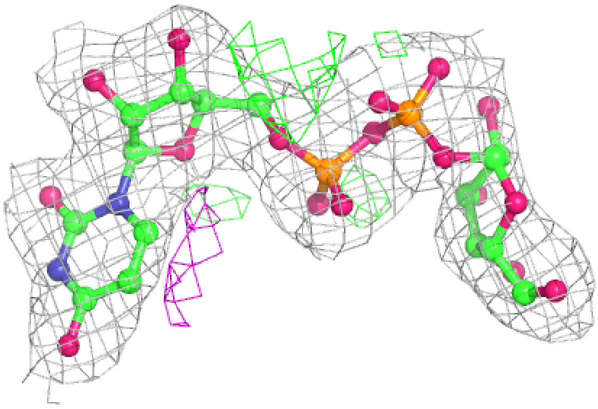


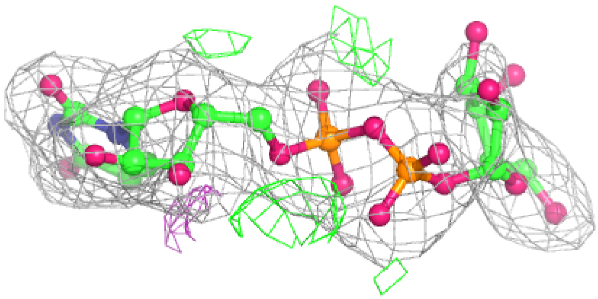


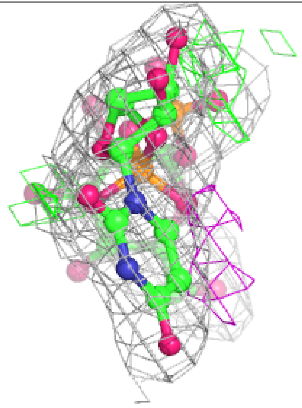


Electron density around GDU A 802:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

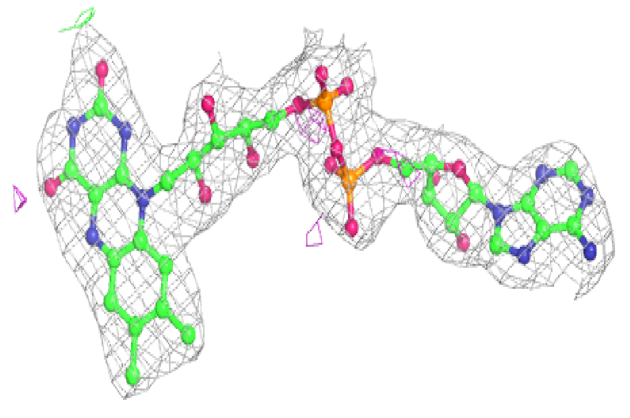


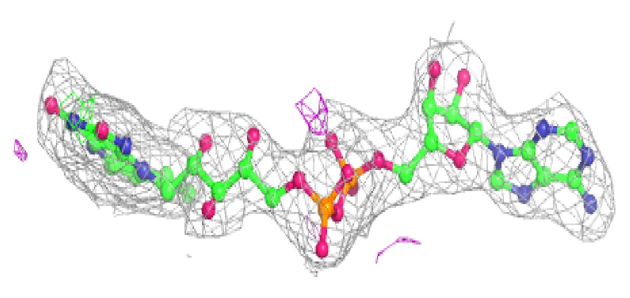


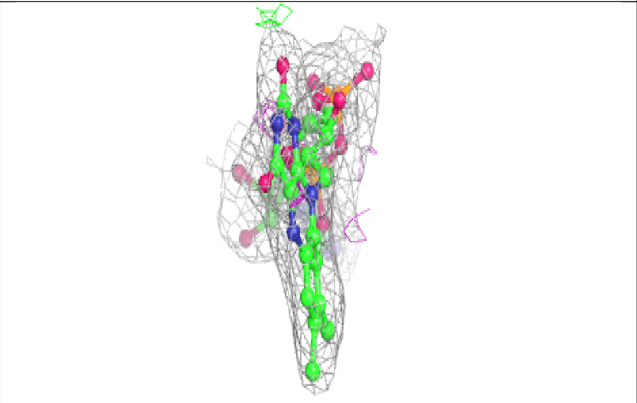


Electron density around FDA C 600:

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

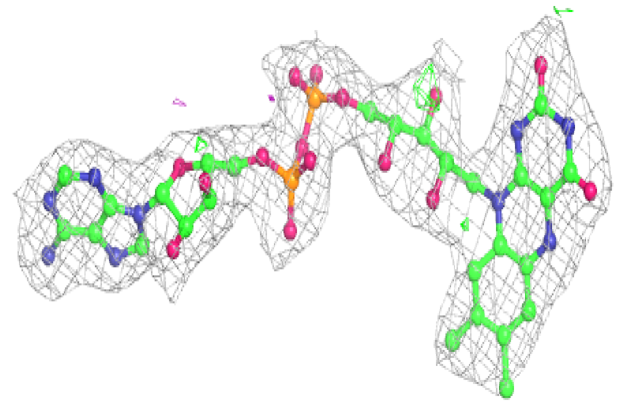


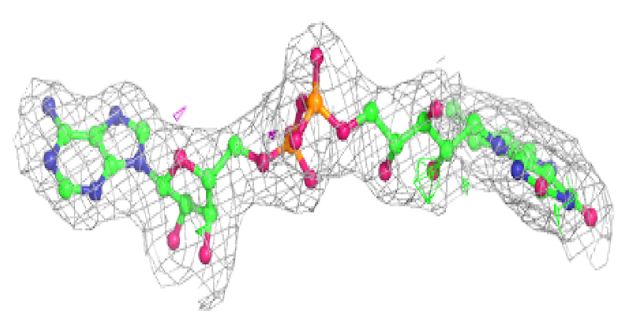


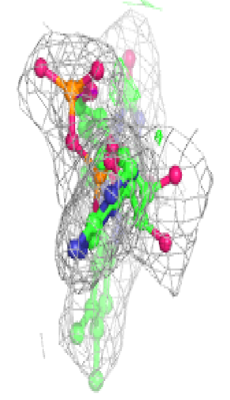


Electron density around FDA A 600:

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







6.5 Other polymers ⓘ

There are no such residues in this entry.