Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 06:07 PM JST

PDB ID	:	5H3T
Title	:	m7G cap bound to GEMIN5-WD
Authors	:	Bharath, S.R.; Tang, X.; Song, H.
Deposited on	:	2016-10-27
Resolution	:	2.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

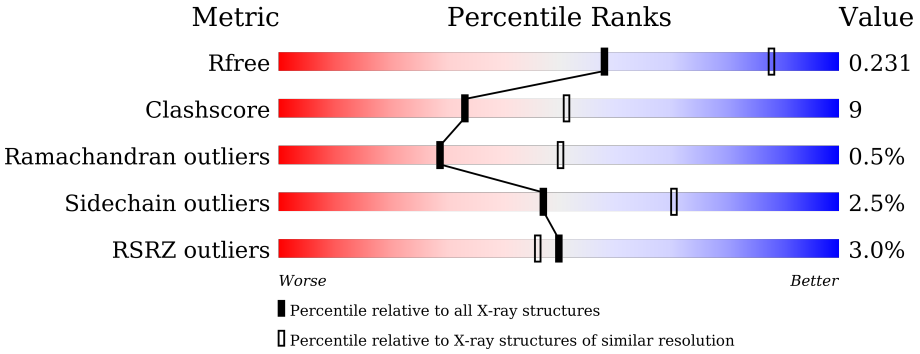
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	740	5% 69% 17% • 12%
1	B	740	.% 73% 15% 12%
1	C	740	2% 69% 19% • 11%
1	D	740	3% 70% 18% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	802	-	-	-	X

2 Entry composition (i)

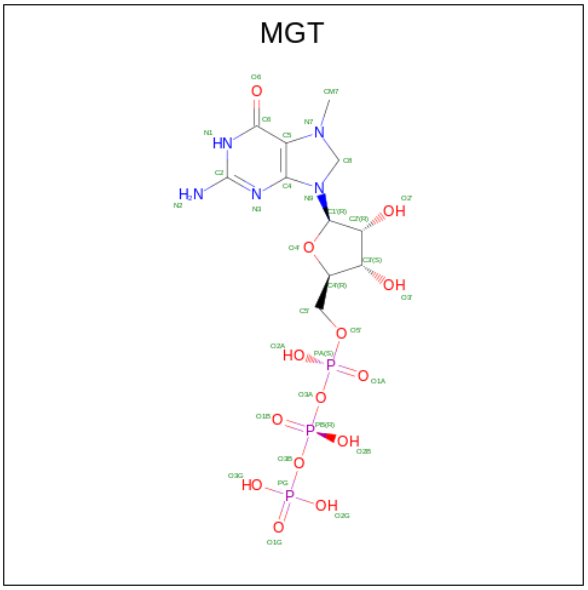
There are 4 unique types of molecules in this entry. The entry contains 20448 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Gem-associated protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	652	5026	3205	867	928	26	0	0	0
1	B	652	5042	3213	869	934	26	0	0	0
1	C	657	5072	3233	877	935	27	0	0	0
1	D	657	5050	3217	871	936	26	0	0	0

- Molecule 2 is 7N-METHYL-8-HYDROGUANOSINE-5'-TRIPHOSPHATE (three-letter code: MGT) (formula: $C_{11}H_{20}N_5O_{14}P_3$).



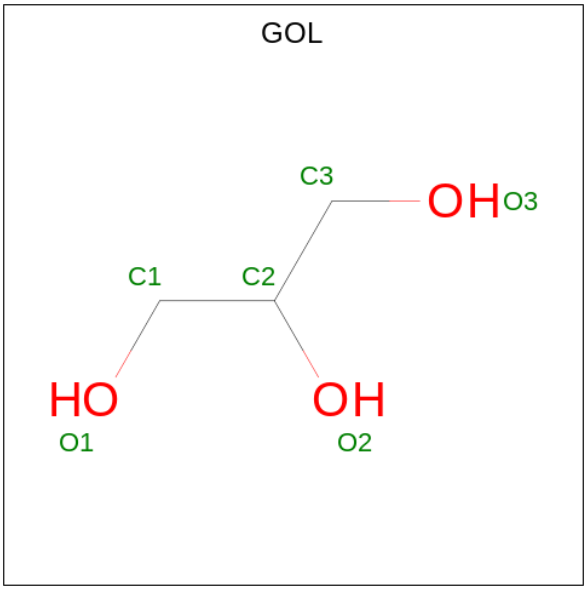
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	33	11	5	14	3	0	0
2	B	1	33	11	5	14	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	33	11	5	14	3	0	0
2	D	1	33	11	5	14	3	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
3	B	1	6	3	3	0	0

- Molecule 4 is water.

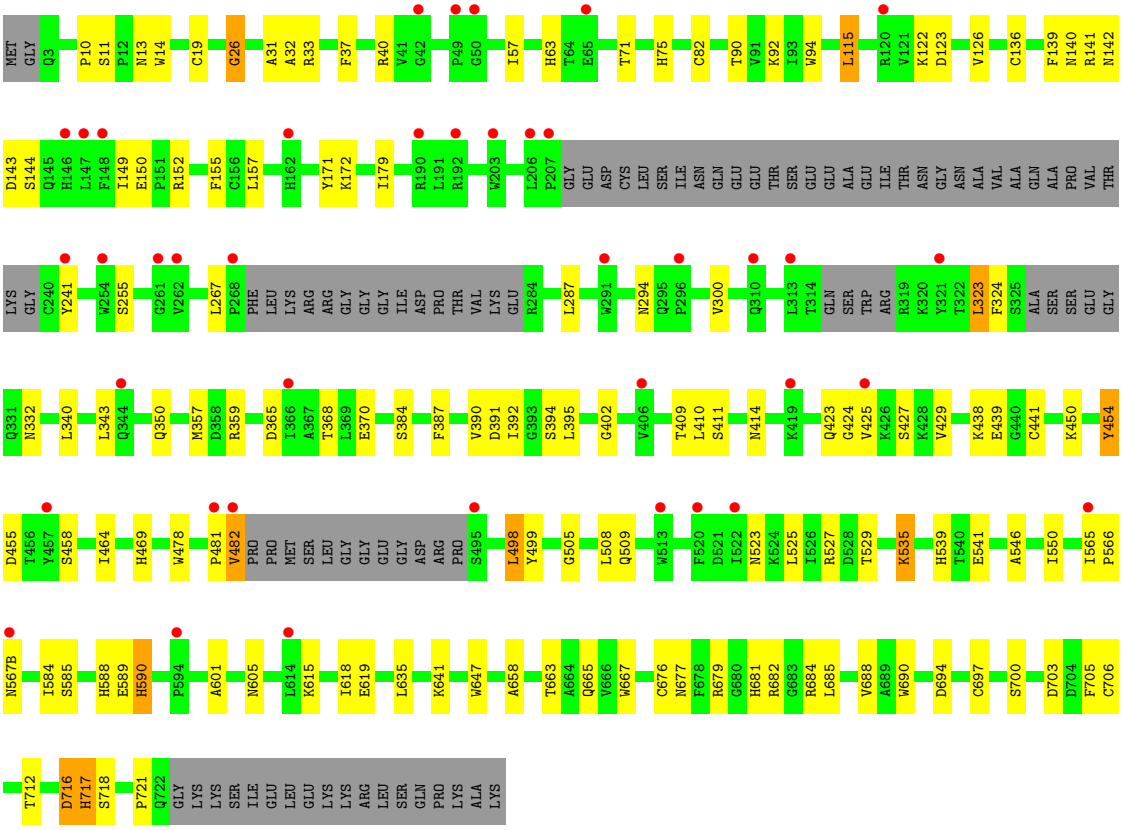
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	9	9	9	0	0
4	B	26	26	26	0	0
4	C	54	54	54	0	0
4	D	25	25	25	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

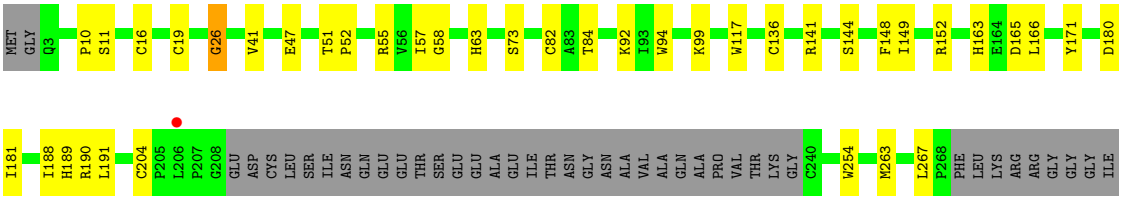
• Molecule 1: Gem-associated protein 5

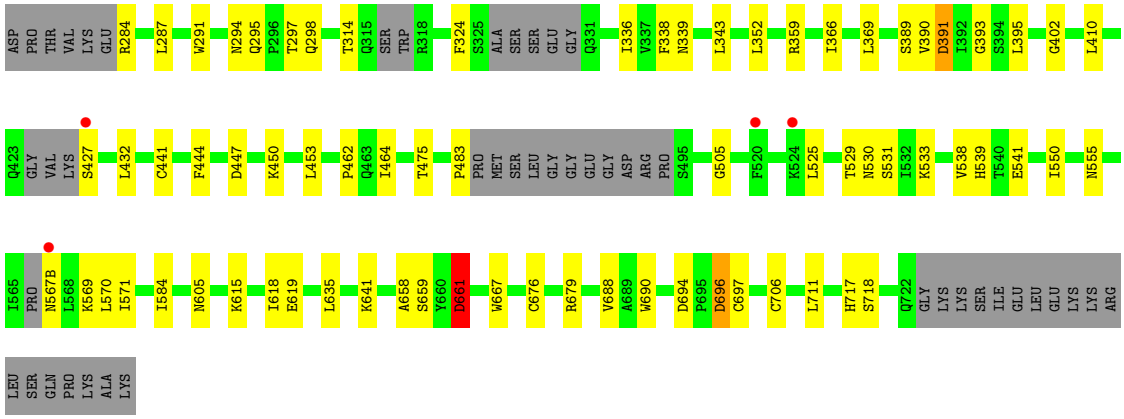
Chain A:



• Molecule 1: Gem-associated protein 5

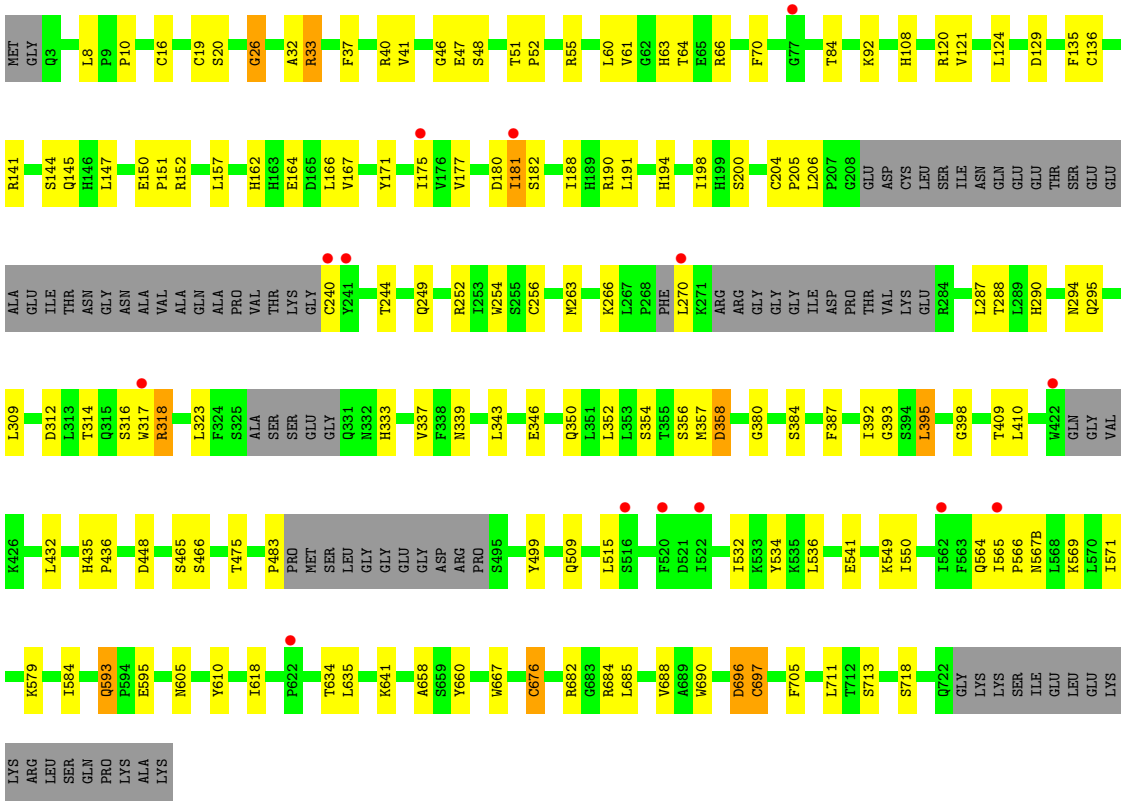
Chain B:





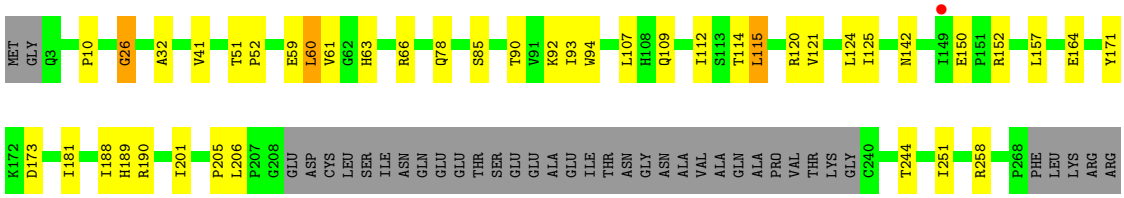
• Molecule 1: Gem-associated protein 5

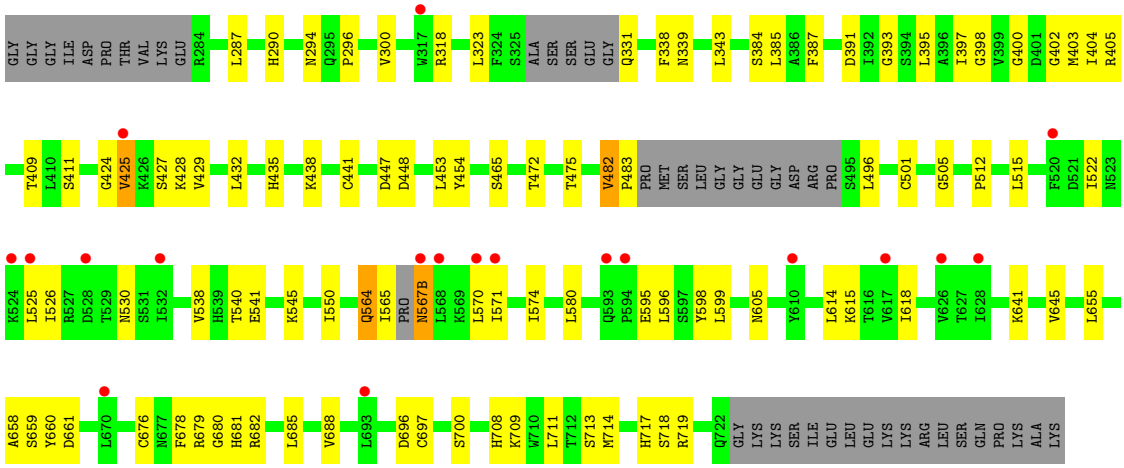
Chain C:



• Molecule 1: Gem-associated protein 5

Chain D:




GLY
GLY
GLY
ILE
ASP
PRO
THR
VAL
LYS
GLU
R284
L287
H290
N294
Q295
P296
V300
W317
R318
L323
F324
S325
ALA
SER
SER
GLU
GLY
Q331
F338
N339
L343
S384
L385
A386
F387
D391
I392
G393
S394
L395
A396
I397
G398
V399
G400
D401
G402
M403
I404
R405
T409
L410
S411
G424
V425
K426
S427
K428
V429
L432
H435
K438
C441
D447
D448
L453
Y454
S465
T472
T475
V482
P483
PRO
MET
SER
LEU
GLY
GLY
GLU
GLY
ASP
ARG
PRO
S495
L496
C501
G505
P512
L515
F520
D521
I522
N523
K524
L525
I526
R527
D528
T529
N530
S531
T532
V538
H539
T540
E541
K545
I550
Q564
I565
PRO
N567B
L568
K569
L570
I571
I574
L580
Q593
P594
E595
L596
S597
Y598
L599
N605
Y610
L614
K615
T616
V617
I618
V626
T627
I628
K641
V645
L655
A658
S659
Y660
D661
L670
C676
N677
F678
R679
G680
H681
R682
L685
V688
L693
D696
C697
S700
H708
K709
W710
L711
T712
S713
M714
H717
S718
R719
Q722
GLY
LYS
LYS
SER
ILE
GLU
LEU
GLU
LYS
LYS
ARG
LEU
SER
GLN
PRO
LYS
ALA
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	113.16Å 91.01Å 153.72Å 90.00° 100.59° 90.00°	Depositor
Resolution (Å)	49.33 – 2.57 49.33 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.33-2.57) 97.8 (49.33-2.57)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.58Å)	Xtriage
Refinement program	PHENIX (dev_2386: ???)	Depositor
R, R_{free}	0.171 , 0.228 0.178 , 0.231	Depositor DCC
R_{free} test set	4808 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 74.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20448	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4853e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.39	0/5171	0.57	0/7061
1	B	0.48	1/5185 (0.0%)	0.65	0/7076
1	C	0.51	1/5217 (0.0%)	0.69	4/7122 (0.1%)
1	D	0.43	0/5196	0.61	1/7099 (0.0%)
All	All	0.45	2/20769 (0.0%)	0.63	5/28358 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	697	CYS	CB-SG	-5.87	1.72	1.81
1	B	52	PRO	C-N	-5.52	1.23	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	157	LEU	CA-CB-CG	5.24	127.34	115.30
1	C	157	LEU	CA-CB-CG	5.20	127.26	115.30
1	C	392	ILE	C-N-CA	-5.16	111.47	122.30
1	C	252	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	358	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5026	0	4807	90	0
1	B	5042	0	4828	72	0
1	C	5072	0	4861	94	0
1	D	5050	0	4805	88	0
2	A	33	0	16	1	0
2	B	33	0	16	0	0
2	C	33	0	16	0	0
2	D	33	0	16	0	0
3	A	6	0	8	3	0
3	B	6	0	8	2	0
4	A	9	0	0	0	0
4	B	26	0	0	0	0
4	C	54	0	0	6	0
4	D	25	0	0	2	0
All	All	20448	0	19381	342	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (342) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ASP:OD2	1:A:458:SER:HB3	1.51	1.10
1:A:717:HIS:HB3	3:A:802:GOL:H2	1.44	0.98
1:A:13:ASN:HD21	1:A:33:ARG:H	1.21	0.89
1:D:530:ASN:HD21	1:D:570:LEU:H	1.25	0.85
1:B:530:ASN:HD21	1:B:569:LYS:HA	1.44	0.83
1:A:529:THR:HG21	1:A:567(B):ASN:HB3	1.62	0.81
1:A:482:VAL:H	1:A:509:GLN:HE22	1.32	0.78
1:B:539:HIS:HA	1:B:555:ASN:HD22	1.50	0.77
1:D:26:GLY:HA2	1:D:343:LEU:HD21	1.65	0.77
1:B:84:THR:CG2	1:B:94:TRP:HE1	1.99	0.76
1:B:149:ILE:HD13	1:B:149:ILE:N	2.03	0.74
1:B:84:THR:HG22	1:B:94:TRP:HE1	1.53	0.73
1:C:393:GLY:O	1:C:409:THR:HB	1.89	0.72
1:A:717:HIS:N	1:A:717:HIS:CD2	2.56	0.72
1:C:150:GLU:HG2	1:C:152:ARG:HH11	1.54	0.72
1:C:333:HIS:HE1	1:C:354:SER:OG	1.73	0.71
1:C:317:TRP:O	1:C:318:ARG:CB	2.39	0.70
1:A:75:HIS:CE1	1:A:122:LYS:HA	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLU:HG3	1:C:151:PRO:HD2	1.73	0.69
1:D:540:THR:HG21	1:D:580:LEU:HG	1.75	0.68
1:B:148:PHE:C	1:B:149:ILE:HD13	2.14	0.68
1:C:565:ILE:HG23	1:C:566:PRO:HD3	1.76	0.67
1:A:368:THR:HG23	1:A:370:GLU:H	1.60	0.67
1:D:152:ARG:HB2	1:D:171:TYR:CD1	2.29	0.67
1:A:535:LYS:H	1:A:535:LYS:HD2	1.58	0.67
1:D:598:TYR:CD2	1:D:615:LYS:HA	2.29	0.67
1:C:26:GLY:HA2	1:C:343:LEU:HD21	1.77	0.66
1:B:165:ASP:HB3	1:B:180:ASP:OD1	1.95	0.66
1:B:297:THR:HG23	1:B:314:THR:HG23	1.78	0.66
1:D:402:GLY:HA2	1:D:427:SER:O	1.96	0.66
1:A:565:ILE:HG23	1:A:566:PRO:HD3	1.77	0.66
1:C:177:VAL:HG12	1:C:190:ARG:HG3	1.79	0.65
1:C:150:GLU:HG2	1:C:152:ARG:NH1	2.12	0.65
1:B:63:HIS:NE2	1:B:84:THR:HG23	2.12	0.64
1:B:676:CYS:HA	1:B:718:SER:HA	1.80	0.64
1:D:482:VAL:N	1:D:483:PRO:CD	2.61	0.63
1:B:550:ILE:HG13	1:B:618:ILE:HD13	1.79	0.63
1:A:676:CYS:HA	1:A:718:SER:HA	1.81	0.63
1:A:679:ARG:CZ	1:A:717:HIS:ND1	2.62	0.63
1:D:645:VAL:HG13	1:D:655:LEU:HD11	1.81	0.63
1:A:411:SER:CB	1:A:414:ASN:O	2.47	0.62
1:A:391:ASP:HB3	1:A:394:SER:HB2	1.83	0.61
1:A:550:ILE:HG13	1:A:618:ILE:HD13	1.83	0.61
1:C:191:LEU:HD13	1:C:254:TRP:CG	2.35	0.61
1:A:681:HIS:NE2	1:A:700:SER:HB3	2.16	0.60
1:B:483:PRO:HB2	1:B:525:LEU:HD13	1.82	0.60
1:A:365:ASP:HB3	1:A:368:THR:HG22	1.83	0.60
1:B:352:LEU:HB2	1:B:366:ILE:HD11	1.83	0.59
1:A:26:GLY:HA2	1:A:343:LEU:HD21	1.83	0.59
1:B:26:GLY:HA2	1:B:343:LEU:HD21	1.83	0.59
1:C:46:GLY:O	1:C:55:ARG:NH2	2.34	0.59
1:B:297:THR:HG22	1:B:298:GLN:HE21	1.68	0.59
1:D:188:ILE:HG22	1:D:189:HIS:CD2	2.38	0.58
1:A:409:THR:O	1:A:410:LEU:HD23	2.04	0.58
1:A:482:VAL:H	1:A:509:GLN:NE2	2.01	0.58
1:B:530:ASN:ND2	1:B:570:LEU:H	2.01	0.58
1:A:152:ARG:HB2	1:A:171:TYR:CD1	2.38	0.57
1:A:324:PHE:O	1:A:332:ASN:ND2	2.37	0.57
1:A:90:THR:CG2	1:A:92:LYS:HG3	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ARG:HG2	1:B:336:ILE:HD13	1.86	0.57
1:B:605:ASN:HA	1:B:641:LYS:HB2	1.86	0.57
1:B:190:ARG:HH11	1:B:190:ARG:HB3	1.70	0.57
1:B:717:HIS:ND1	3:B:802:GOL:O2	2.26	0.56
1:C:164:GLU:O	1:C:164:GLU:HG2	2.04	0.56
1:C:194:HIS:CE1	1:C:244:THR:HG22	2.39	0.56
1:D:90:THR:CG2	1:D:92:LYS:HG3	2.36	0.56
1:D:115:LEU:HD12	1:D:115:LEU:O	2.06	0.56
1:D:676:CYS:HA	1:D:718:SER:HA	1.86	0.56
1:C:48:SER:O	1:C:51:THR:OG1	2.22	0.56
1:A:482:VAL:HG22	1:A:499:TYR:OH	2.06	0.56
1:A:424:GLY:O	1:A:450:LYS:NZ	2.39	0.55
1:D:331:GLN:N	4:D:901:HOH:O	2.39	0.55
1:D:90:THR:HG21	1:D:92:LYS:NZ	2.21	0.55
1:A:665:GLN:HE22	1:A:677:ASN:HB2	1.71	0.55
1:C:19:CYS:H	1:C:339:ASN:HD21	1.55	0.55
1:C:108:HIS:ND1	1:C:129:ASP:HB3	2.22	0.55
1:D:150:GLU:CD	1:D:190:ARG:HH12	2.10	0.55
1:D:596:LEU:O	1:D:599:LEU:HD12	2.07	0.55
1:D:121:VAL:CG2	1:D:124:LEU:HB3	2.36	0.55
1:C:26:GLY:HA3	1:C:41:VAL:O	2.07	0.55
1:A:19:CYS:HB2	1:A:31:ALA:HB3	1.89	0.54
1:B:26:GLY:HA3	1:B:41:VAL:O	2.07	0.54
1:C:333:HIS:CE1	1:C:354:SER:OG	2.59	0.54
1:B:541:GLU:HG2	1:B:584:ILE:HG13	1.89	0.54
1:A:149:ILE:HG12	1:A:179:ILE:HG21	1.90	0.54
3:A:802:GOL:O2	1:D:717:HIS:ND1	2.37	0.54
1:C:66:ARG:HD2	4:C:946:HOH:O	2.07	0.54
1:C:166:LEU:HD22	1:C:188:ILE:HD12	1.90	0.53
1:A:33:ARG:HD2	1:A:705:PHE:CG	2.44	0.53
1:A:63:HIS:CE1	1:A:92:LYS:HE2	2.43	0.53
1:D:605:ASN:HA	1:D:641:LYS:HB2	1.91	0.53
1:D:681:HIS:CE1	1:D:708:HIS:HD2	2.26	0.53
1:D:121:VAL:HG23	1:D:124:LEU:HB3	1.91	0.53
1:A:142:ASN:O	1:A:143:ASP:OD1	2.27	0.52
1:A:716:ASP:HB2	1:A:717:HIS:CD2	2.44	0.52
1:B:58:GLY:HA3	1:B:99:LYS:HE3	1.90	0.52
1:C:152:ARG:CZ	1:C:175:ILE:HD12	2.39	0.52
1:D:26:GLY:HA3	1:D:41:VAL:O	2.10	0.52
1:C:290:HIS:HE1	4:C:952:HOH:O	1.91	0.52
1:A:679:ARG:NH1	1:A:721:PRO:HG3	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:549:LYS:HA	1:C:565:ILE:HB	1.90	0.52
1:D:201:ILE:HG12	1:D:244:THR:HG22	1.91	0.52
1:D:679:ARG:NH2	1:D:719:ARG:O	2.43	0.52
1:B:569:LYS:HE2	1:B:571:ILE:HG22	1.90	0.52
1:C:194:HIS:CE1	1:C:244:THR:CG2	2.92	0.52
1:C:200:SER:OG	1:C:288:THR:HA	2.08	0.52
1:C:249:GLN:HE21	1:C:266:LYS:NZ	2.07	0.52
1:C:52:PRO:HB2	4:C:937:HOH:O	2.10	0.52
1:C:181:ILE:O	1:C:181:ILE:HG13	2.07	0.52
1:D:465:SER:HA	1:D:515:LEU:O	2.09	0.52
1:A:10:PRO:HD2	1:A:37:PHE:CE1	2.45	0.52
1:B:462:PRO:HG2	1:B:464:ILE:HD11	1.90	0.52
1:B:533:LYS:HE2	1:D:142:ASN:OD1	2.09	0.52
1:C:47:GLU:HA	1:C:47:GLU:OE1	2.10	0.52
1:C:658:ALA:HB1	1:C:685:LEU:HB3	1.92	0.52
1:D:711:LEU:HD12	1:D:714:MET:SD	2.50	0.51
1:A:390:VAL:HG11	1:A:439:GLU:HB3	1.91	0.51
1:D:574:ILE:HD11	1:D:614:LEU:HD21	1.92	0.51
1:B:136:CYS:O	1:B:144:SER:HA	2.10	0.51
1:D:522:ILE:O	1:D:526:ILE:HG13	2.11	0.50
1:A:150:GLU:OE1	1:A:152:ARG:HD2	2.11	0.50
1:A:71:THR:HG22	1:A:115:LEU:HD13	1.92	0.50
1:A:155:PHE:CE1	1:A:172:LYS:HG3	2.45	0.50
1:C:10:PRO:HB2	1:C:32:ALA:HB1	1.93	0.50
1:A:665:GLN:HE21	1:A:677:ASN:HD22	1.58	0.50
1:B:450:LYS:HD2	1:B:464:ILE:HG12	1.93	0.50
1:C:380:GLY:HA2	1:C:705:PHE:CE2	2.47	0.50
1:A:665:GLN:NE2	1:A:677:ASN:HD22	2.10	0.50
1:B:635:LEU:HD13	1:B:667:TRP:CG	2.46	0.50
1:B:84:THR:HG21	1:B:94:TRP:HE1	1.76	0.50
1:C:641:LYS:HD3	1:C:660:TYR:CE2	2.47	0.49
1:D:120:ARG:HB3	1:D:164:GLU:HG3	1.93	0.49
1:C:52:PRO:HG2	4:C:918:HOH:O	2.11	0.49
1:A:10:PRO:HD3	1:A:706:CYS:SG	2.52	0.49
1:D:435:HIS:CE1	1:D:438:LYS:HG2	2.47	0.49
1:B:267:LEU:HD11	1:B:287:LEU:HD22	1.94	0.49
1:B:539:HIS:HA	1:B:555:ASN:ND2	2.23	0.49
1:A:14:TRP:CE3	1:A:357:MET:HE2	2.47	0.49
1:B:441:CYS:SG	1:B:453:LEU:HD11	2.53	0.49
1:C:635:LEU:HD13	1:C:667:TRP:CG	2.47	0.49
1:A:365:ASP:HB3	1:A:368:THR:CG2	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ASN:O	1:A:527:ARG:HG3	2.12	0.49
1:A:565:ILE:HG23	1:A:566:PRO:CD	2.43	0.49
1:C:346:GLU:O	1:C:346:GLU:OE2	2.30	0.49
1:D:596:LEU:HA	1:D:599:LEU:HD12	1.95	0.49
1:A:267:LEU:HD11	1:A:287:LEU:HD22	1.95	0.49
1:A:450:LYS:HG3	1:A:464:ILE:HG23	1.95	0.49
1:A:40:ARG:HB2	1:A:57:ILE:HD13	1.95	0.48
1:D:475:THR:HG23	1:D:501:CYS:HB3	1.95	0.48
1:C:61:VAL:HG21	1:C:682:ARG:HD2	1.96	0.48
1:D:63:HIS:CE1	1:D:92:LYS:HD2	2.48	0.48
1:A:601:ALA:HB2	1:A:647:TRP:CZ2	2.49	0.48
1:C:566:PRO:HD2	4:C:944:HOH:O	2.14	0.48
1:A:505:GLY:HA2	1:A:539:HIS:O	2.13	0.48
1:A:717:HIS:N	1:A:717:HIS:HD2	2.08	0.48
1:B:694:ASP:HB3	1:B:697:CYS:HB3	1.96	0.48
1:C:152:ARG:HB2	1:C:171:TYR:CD2	2.49	0.48
1:A:11:SER:OG	1:A:359:ARG:HD3	2.14	0.48
1:A:402:GLY:HA2	1:A:427:SER:O	2.14	0.48
1:B:659:SER:OG	1:B:661:ASP:HB2	2.13	0.48
1:C:180:ASP:C	1:C:182:SER:H	2.17	0.48
1:A:126:VAL:HG12	1:A:157:LEU:HD11	1.95	0.48
1:D:424:GLY:O	1:D:425:VAL:C	2.52	0.48
1:C:333:HIS:HD2	1:C:358:ASP:OD2	1.96	0.48
1:A:679:ARG:CZ	1:A:721:PRO:HG3	2.43	0.47
1:D:545:LYS:HB2	1:D:550:ILE:HB	1.96	0.47
1:D:641:LYS:HD3	1:D:660:TYR:CD2	2.49	0.47
1:D:678:PHE:CZ	1:D:680:GLY:HA3	2.48	0.47
1:A:300:VAL:HG12	1:A:340:LEU:HD13	1.96	0.47
1:D:59:GLU:HG2	1:D:61:VAL:HG23	1.96	0.47
1:D:400:GLY:O	1:D:428:LYS:HG2	2.13	0.47
1:C:63:HIS:CE1	1:C:92:LYS:HG3	2.48	0.47
1:B:659:SER:CB	1:B:661:ASP:HB2	2.45	0.47
1:A:658:ALA:HB1	1:A:685:LEU:HB3	1.96	0.47
1:C:198:ILE:HG23	1:C:244:THR:HG23	1.96	0.47
1:D:90:THR:HG21	1:D:92:LYS:HG3	1.97	0.47
1:D:696:ASP:OD2	1:D:713:SER:OG	2.26	0.47
1:A:294:ASN:ND2	1:A:350:GLN:HG3	2.30	0.47
1:D:51:THR:HG23	1:D:52:PRO:HD2	1.95	0.47
1:D:403:MET:HB2	1:D:405:ARG:NH1	2.30	0.47
1:B:163:HIS:HB3	1:B:166:LEU:HG	1.97	0.47
1:C:61:VAL:HG11	1:C:682:ARG:HD3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:GLY:O	1:C:40:ARG:HD3	2.15	0.47
1:D:404:ILE:HG13	1:D:429:VAL:HG21	1.97	0.47
1:C:610:TYR:CD1	1:C:634:THR:HG22	2.49	0.46
1:D:505:GLY:HA3	1:D:538:VAL:HG13	1.96	0.46
1:A:679:ARG:HH22	3:A:802:GOL:H12	1.79	0.46
1:D:393:GLY:O	1:D:409:THR:HB	2.15	0.46
1:D:688:VAL:HG12	1:D:700:SER:HB3	1.98	0.46
1:A:694:ASP:HB3	1:A:697:CYS:HB3	1.97	0.46
1:B:659:SER:HB3	1:B:661:ASP:HB2	1.96	0.46
1:B:338:PHE:C	1:B:339:ASN:HD22	2.19	0.46
1:C:249:GLN:HE21	1:C:266:LYS:HZ3	1.62	0.46
1:C:205:PRO:O	1:C:206:LEU:HD23	2.15	0.46
1:D:398:GLY:N	1:D:432:LEU:HD11	2.31	0.46
1:D:447:ASP:HA	1:D:472:THR:HG23	1.98	0.46
1:B:73:SER:HB2	1:B:117:TRP:CE2	2.51	0.46
1:B:402:GLY:HA2	1:B:427:SER:O	2.16	0.46
1:D:205:PRO:O	1:D:206:LEU:HD23	2.16	0.46
1:B:16:CYS:HB2	1:B:19:CYS:SG	2.55	0.46
1:B:63:HIS:CE1	1:B:92:LYS:HE2	2.51	0.46
1:B:152:ARG:HB2	1:B:171:TYR:CD1	2.51	0.46
1:B:188:ILE:HG22	1:B:189:HIS:CD2	2.50	0.46
1:C:136:CYS:O	1:C:144:SER:HA	2.16	0.46
1:C:337:VAL:HG22	1:C:356:SER:HB2	1.98	0.46
1:D:152:ARG:HD3	1:D:173:ASP:OD2	2.16	0.46
1:D:120:ARG:HE	1:D:120:ARG:HA	1.81	0.46
1:D:387:PHE:CE1	1:D:395:LEU:HB2	2.51	0.46
1:B:190:ARG:HB3	1:B:190:ARG:NH1	2.30	0.45
1:A:635:LEU:HD13	1:A:667:TRP:CG	2.51	0.45
1:B:10:PRO:HD3	1:B:706:CYS:SG	2.56	0.45
1:B:204:CYS:HB2	1:B:291:TRP:CH2	2.51	0.45
1:C:263:MET:HE3	1:C:316:SER:HA	1.96	0.45
1:D:596:LEU:HA	1:D:599:LEU:CD1	2.45	0.45
1:A:615:LYS:HE2	1:A:619:GLU:OE1	2.16	0.45
1:A:658:ALA:HB2	1:A:688:VAL:HG13	1.97	0.45
1:C:483:PRO:HG2	1:C:567(B):ASN:OD1	2.16	0.45
1:C:593:GLN:HE22	1:C:595:GLU:CB	2.29	0.45
1:A:241:TYR:HD1	1:A:255:SER:HA	1.82	0.45
1:A:541:GLU:HG2	1:A:584:ILE:HG13	1.97	0.45
1:B:390:VAL:HG13	1:B:391:ASP:H	1.82	0.45
1:C:145:GLN:HG2	1:C:147:LEU:CD1	2.47	0.45
1:D:385:LEU:HD23	1:D:397:ILE:HG12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:ILE:O	1:D:567(B):ASN:N	2.49	0.45
1:A:478:TRP:CH2	1:A:498:LEU:HG	2.52	0.45
1:B:432:LEU:HD23	1:B:444:PHE:HB3	1.98	0.45
1:B:615:LYS:NZ	1:B:619:GLU:OE1	2.48	0.45
1:C:534:TYR:CE1	1:C:536:LEU:HD23	2.52	0.45
1:B:47:GLU:HG3	1:B:51:THR:HB	1.99	0.45
1:B:55:ARG:O	1:B:57:ILE:HG23	2.17	0.45
1:A:605:ASN:HA	1:A:641:LYS:HB2	1.97	0.44
1:C:410:LEU:HD23	1:C:410:LEU:HA	1.72	0.44
1:C:532:ILE:HG23	1:C:534:TYR:CE2	2.52	0.44
1:D:482:VAL:N	1:D:483:PRO:HD3	2.31	0.44
1:A:425:VAL:HG11	1:A:429:VAL:HG22	2.00	0.44
1:A:481:PRO:HA	1:A:509:GLN:NE2	2.31	0.44
1:C:16:CYS:HB2	1:C:19:CYS:SG	2.58	0.44
1:A:438:LYS:HG2	1:A:441:CYS:HB2	2.00	0.44
1:B:529:THR:HG22	1:B:530:ASN:ND2	2.33	0.44
1:D:598:TYR:CG	1:D:615:LYS:HB2	2.52	0.44
1:C:33:ARG:HD2	1:C:705:PHE:CD1	2.53	0.44
1:C:162:HIS:HE1	1:C:204:CYS:O	2.01	0.44
1:D:251:ILE:HG13	1:D:287:LEU:HD21	1.99	0.44
1:D:496:LEU:O	1:D:512:PRO:HG3	2.18	0.44
1:D:658:ALA:HB1	1:D:685:LEU:HB3	1.99	0.44
1:D:697:CYS:SG	1:D:709:LYS:HG3	2.58	0.44
1:A:90:THR:HG21	1:A:92:LYS:HG3	1.99	0.44
1:C:579:LYS:HB3	1:C:605:ASN:HB2	2.00	0.44
1:D:290:HIS:HB3	1:D:300:VAL:HG22	2.00	0.44
1:A:63:HIS:ND1	1:A:92:LYS:HE2	2.33	0.44
1:D:564:GLN:HB3	1:D:571:ILE:HD13	2.00	0.44
1:A:717:HIS:CD2	1:A:717:HIS:H	2.34	0.43
1:B:505:GLY:HA2	1:B:539:HIS:O	2.18	0.43
1:A:663:THR:HG21	1:A:721:PRO:CD	2.48	0.43
1:B:427:SER:HB2	1:B:447:ASP:OD1	2.19	0.43
1:C:658:ALA:HB2	1:C:688:VAL:HG13	2.00	0.43
1:D:530:ASN:ND2	1:D:570:LEU:H	2.04	0.43
1:C:515:LEU:HD23	1:C:515:LEU:HA	1.82	0.43
1:C:676:CYS:HA	1:C:718:SER:HA	1.99	0.43
1:B:11:SER:OG	1:B:359:ARG:HD3	2.18	0.43
1:B:324:PHE:CZ	1:B:369:LEU:HD22	2.54	0.43
1:C:141:ARG:HH21	1:C:141:ARG:HG2	1.84	0.43
1:D:441:CYS:SG	1:D:453:LEU:HD11	2.59	0.43
1:D:614:LEU:O	1:D:618:ILE:HG13	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:LYS:HE2	1:C:571:ILE:HG22	2.01	0.43
1:D:435:HIS:HB2	1:D:441:CYS:HB3	2.00	0.43
1:B:533:LYS:HD2	1:D:107:LEU:HD21	2.01	0.43
1:C:398:GLY:N	1:C:432:LEU:HD11	2.34	0.43
1:C:541:GLU:HG2	1:C:584:ILE:HG13	2.01	0.43
1:C:696:ASP:O	1:C:711:LEU:HA	2.19	0.43
1:C:290:HIS:HD2	4:C:954:HOH:O	2.01	0.43
1:C:435:HIS:CG	1:C:436:PRO:HD2	2.54	0.43
1:C:499:TYR:CE2	1:C:509:GLN:HG3	2.54	0.43
1:C:191:LEU:HD13	1:C:254:TRP:CD2	2.54	0.43
1:D:59:GLU:OE1	1:D:682:ARG:HD3	2.19	0.42
1:B:63:HIS:NE2	1:B:84:THR:CG2	2.80	0.42
1:D:93:ILE:HD11	1:D:125:ILE:HG13	2.01	0.42
1:D:338:PHE:C	1:D:339:ASN:HD22	2.23	0.42
1:B:141:ARG:H	1:B:141:ARG:HG3	1.66	0.42
1:A:10:PRO:HB2	1:A:32:ALA:HB1	2.00	0.42
1:B:191:LEU:HB3	1:B:254:TRP:CE3	2.54	0.42
1:B:393:GLY:HA3	1:B:410:LEU:HG	2.01	0.42
1:D:60:LEU:HG	1:D:94:TRP:CD2	2.54	0.42
1:A:123:ASP:OD2	1:A:140:ASN:HB2	2.20	0.42
1:B:505:GLY:HA3	1:B:538:VAL:HG13	2.01	0.42
1:C:294:ASN:HB3	1:C:295:GLN:HG3	2.01	0.42
1:C:697:CYS:HA	1:C:711:LEU:HD23	2.02	0.42
1:A:469:HIS:NE2	1:A:508:LEU:HD12	2.34	0.42
1:C:70:PHE:HD1	1:C:84:THR:HG22	1.84	0.42
1:C:240:CYS:O	1:C:256:CYS:HB2	2.20	0.42
1:C:312:ASP:OD1	1:C:314:THR:HB	2.20	0.42
1:D:181:ILE:HD13	1:D:181:ILE:HA	1.80	0.42
1:A:387:PHE:CE1	1:A:395:LEU:HB2	2.55	0.42
1:B:658:ALA:HB2	1:B:688:VAL:HG13	2.01	0.42
1:C:120:ARG:HA	1:C:120:ARG:HD2	1.85	0.42
1:C:387:PHE:CZ	1:C:395:LEU:HG	2.55	0.42
1:C:696:ASP:OD2	1:C:713:SER:HB3	2.19	0.42
1:D:52:PRO:HB2	4:D:922:HOH:O	2.19	0.42
1:A:546:ALA:HB3	1:A:589:GLU:HG3	2.02	0.41
1:B:82:CYS:SG	1:B:94:TRP:HB2	2.60	0.41
1:A:423:GLN:O	1:A:454:TYR:OH	2.29	0.41
1:C:536:LEU:HD23	1:C:536:LEU:HA	1.90	0.41
1:D:596:LEU:HD23	1:D:599:LEU:HD11	2.01	0.41
1:B:696:ASP:O	1:B:711:LEU:HA	2.20	0.41
1:C:10:PRO:HD2	1:C:37:PHE:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:VAL:HB	1:C:124:LEU:HB3	2.02	0.41
1:D:641:LYS:HG2	1:D:660:TYR:HB2	2.02	0.41
1:A:123:ASP:HB2	1:A:139:PHE:CD1	2.56	0.41
1:C:333:HIS:CD2	1:C:358:ASP:OD2	2.74	0.41
1:D:120:ARG:HA	1:D:120:ARG:NE	2.36	0.41
1:A:525:LEU:HD12	1:A:529:THR:HG23	2.03	0.41
1:A:684:ARG:N	1:A:703:ASP:OD1	2.54	0.41
1:C:393:GLY:HA3	1:C:410:LEU:HG	2.02	0.41
1:D:85:SER:HB2	1:D:112:ILE:HG21	2.03	0.41
1:A:142:ASN:C	1:A:143:ASP:OD1	2.59	0.41
1:B:531:SER:HB2	1:D:109:GLN:NE2	2.36	0.41
1:C:108:HIS:CD2	1:C:135:PHE:HD2	2.39	0.41
1:A:323:LEU:HA	1:A:323:LEU:HD23	1.87	0.41
1:B:679:ARG:HH22	3:B:802:GOL:H11	1.86	0.41
1:C:8:LEU:HD23	1:C:8:LEU:HA	1.88	0.41
1:D:294:ASN:O	1:D:296:PRO:HD3	2.21	0.41
1:A:82:CYS:SG	1:A:94:TRP:HB2	2.61	0.41
1:C:63:HIS:CE1	1:C:92:LYS:HE2	2.56	0.41
1:C:352:LEU:HD12	1:C:352:LEU:HA	1.88	0.41
1:D:10:PRO:HB2	1:D:32:ALA:HB1	2.03	0.41
1:D:51:THR:O	1:D:52:PRO:C	2.58	0.41
1:B:181:ILE:HD13	1:B:181:ILE:HG21	1.83	0.41
1:C:270:LEU:HD11	1:C:309:LEU:HD21	2.02	0.41
1:D:475:THR:HG21	1:D:541:GLU:HA	2.03	0.41
1:D:482:VAL:O	1:D:525:LEU:HD22	2.20	0.41
1:D:659:SER:HB3	1:D:661:ASP:OD1	2.21	0.41
1:A:392:ILE:HD12	1:A:392:ILE:HA	1.79	0.40
1:A:588:HIS:ND1	1:A:590:HIS:HB2	2.37	0.40
1:B:295:GLN:OE1	1:B:298:GLN:HG3	2.20	0.40
1:C:564:GLN:HG3	1:C:565:ILE:H	1.86	0.40
1:A:676:CYS:SG	1:A:712:THR:HG23	2.60	0.40
2:A:801:MGT:H81	2:A:801:MGT:O5'	2.21	0.40
1:C:294:ASN:HD21	1:C:350:GLN:HG3	1.86	0.40
1:C:550:ILE:HG13	1:C:618:ILE:HD13	2.04	0.40
1:A:136:CYS:O	1:A:144:SER:HA	2.21	0.40
1:D:641:LYS:HD3	1:D:660:TYR:CE2	2.56	0.40
1:B:530:ASN:HD21	1:B:570:LEU:H	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	640/740 (86%)	598 (93%)	40 (6%)	2 (0%)	41	62
1	B	636/740 (86%)	607 (95%)	27 (4%)	2 (0%)	41	62
1	C	643/740 (87%)	602 (94%)	38 (6%)	3 (0%)	29	50
1	D	645/740 (87%)	609 (94%)	30 (5%)	6 (1%)	17	34
All	All	2564/2960 (87%)	2416 (94%)	135 (5%)	13 (0%)	29	50

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	GLY
1	B	26	GLY
1	B	661	ASP
1	C	26	GLY
1	C	318	ARG
1	D	318	ARG
1	A	590	HIS
1	C	357	MET
1	D	26	GLY
1	D	595	GLU
1	D	425	VAL
1	D	258	ARG
1	D	482	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	546/642 (85%)	533 (98%)	13 (2%)	49	72
1	B	551/642 (86%)	541 (98%)	10 (2%)	59	78
1	C	553/642 (86%)	534 (97%)	19 (3%)	37	60
1	D	547/642 (85%)	534 (98%)	13 (2%)	49	72
All	All	2197/2568 (86%)	2142 (98%)	55 (2%)	47	70

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	141	ARG
1	A	323	LEU
1	A	384	SER
1	A	454	TYR
1	A	482	VAL
1	A	498	LEU
1	A	535	LYS
1	A	585	SER
1	A	682	ARG
1	A	690	TRP
1	A	716	ASP
1	A	717	HIS
1	B	263	MET
1	B	294	ASN
1	B	389	SER
1	B	391	ASP
1	B	395	LEU
1	B	475	THR
1	B	567(B)	ASN
1	B	661	ASP
1	B	690	TRP
1	B	696	ASP
1	C	20	SER
1	C	33	ARG
1	C	60	LEU
1	C	64	THR
1	C	167	VAL
1	C	181	ILE
1	C	287	LEU
1	C	323	LEU
1	C	384	SER
1	C	395	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	448	ASP
1	C	465	SER
1	C	466	SER
1	C	475	THR
1	C	593	GLN
1	C	676	CYS
1	C	684	ARG
1	C	690	TRP
1	C	696	ASP
1	D	60	LEU
1	D	66	ARG
1	D	78	GLN
1	D	114	THR
1	D	115	LEU
1	D	323	LEU
1	D	384	SER
1	D	391	ASP
1	D	411	SER
1	D	448	ASP
1	D	454	TYR
1	D	564	GLN
1	D	567(B)	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	146	HIS
1	A	249	GLN
1	A	339	ASN
1	A	350	GLN
1	A	509	GLN
1	A	665	GLN
1	B	189	HIS
1	B	298	GLN
1	B	310	GLN
1	B	530	ASN
1	B	555	ASN
1	B	708	HIS
1	C	109	GLN
1	C	194	HIS
1	C	249	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	333	HIS
1	C	415	ASN
1	C	593	GLN
1	C	665	GLN
1	D	109	GLN
1	D	142	ASN
1	D	145	GLN
1	D	189	HIS
1	D	344	GLN
1	D	530	ASN
1	D	708	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	802	-	5,5,5	0.25	0	5,5,5	0.18	0
2	MGT	A	801	-	30,35,35	1.25	4 (13%)	42,56,56	2.41	11 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MGT	C	801	-	30,35,35	1.24	4 (13%)	42,56,56	2.38	11 (26%)
3	GOL	B	802	-	5,5,5	0.26	0	5,5,5	0.28	0
2	MGT	D	801	-	30,35,35	1.23	4 (13%)	42,56,56	2.40	11 (26%)
2	MGT	B	801	-	30,35,35	1.25	4 (13%)	42,56,56	2.40	11 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	802	-	-	3/4/4/4	-
2	MGT	A	801	-	-	6/22/50/50	0/3/3/3
2	MGT	C	801	-	-	3/22/50/50	0/3/3/3
3	GOL	B	802	-	-	2/4/4/4	-
2	MGT	D	801	-	-	1/22/50/50	0/3/3/3
2	MGT	B	801	-	-	4/22/50/50	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	MGT	C5-C4	2.95	1.47	1.38
2	B	801	MGT	C5-C4	2.94	1.47	1.38
2	C	801	MGT	C5-C4	2.93	1.47	1.38
2	D	801	MGT	C5-C4	2.91	1.47	1.38
2	C	801	MGT	C4-N9	-2.83	1.34	1.37
2	D	801	MGT	C4-N9	-2.81	1.34	1.37
2	B	801	MGT	C4-N9	-2.80	1.34	1.37
2	A	801	MGT	C4-N9	-2.72	1.34	1.37
2	B	801	MGT	C6-N1	-2.41	1.34	1.38
2	C	801	MGT	C6-N1	-2.39	1.34	1.38
2	A	801	MGT	C6-N1	-2.35	1.34	1.38
2	D	801	MGT	C6-N1	-2.30	1.34	1.38
2	A	801	MGT	C8-N9	2.28	1.47	1.46
2	C	801	MGT	C8-N9	2.24	1.47	1.46
2	B	801	MGT	C8-N9	2.21	1.47	1.46
2	D	801	MGT	C8-N9	2.11	1.47	1.46

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	MGT	N9-C4-N3	8.94	138.85	125.47
2	C	801	MGT	N9-C4-N3	8.85	138.71	125.47
2	B	801	MGT	N9-C4-N3	8.85	138.71	125.47
2	D	801	MGT	N9-C4-N3	8.84	138.69	125.47
2	A	801	MGT	C5-C4-N3	-5.57	117.51	128.13
2	C	801	MGT	C5-C4-N3	-5.53	117.60	128.13
2	B	801	MGT	C5-C4-N3	-5.51	117.62	128.13
2	D	801	MGT	C5-C4-N3	-5.51	117.64	128.13
2	C	801	MGT	N9-C8-N7	-5.07	96.12	103.38
2	B	801	MGT	N9-C8-N7	-5.04	96.17	103.38
2	D	801	MGT	N9-C8-N7	-5.00	96.22	103.38
2	A	801	MGT	N9-C8-N7	-5.00	96.22	103.38
2	C	801	MGT	C2-N3-C4	4.35	120.06	112.30
2	B	801	MGT	C2-N3-C4	4.35	120.05	112.30
2	A	801	MGT	C2-N3-C4	4.34	120.04	112.30
2	D	801	MGT	C2-N3-C4	4.32	120.00	112.30
2	B	801	MGT	PB-O3B-PG	-3.79	119.84	132.83
2	C	801	MGT	PB-O3B-PG	-3.77	119.89	132.83
2	A	801	MGT	PB-O3B-PG	-3.77	119.90	132.83
2	D	801	MGT	PB-O3B-PG	-3.67	120.22	132.83
2	A	801	MGT	PA-O3A-PB	-3.58	120.55	132.83
2	B	801	MGT	PA-O3A-PB	-3.55	120.64	132.83
2	D	801	MGT	PA-O3A-PB	-3.52	120.74	132.83
2	D	801	MGT	O4'-C1'-N9	3.42	113.96	109.30
2	B	801	MGT	O4'-C1'-N9	3.37	113.89	109.30
2	A	801	MGT	O4'-C1'-N9	3.34	113.85	109.30
2	C	801	MGT	O4'-C1'-N9	3.33	113.84	109.30
2	C	801	MGT	PA-O3A-PB	-3.25	121.67	132.83
2	B	801	MGT	C5-C6-N1	2.71	115.77	110.99
2	C	801	MGT	C5-C6-N1	2.71	115.77	110.99
2	D	801	MGT	C5-C6-N1	2.69	115.72	110.99
2	A	801	MGT	C5-C6-N1	2.67	115.70	110.99
2	D	801	MGT	C3'-C2'-C1'	2.39	105.97	101.43
2	A	801	MGT	C3'-C2'-C1'	2.33	105.86	101.43
2	B	801	MGT	C3'-C2'-C1'	2.27	105.73	101.43
2	B	801	MGT	O6-C6-C5	-2.23	122.07	127.54
2	C	801	MGT	C3'-C2'-C1'	2.22	105.65	101.43
2	C	801	MGT	O6-C6-C5	-2.20	122.13	127.54
2	D	801	MGT	O6-C6-C5	-2.20	122.14	127.54
2	A	801	MGT	O6-C6-C5	-2.20	122.15	127.54
2	A	801	MGT	C5-C4-N9	-2.08	103.65	106.35
2	D	801	MGT	C5-C4-N9	-2.06	103.67	106.35
2	B	801	MGT	C5-C4-N9	-2.06	103.67	106.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	MGT	C5-C4-N9	-2.05	103.69	106.35

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	MGT	C5'-O5'-PA-O1A
2	A	801	MGT	C5'-O5'-PA-O2A
2	C	801	MGT	PB-O3A-PA-O5'
2	C	801	MGT	C5'-O5'-PA-O3A
3	A	802	GOL	C1-C2-C3-O3
3	B	802	GOL	C1-C2-C3-O3
3	A	802	GOL	O1-C1-C2-C3
3	A	802	GOL	O2-C2-C3-O3
3	B	802	GOL	O2-C2-C3-O3
2	D	801	MGT	PB-O3A-PA-O5'
2	A	801	MGT	C5'-O5'-PA-O3A
2	A	801	MGT	PB-O3A-PA-O2A
2	C	801	MGT	C5'-O5'-PA-O1A
2	B	801	MGT	PB-O3B-PG-O1G
2	B	801	MGT	O4'-C4'-C5'-O5'
2	A	801	MGT	PB-O3B-PG-O2G
2	B	801	MGT	PB-O3B-PG-O3G
2	A	801	MGT	PB-O3A-PA-O1A
2	B	801	MGT	PB-O3A-PA-O2A

There are no ring outliers.

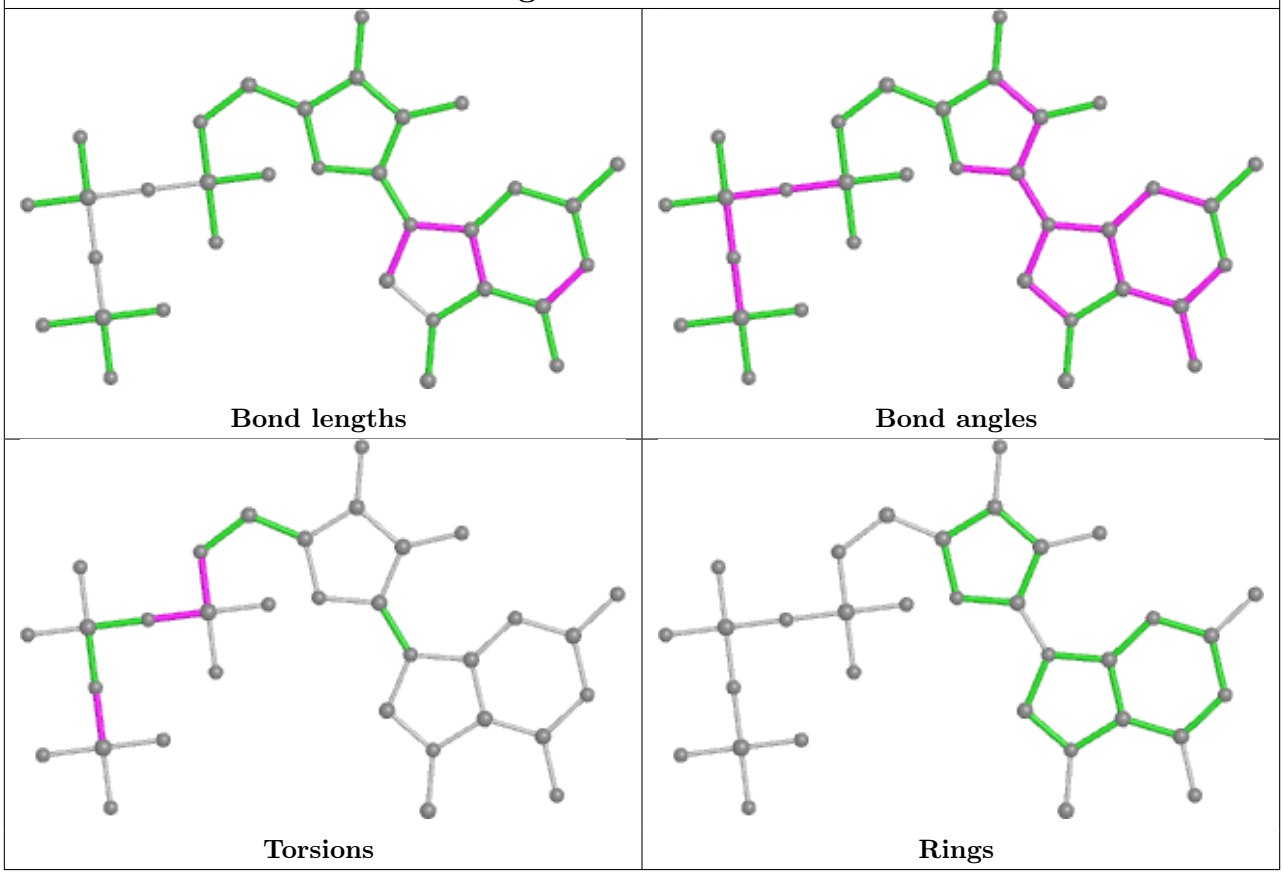
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	GOL	3	0
2	A	801	MGT	1	0
3	B	802	GOL	2	0

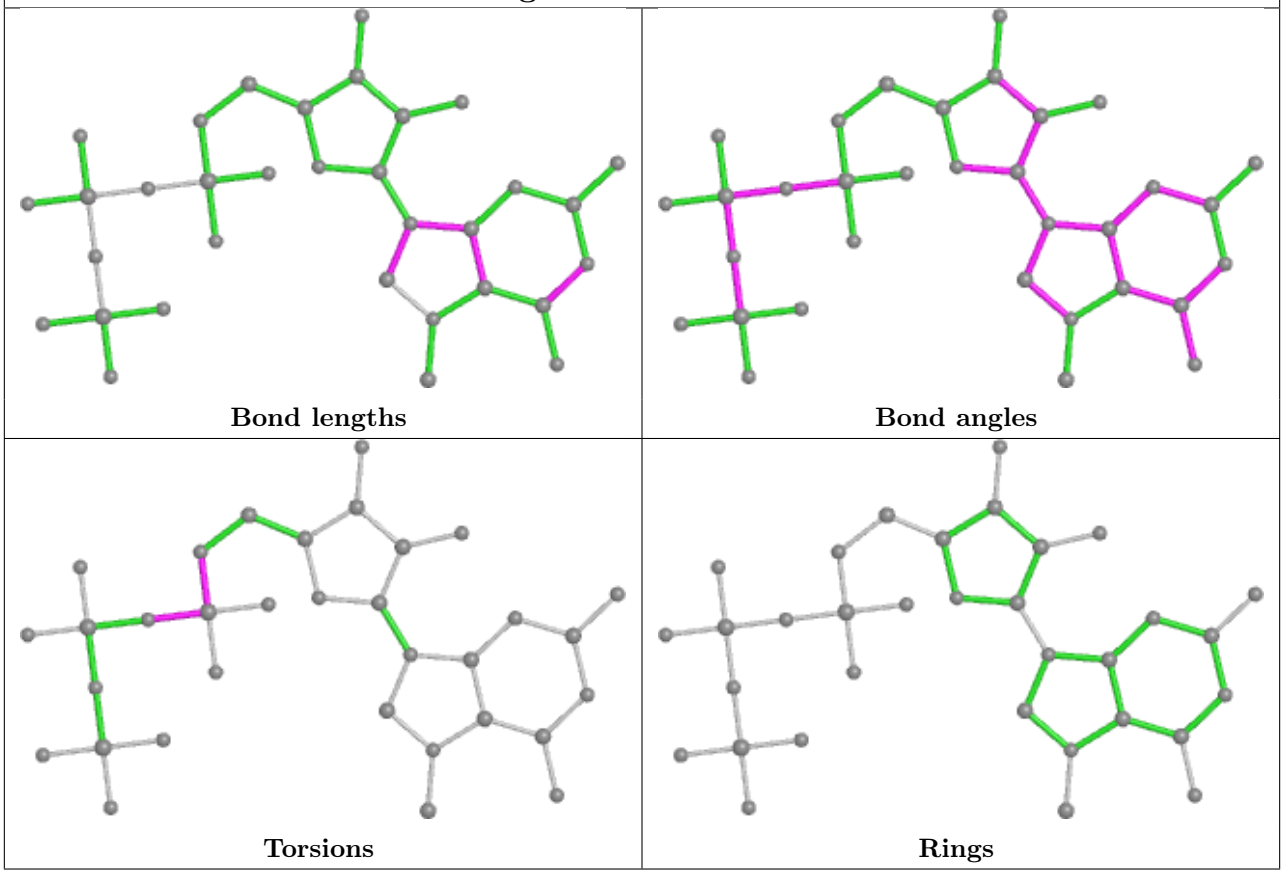
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

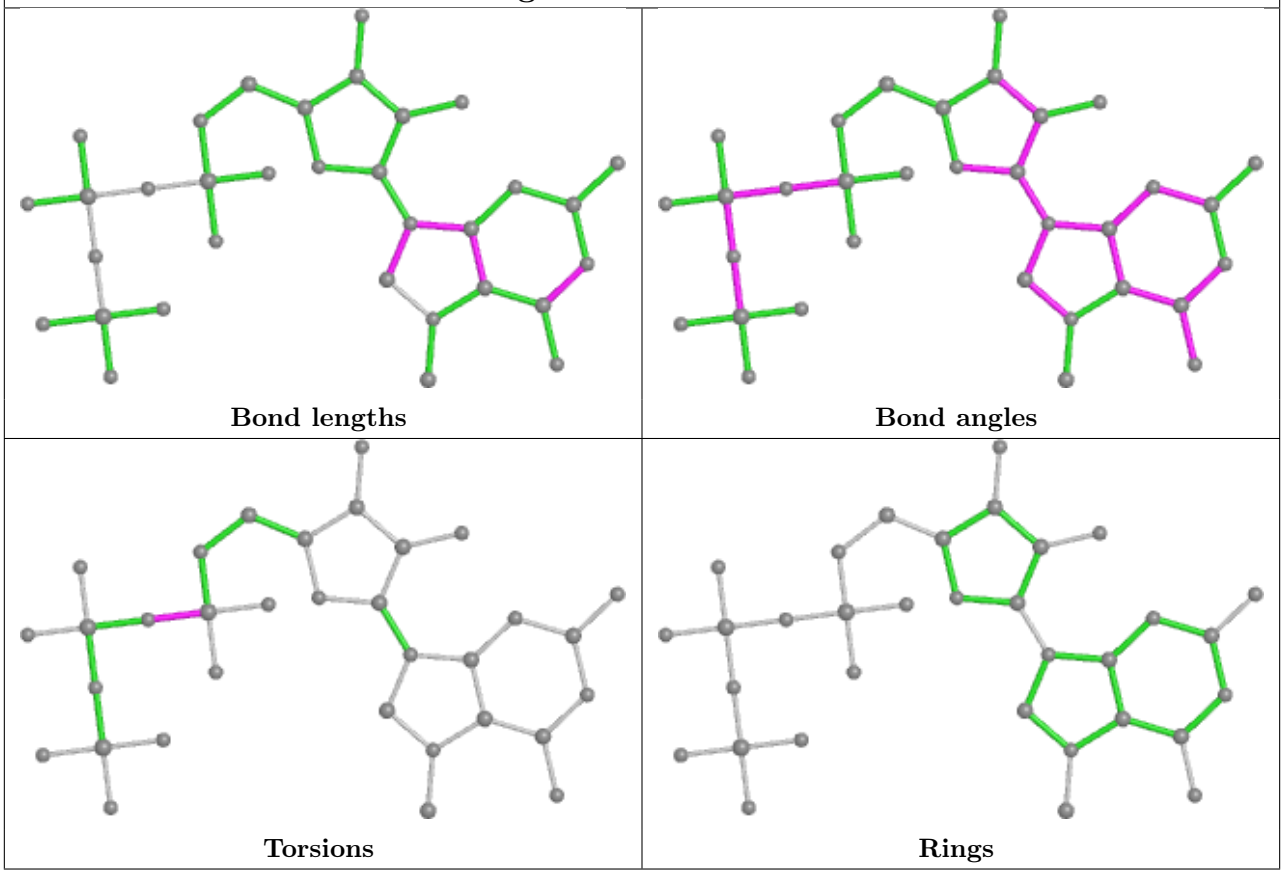
Ligand MGT A 801



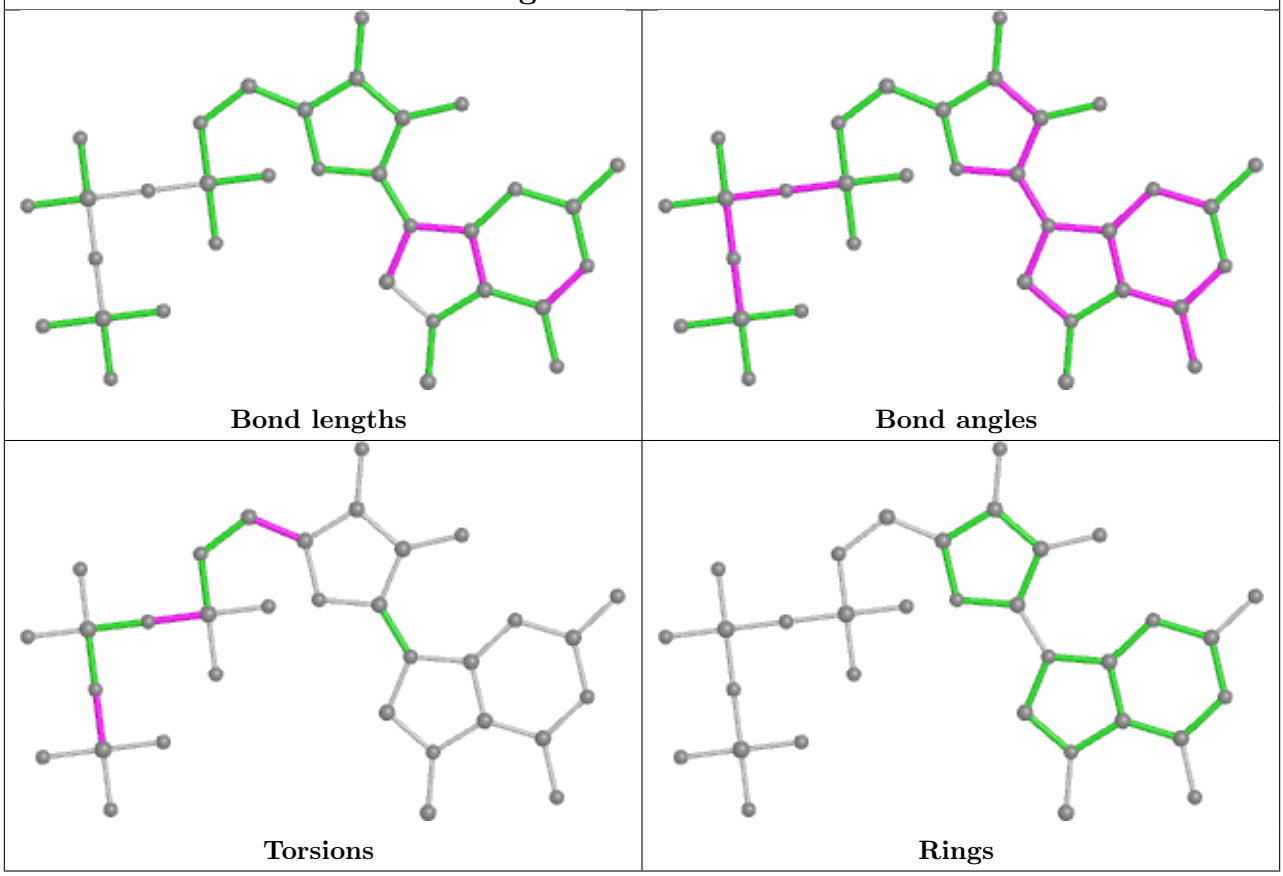
Ligand MGT C 801



Ligand MGT D 801



Ligand MGT B 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	652/740 (88%)	0.41	40 (6%)	21	17	52, 78, 114, 141	0
1	B	652/740 (88%)	0.13	5 (0%)	86	85	35, 55, 88, 118	0
1	C	657/740 (88%)	0.27	14 (2%)	63	60	29, 52, 94, 134	0
1	D	657/740 (88%)	0.26	20 (3%)	50	46	39, 63, 109, 158	0
All	All	2618/2960 (88%)	0.27	79 (3%)	50	46	29, 63, 106, 158	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	LEU	6.3
1	D	317	TRP	4.5
1	A	565	ILE	4.3
1	D	626	VAL	3.7
1	C	520	PHE	3.6
1	C	181	ILE	3.6
1	C	422	TRP	3.4
1	B	524	LYS	3.4
1	A	513	TRP	3.3
1	A	310	GLN	3.2
1	A	495	SER	3.2
1	D	149	ILE	3.2
1	D	525	LEU	3.1
1	A	203	TRP	2.9
1	D	528	ASP	2.9
1	A	520	PHE	2.9
1	D	693	LEU	2.8
1	A	49	PRO	2.8
1	A	291	TRP	2.8
1	A	262	VAL	2.7
1	A	296	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	482	VAL	2.7
1	D	670	LEU	2.6
1	A	207	PRO	2.6
1	A	254	TRP	2.6
1	A	192	ARG	2.6
1	A	162	HIS	2.6
1	B	206	LEU	2.6
1	C	565	ILE	2.6
1	D	570	LEU	2.6
1	D	568	LEU	2.5
1	C	317	TRP	2.5
1	A	594	PRO	2.5
1	A	65	GLU	2.5
1	A	457	TYR	2.5
1	D	520	PHE	2.5
1	C	516	SER	2.5
1	C	77	GLY	2.5
1	C	522	ILE	2.4
1	A	567(B)	ASN	2.4
1	A	366	ILE	2.4
1	C	175	ILE	2.4
1	D	628	ILE	2.4
1	C	622	PRO	2.4
1	A	614	LEU	2.4
1	A	425	VAL	2.4
1	D	532	ILE	2.4
1	A	313	LEU	2.3
1	D	571	ILE	2.3
1	A	481	PRO	2.3
1	A	419	LYS	2.3
1	B	567(B)	ASN	2.2
1	D	617	VAL	2.2
1	D	610	TYR	2.2
1	A	261	GLY	2.2
1	A	522	ILE	2.2
1	D	524	LYS	2.2
1	D	594	PRO	2.2
1	B	427	SER	2.2
1	D	425	VAL	2.2
1	B	520	PHE	2.2
1	A	146	HIS	2.2
1	A	50	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	321	TYR	2.2
1	A	42	GLY	2.1
1	C	562	ILE	2.1
1	A	120	ARG	2.1
1	A	241	TYR	2.1
1	D	593	GLN	2.1
1	A	148	PHE	2.1
1	A	147	LEU	2.1
1	C	270	LEU	2.1
1	C	241	TYR	2.1
1	C	240	CYS	2.1
1	A	190	ARG	2.0
1	A	268	PRO	2.0
1	A	406	VAL	2.0
1	A	344	GLN	2.0
1	D	567(B)	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

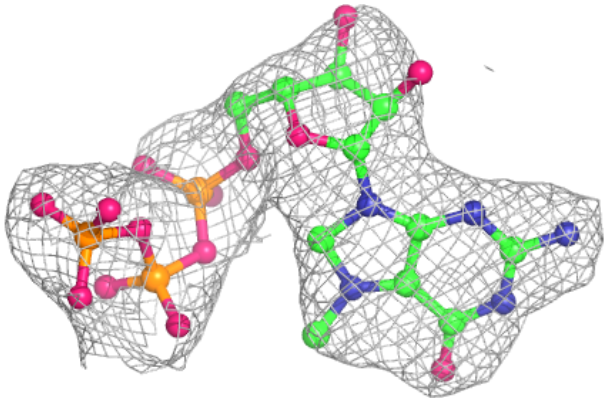
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

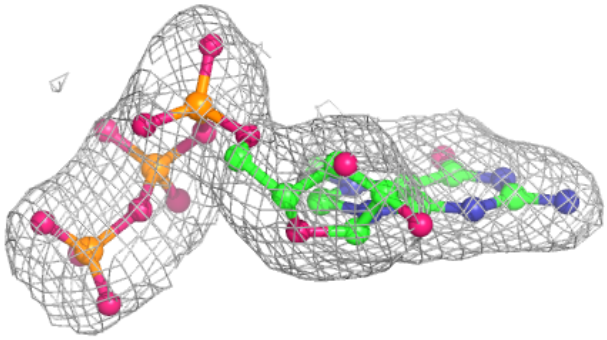
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	802	6/6	0.80	0.53	5,59,65,75	0
3	GOL	A	802	6/6	0.84	0.39	11,37,46,49	0
2	MGT	A	801	33/33	0.94	0.16	49,81,119,120	0
2	MGT	D	801	33/33	0.94	0.14	46,68,99,104	0
2	MGT	C	801	33/33	0.96	0.14	28,61,95,99	0
2	MGT	B	801	33/33	0.96	0.16	41,62,99,101	0

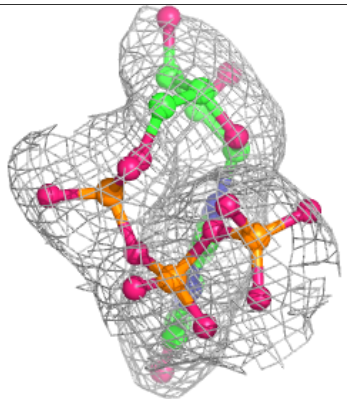
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGT A 801:

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

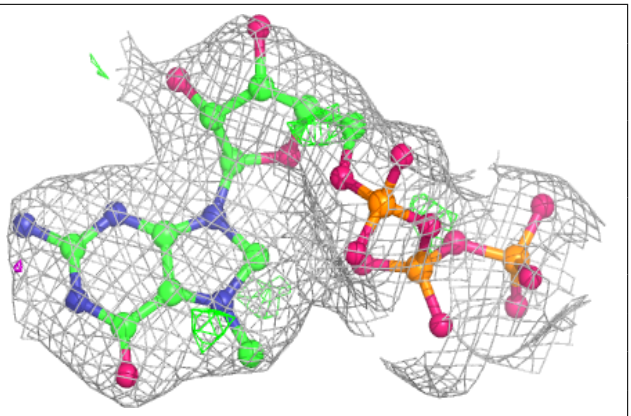


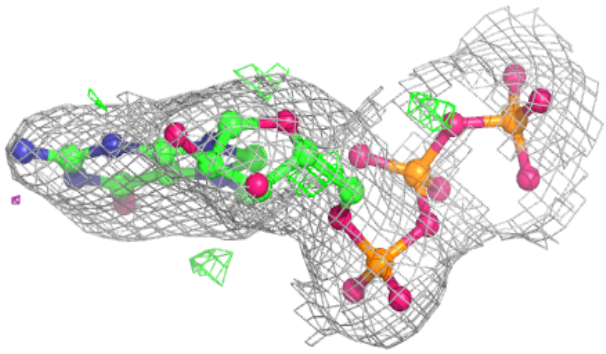


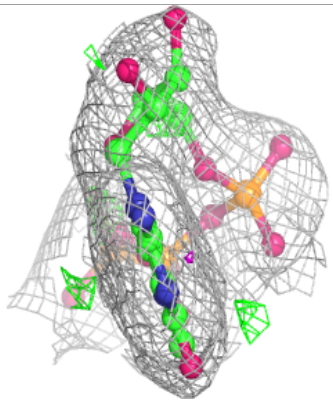


Electron density around MGT D 801:

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

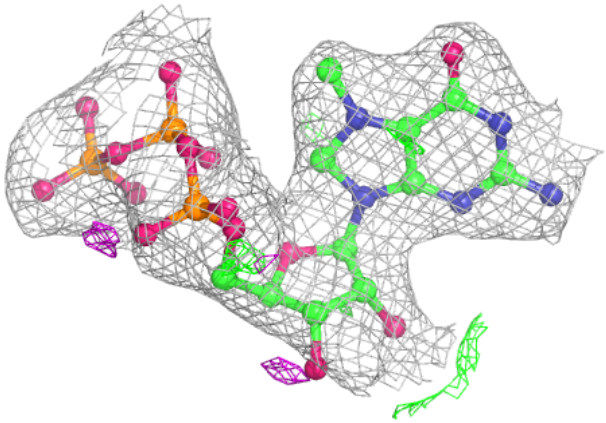


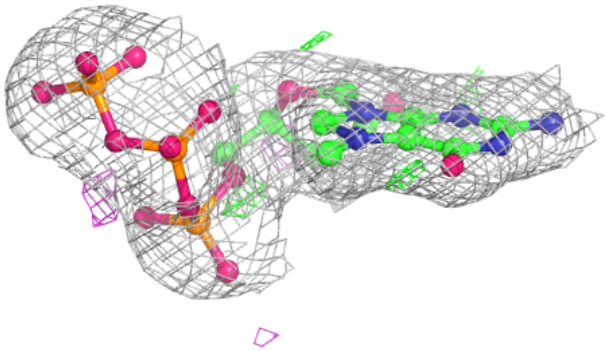


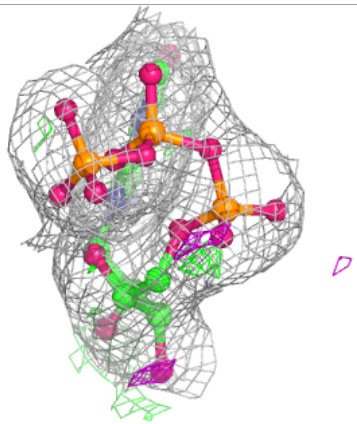


Electron density around MGT C 801:

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

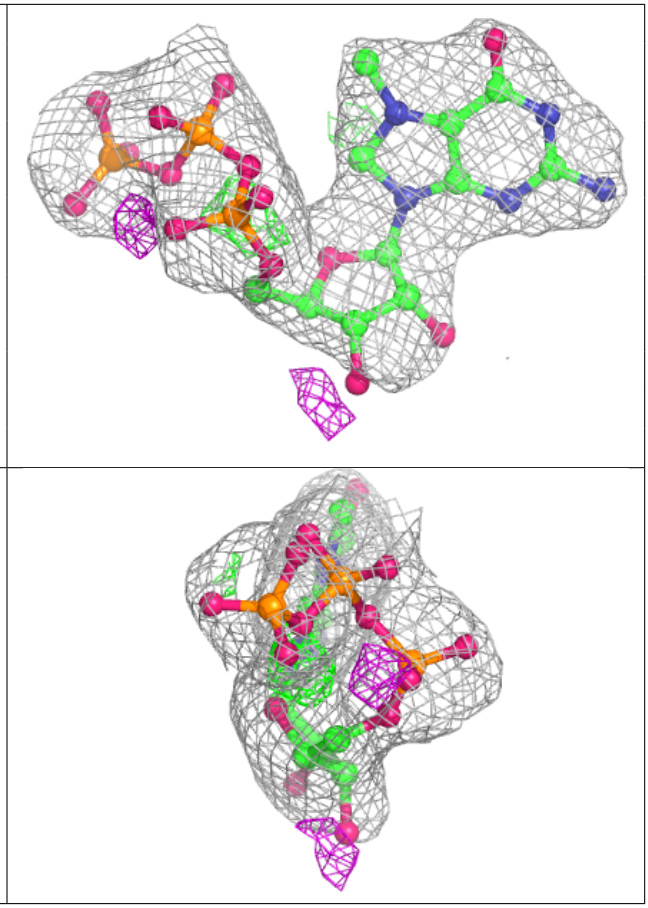






Electron density around MGT B 801:

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



6.5 Other polymers (i)

There are no such residues in this entry.