



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:07 PM EDT

PDB ID : 5H3T / pdb_00005h3t
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

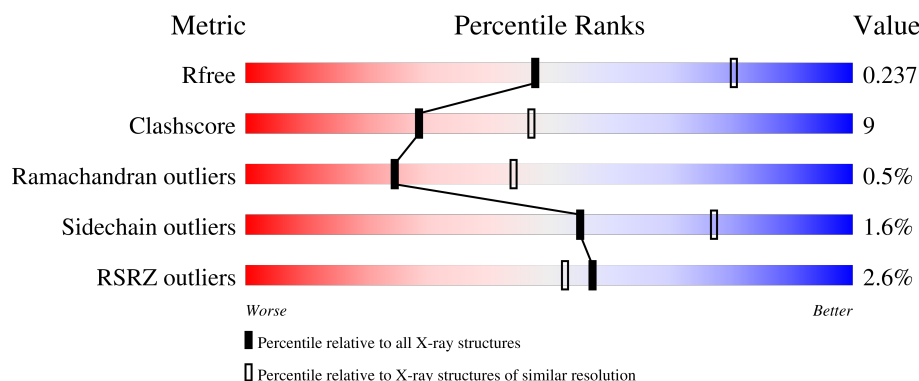
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	740	 2% 70% 18% 12%
1	B	740	 % 74% 14% 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 criteria:

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

2 Entry composition [i](#)

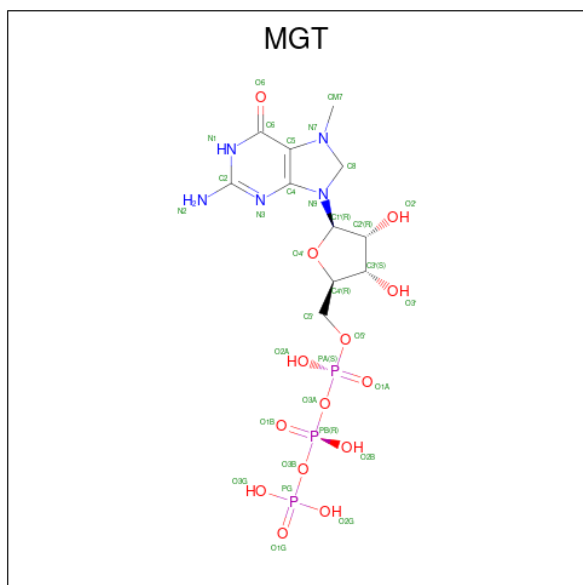
There are 4 unique types of molecules in this entry. The entry contains 20448 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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



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

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

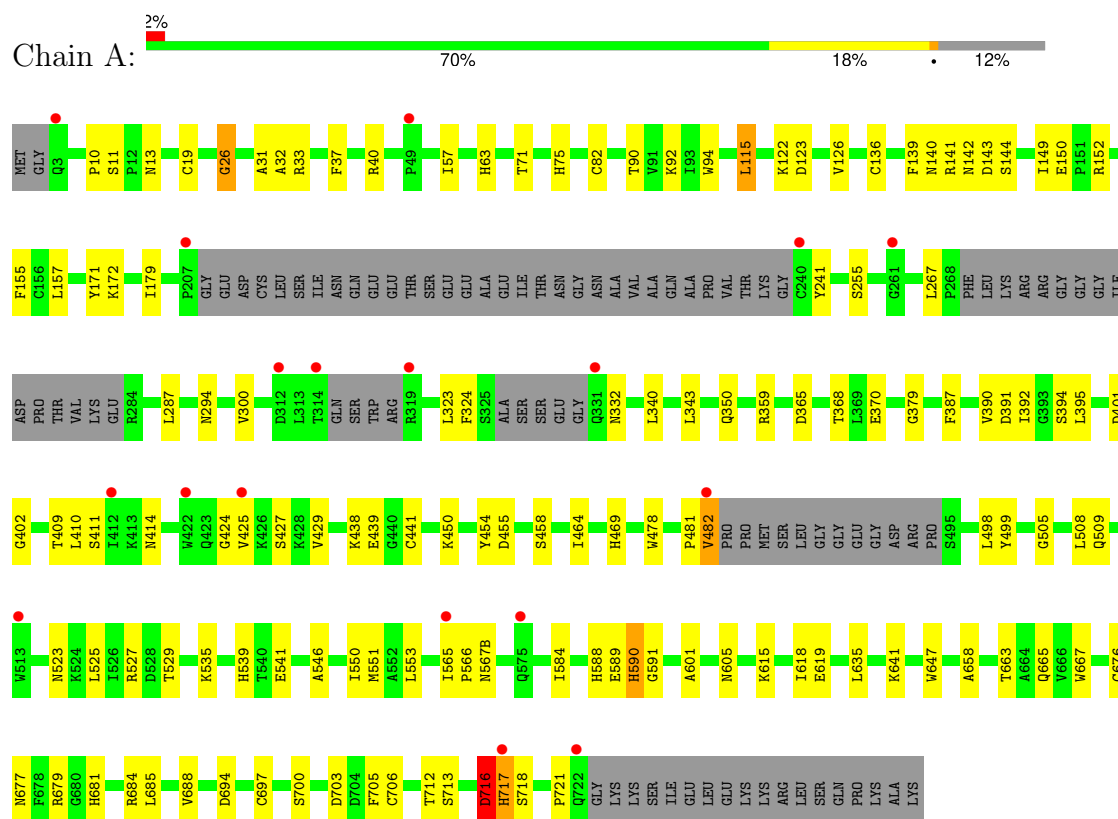
- Molecule 4 is water.

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

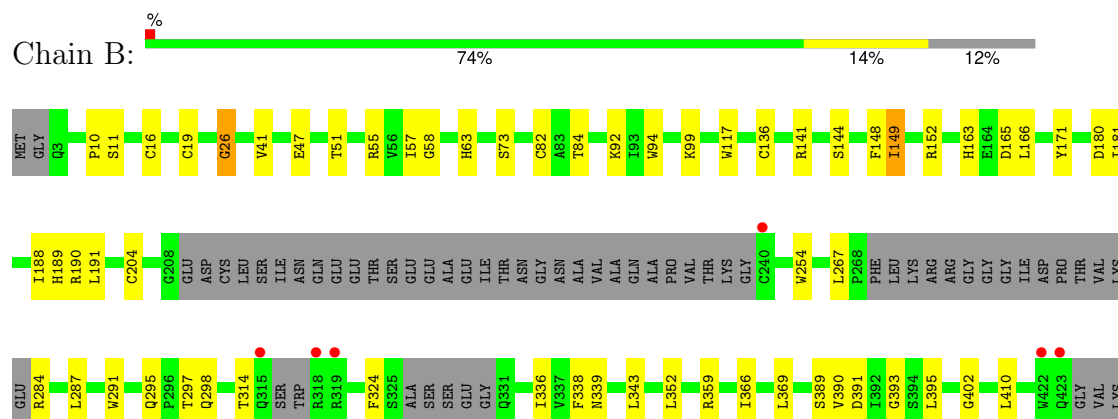
3 Residue-property plots

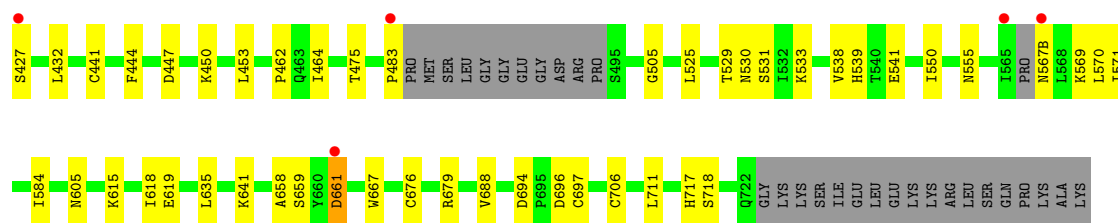
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Gem-associated protein 5

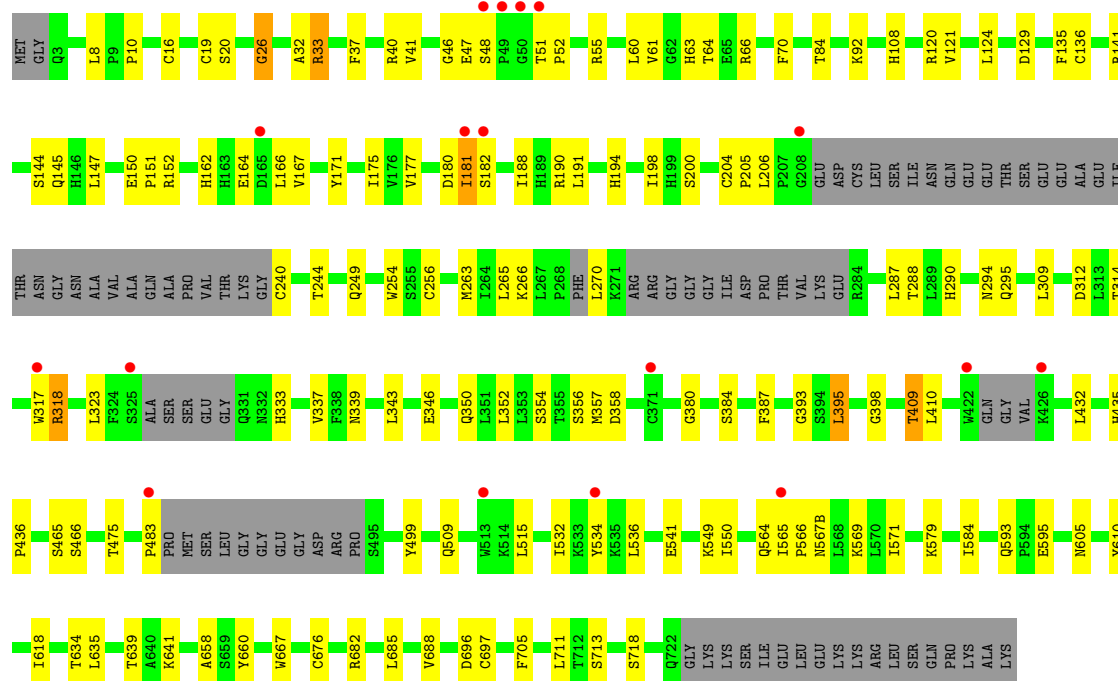


• Molecule 1: Gem-associated protein 5

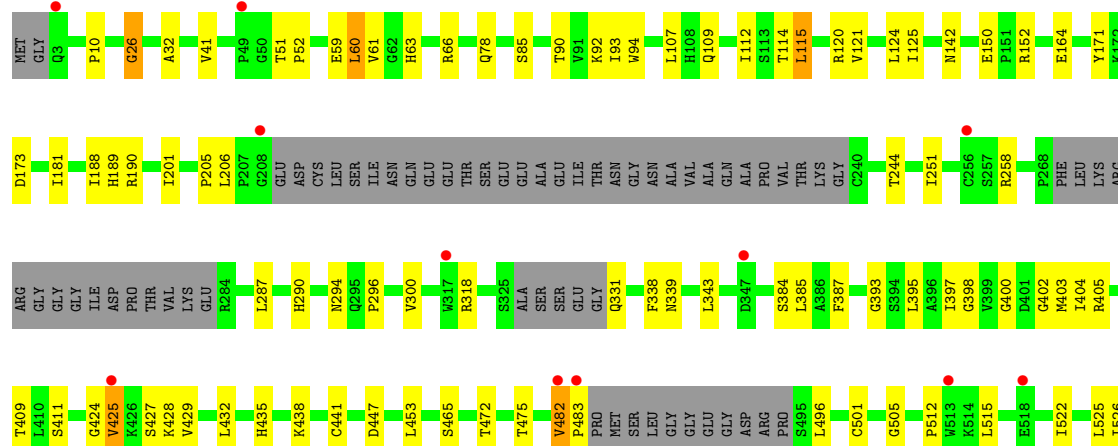


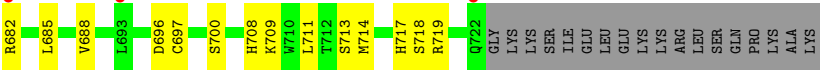
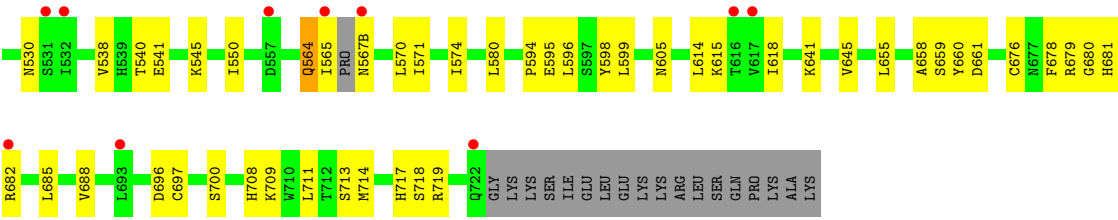


• Molecule 1: Gem-associated protein 5



• Molecule 1: Gem-associated protein 5





4 Data and refinement statistics

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) 98.2 (49.33-2.57)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.58Å)	Xtriage
Refinement program	PHENIX (dev_2386: ???)	Depositor
R, R_{free}	0.171 , 0.228 0.186 , 0.237	Depositor DCC
R_{free} test set	4808 reflections (4.89%)	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 , 70.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	1/5171 (0.0%)	0.53	0/7061
1	B	0.42	0/5185	0.62	0/7076
1	C	0.45	0/5217	0.69	0/7122
1	D	0.37	0/5196	0.60	0/7099
All	All	0.40	1/20769 (0.0%)	0.61	0/28358

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	716	ASP	C-N	5.04	1.40	1.33

There are no bond angle outliers.

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	93	0
1	B	5042	0	4828	72	0
1	C	5072	0	4861	95	0
1	D	5050	0	4805	92	0
2	A	33	0	16	1	0
2	B	33	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	350	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 (350) 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:B:148:PHE:C	1:B:149:ILE:HD13	2.14	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:150:GLU:CD	1:D:190:ARG:HH12	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:180:ASP:C	1:C:182:SER:H	2.17	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:D:424:GLY:O	1:D:425:VAL:C	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:338:PHE:C	1:B:339:ASN:HD22	2.19	0.51
1:B:136:CYS:O	1:B:144:SER:HA	2.10	0.51
1:A:551:MET:HE3	1:A:553:LEU:HG	1.93	0.50
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:A:455:ASP:CG	1:A:458:SER:HB3	2.34	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:403:MET:HE3	1:D:405:ARG:CZ	2.43	0.49
1:A:40:ARG:HB2	1:A:57:ILE:HD13	1.95	0.48
1:C:263:MET:HE2	1:C:265:LEU:HD21	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:A:126:VAL:HG12	1:A:157:LEU:HD11	1.95	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:D:338:PHE:C	1:D:339:ASN:HD22	2.23	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:696:ASP:OD2	1:D:713:SER:OG	2.26	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:D:51:THR:O	1:D:52:PRO:C	2.58	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: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:A:142:ASN:C	1:A:143:ASP:OD1	2.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:90:THR:HG21	1:D:92:LYS:HZ3	1.83	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:164:GLU:H	1:C:164:GLU:CD	2.26	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:409:THR:C	1:A:410:LEU:HD23	2.43	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:A:589:GLU:C	1:A:591:GLY:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:115:LEU:C	1:D:115:LEU:CD1	2.92	0.43
1:D:59:GLU:OE1	1:D:682:ARG:HD3	2.19	0.42
1:D:594:PRO:C	1:D:596:LEU:H	2.27	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:379:GLY:C	1:A:401:ASP:HB3	2.46	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: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%)	36	56
1	B	636/740 (86%)	607 (95%)	27 (4%)	2 (0%)	36	56
1	C	643/740 (87%)	602 (94%)	38 (6%)	3 (0%)	24	44
1	D	645/740 (87%)	609 (94%)	30 (5%)	6 (1%)	14	29
All	All	2564/2960 (87%)	2416 (94%)	135 (5%)	13 (0%)	24	44

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%)	539 (99%)	7 (1%)	61	81
1	B	551/642 (86%)	546 (99%)	5 (1%)	70	85
1	C	553/642 (86%)	538 (97%)	15 (3%)	39	65
1	D	547/642 (85%)	539 (98%)	8 (2%)	57	78
All	All	2197/2568 (86%)	2162 (98%)	35 (2%)	55	77

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	141	ARG
1	A	454	TYR
1	A	482	VAL
1	A	713	SER
1	A	716	ASP
1	A	717	HIS
1	B	149	ILE
1	B	389	SER
1	B	395	LEU
1	B	475	THR
1	B	567(B)	ASN
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
1	C	409	THR
1	C	465	SER
1	C	466	SER
1	C	475	THR
1	C	639	THR
1	D	60	LEU
1	D	66	ARG
1	D	78	GLN
1	D	114	THR
1	D	115	LEU
1	D	384	SER

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Mol	Chain	Res	Type
1	D	411	SER
1	D	564	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	109	GLN
1	A	146	HIS
1	A	310	GLN
1	A	350	GLN
1	A	509	GLN
1	A	564	GLN
1	A	567(B)	ASN
1	A	575	GLN
1	A	665	GLN
1	A	717	HIS
1	B	109	GLN
1	B	110	HIS
1	B	189	HIS
1	B	530	ASN
1	B	555	ASN
1	B	564	GLN
1	B	567(B)	ASN
1	B	708	HIS
1	C	109	GLN
1	C	110	HIS
1	C	194	HIS
1	C	249	GLN
1	C	295	GLN
1	C	298	GLN
1	C	310	GLN
1	C	333	HIS
1	C	593	GLN
1	C	665	GLN
1	C	715	GLN
1	D	109	GLN
1	D	140	ASN
1	D	189	HIS
1	D	344	GLN
1	D	530	ASN
1	D	564	GLN

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Mol	Chain	Res	Type
1	D	576	GLN
1	D	612	HIS
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MGT	C	801	-	34,35,35	1.29	4 (11%)	45,56,56	2.22	9 (20%)
2	MGT	A	801	-	34,35,35	1.30	4 (11%)	45,56,56	2.23	9 (20%)
2	MGT	D	801	-	34,35,35	1.27	3 (8%)	45,56,56	2.22	9 (20%)
3	GOL	B	802	-	5,5,5	0.26	0	5,5,5	0.32	0
2	MGT	B	801	-	34,35,35	1.29	4 (11%)	45,56,56	2.22	9 (20%)
3	GOL	A	802	-	5,5,5	0.26	0	5,5,5	0.20	0

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	MGT	C	801	-	-	4/22/50/50	0/3/3/3
2	MGT	A	801	-	-	6/22/50/50	0/3/3/3
2	MGT	D	801	-	-	1/22/50/50	0/3/3/3
3	GOL	B	802	-	-	2/4/4/4	-
2	MGT	B	801	-	-	5/22/50/50	0/3/3/3
3	GOL	A	802	-	-	3/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	MGT	C5-C4	3.28	1.47	1.37
2	B	801	MGT	C5-C4	3.26	1.47	1.37
2	C	801	MGT	C5-C4	3.25	1.47	1.37
2	D	801	MGT	C5-C4	3.24	1.47	1.37
2	C	801	MGT	C4-N9	-2.79	1.34	1.37
2	D	801	MGT	C4-N9	-2.77	1.34	1.37
2	B	801	MGT	C4-N9	-2.77	1.34	1.37
2	A	801	MGT	C4-N9	-2.69	1.34	1.37
2	B	801	MGT	C6-N1	-2.40	1.34	1.38
2	C	801	MGT	C6-N1	-2.37	1.34	1.38
2	A	801	MGT	C6-N1	-2.34	1.34	1.38
2	D	801	MGT	C6-N1	-2.29	1.34	1.38
2	A	801	MGT	C8-N9	2.12	1.47	1.45
2	C	801	MGT	C8-N9	2.09	1.47	1.45
2	B	801	MGT	C8-N9	2.06	1.47	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	MGT	N9-C4-N3	9.13	138.85	125.46
2	C	801	MGT	N9-C4-N3	9.04	138.71	125.46
2	B	801	MGT	N9-C4-N3	9.04	138.71	125.46
2	D	801	MGT	N9-C4-N3	9.03	138.69	125.46
2	A	801	MGT	C5-C4-N3	-5.66	117.51	128.13
2	C	801	MGT	C5-C4-N3	-5.61	117.60	128.13
2	B	801	MGT	C5-C4-N3	-5.60	117.62	128.13
2	D	801	MGT	C5-C4-N3	-5.59	117.64	128.13
2	C	801	MGT	N9-C8-N7	-5.12	96.12	103.37
2	B	801	MGT	N9-C8-N7	-5.09	96.17	103.37
2	D	801	MGT	N9-C8-N7	-5.05	96.22	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	MGT	N9-C8-N7	-5.05	96.22	103.37
2	C	801	MGT	C2-N3-C4	4.50	120.06	112.30
2	B	801	MGT	C2-N3-C4	4.50	120.05	112.30
2	A	801	MGT	C2-N3-C4	4.49	120.04	112.30
2	D	801	MGT	C2-N3-C4	4.47	120.00	112.30
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	B	801	MGT	C5-C6-N1	2.75	115.77	110.94
2	C	801	MGT	C5-C6-N1	2.74	115.77	110.94
2	D	801	MGT	C5-C6-N1	2.72	115.72	110.94
2	A	801	MGT	C5-C6-N1	2.70	115.70	110.94
2	D	801	MGT	C3'-C2'-C1'	2.38	105.97	101.46
2	A	801	MGT	C3'-C2'-C1'	2.33	105.86	101.46
2	B	801	MGT	O6-C6-C5	-2.26	122.07	127.62
2	B	801	MGT	C3'-C2'-C1'	2.26	105.73	101.46
2	C	801	MGT	O6-C6-C5	-2.24	122.13	127.62
2	D	801	MGT	O6-C6-C5	-2.23	122.14	127.62
2	A	801	MGT	O6-C6-C5	-2.23	122.15	127.62
2	C	801	MGT	C3'-C2'-C1'	2.21	105.65	101.46
2	A	801	MGT	C5-C4-N9	-2.10	103.65	106.33
2	D	801	MGT	C5-C4-N9	-2.08	103.67	106.33
2	B	801	MGT	C5-C4-N9	-2.08	103.67	106.33
2	C	801	MGT	C5-C4-N9	-2.06	103.69	106.33

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	MGT	C5'-O5'-PA-O3A
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	PB-O3A-PA-O2A

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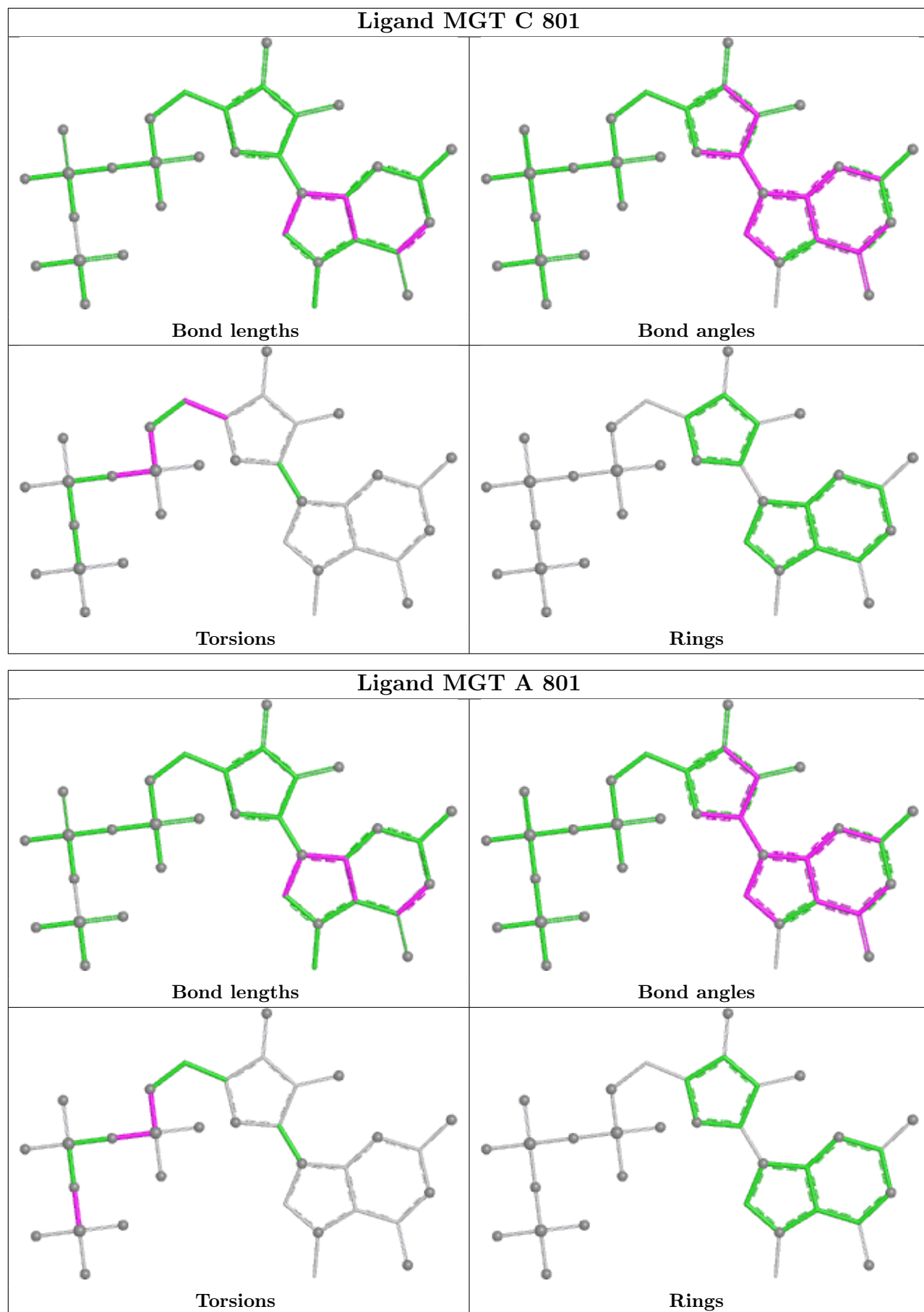
Mol	Chain	Res	Type	Atoms
2	C	801	MGT	C5'-O5'-PA-O1A
2	B	801	MGT	PB-O3B-PG-O1G
2	A	801	MGT	PB-O3B-PG-O2G
2	B	801	MGT	PB-O3B-PG-O3G
2	A	801	MGT	PB-O3A-PA-O1A
2	B	801	MGT	PB-O3A-PA-O2A
2	B	801	MGT	O4'-C4'-C5'-O5'
2	C	801	MGT	O4'-C4'-C5'-O5'
2	B	801	MGT	PB-O3A-PA-O1A

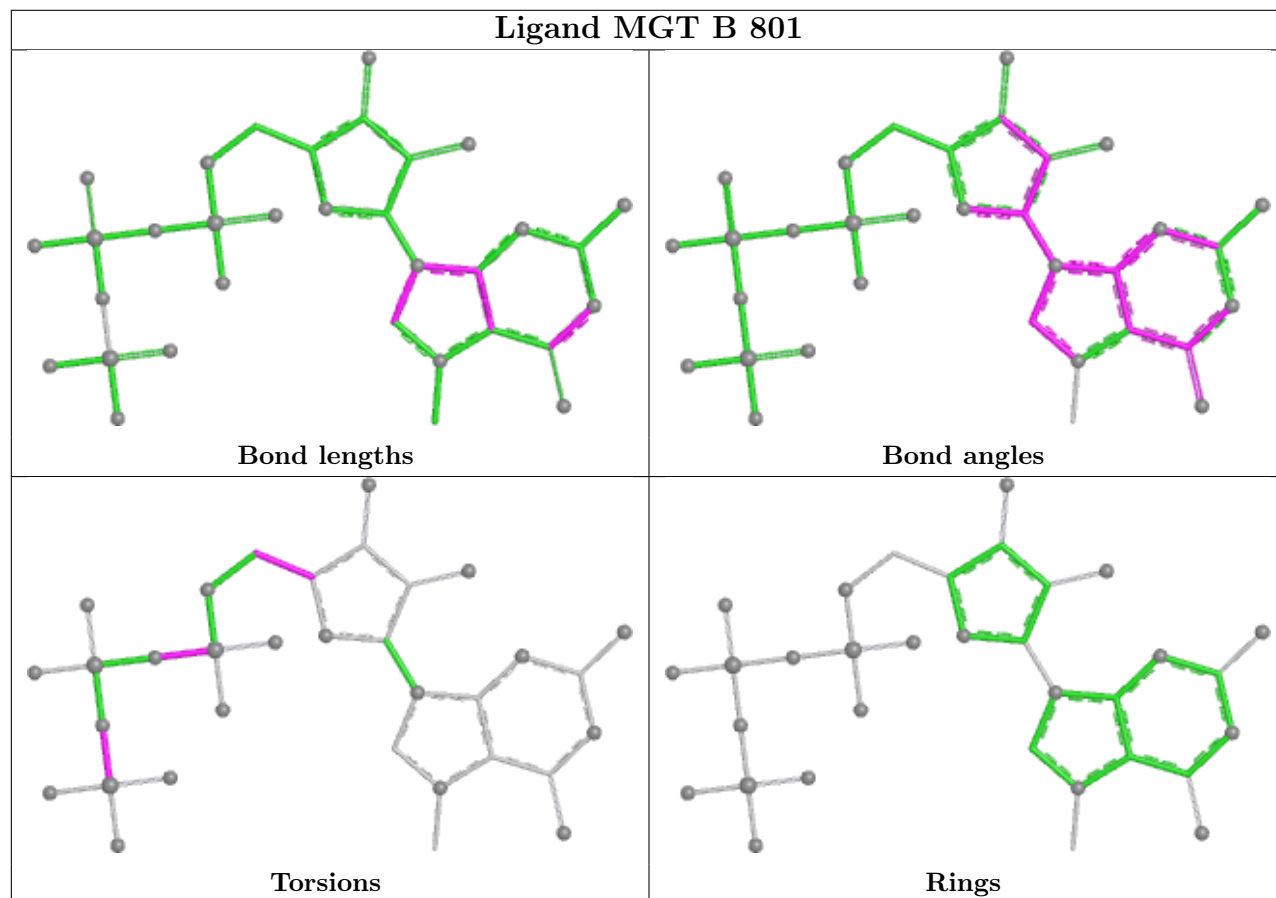
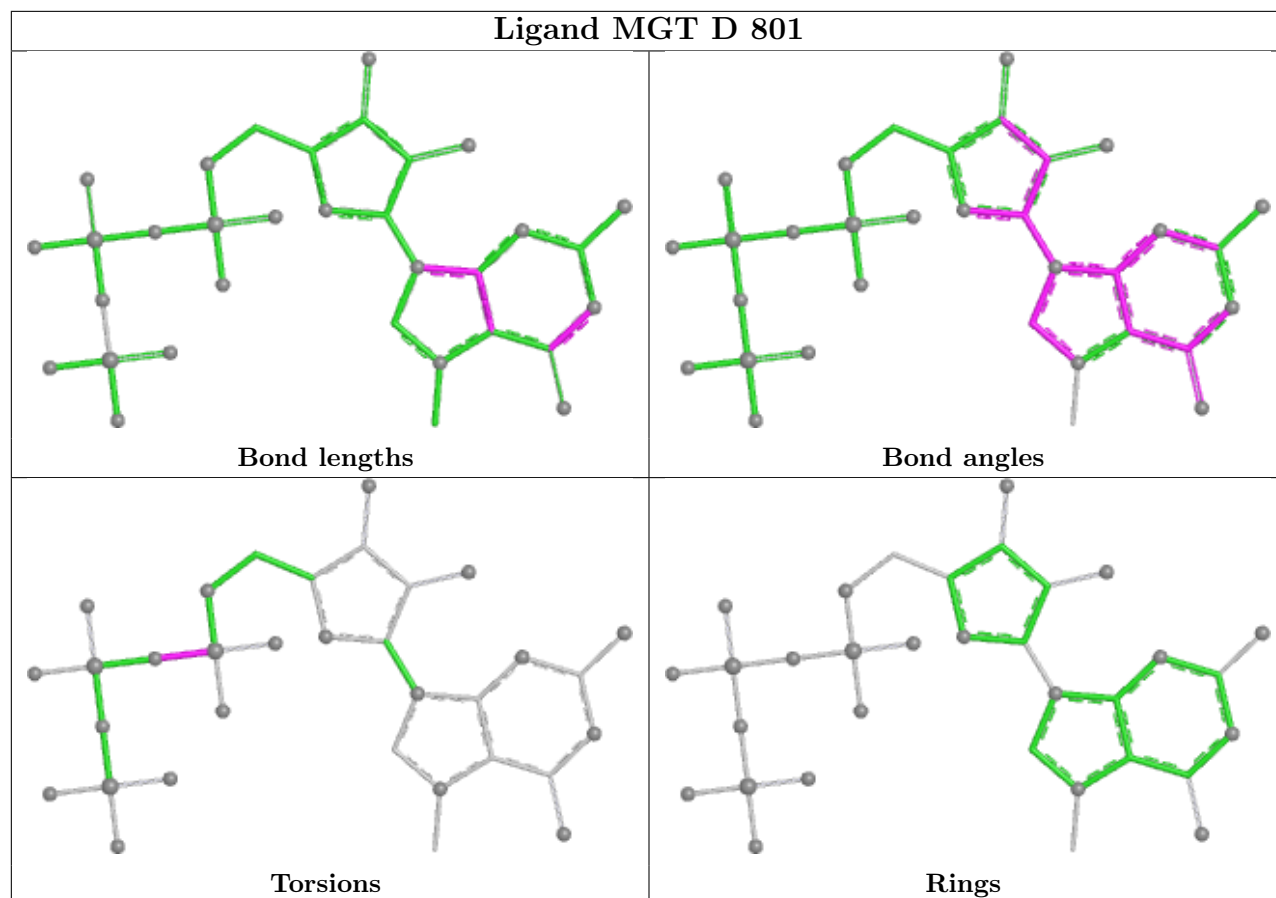
There are no ring outliers.

3 monomers are involved in 6 short contacts:

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

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





5.7 Other polymers [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

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	652/740 (88%)	0.25	18 (2%) 55 50	52, 78, 114, 141	0
1	B	652/740 (88%)	-0.15	11 (1%) 69 65	35, 55, 88, 118	0
1	C	657/740 (88%)	-0.15	17 (2%) 57 52	29, 52, 94, 134	0
1	D	657/740 (88%)	0.03	21 (3%) 50 45	39, 63, 109, 158	0
All	All	2618/2960 (88%)	-0.00	67 (2%) 57 52	29, 63, 106, 158	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	GLN	8.4
1	D	483	PRO	5.9
1	D	565	ILE	5.4
1	B	565	ILE	5.3
1	C	422	TRP	5.2
1	D	531	SER	4.6
1	D	532	ILE	4.5
1	C	317	TRP	4.5
1	A	412	ILE	4.3
1	C	208	GLY	4.1
1	D	208	GLY	3.8
1	A	319	ARG	3.8
1	B	427	SER	3.5
1	A	422	TRP	3.4
1	C	49	PRO	3.4
1	A	240	CYS	3.3
1	C	534	TYR	3.2
1	A	565	ILE	3.2
1	C	48	SER	3.2
1	D	425	VAL	3.2
1	A	207	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	482	VAL	3.1
1	A	513	TRP	3.1
1	D	317	TRP	3.1
1	B	318	ARG	3.1
1	A	722	GLN	3.0
1	C	565	ILE	3.0
1	B	319	ARG	2.9
1	B	422	TRP	2.9
1	C	182	SER	2.9
1	D	617	VAL	2.9
1	D	616	THR	2.8
1	C	181	ILE	2.8
1	C	513	TRP	2.8
1	A	3	GLN	2.8
1	C	483	PRO	2.7
1	C	371	CYS	2.6
1	C	426	LYS	2.6
1	C	50	GLY	2.5
1	C	165	ASP	2.5
1	B	240	CYS	2.5
1	D	3	GLN	2.5
1	D	722	GLN	2.5
1	C	51	THR	2.5
1	D	693	LEU	2.4
1	D	682	ARG	2.4
1	A	331	GLN	2.4
1	A	49	PRO	2.3
1	B	483	PRO	2.3
1	B	315	GLN	2.3
1	B	661	ASP	2.3
1	A	261	GLY	2.2
1	A	312	ASP	2.2
1	D	567(B)	ASN	2.2
1	D	256	CYS	2.2
1	D	482	VAL	2.2
1	A	314	THR	2.2
1	D	518	GLU	2.2
1	D	513	TRP	2.2
1	A	717	HIS	2.1
1	A	575	GLN	2.1
1	C	325	SER	2.1
1	B	567(B)	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	347	ASP	2.1
1	D	557	ASP	2.1
1	D	49	PRO	2.0
1	A	425	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

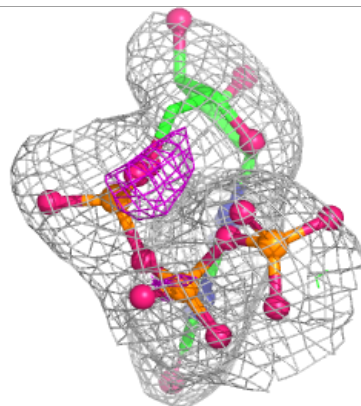
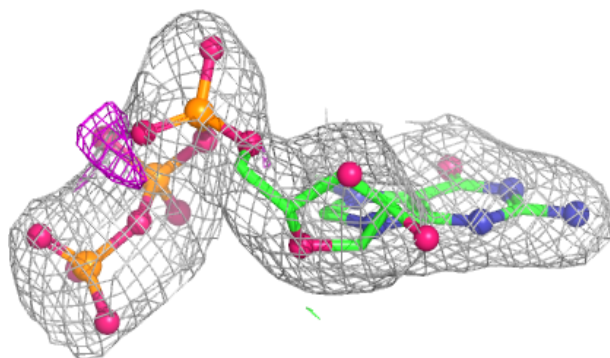
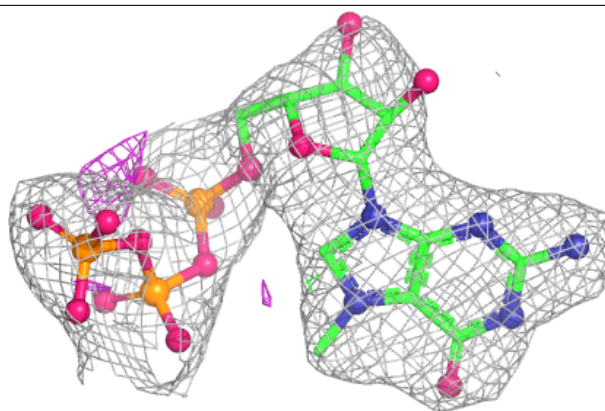
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	802	6/6	0.77	0.47	5,59,65,75	0
3	GOL	A	802	6/6	0.83	0.27	11,37,46,49	0
2	MGT	A	801	33/33	0.90	0.10	49,81,119,120	0
2	MGT	B	801	33/33	0.92	0.09	41,62,99,101	0
2	MGT	C	801	33/33	0.93	0.09	28,61,95,99	0
2	MGT	D	801	33/33	0.93	0.09	46,68,99,104	0

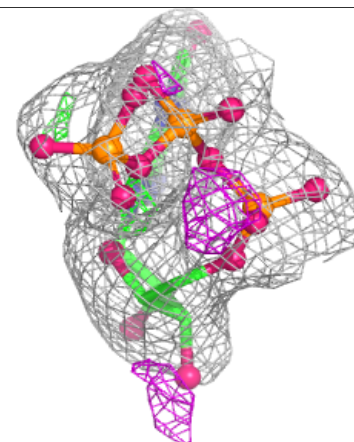
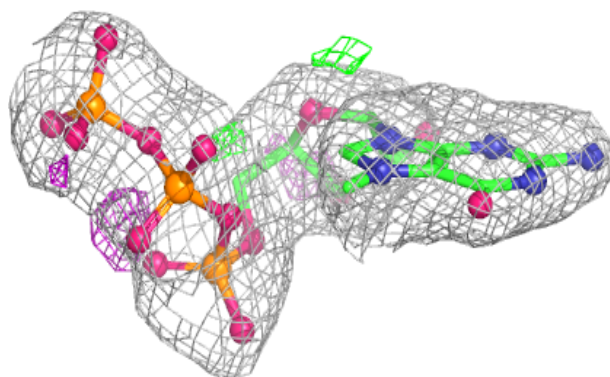
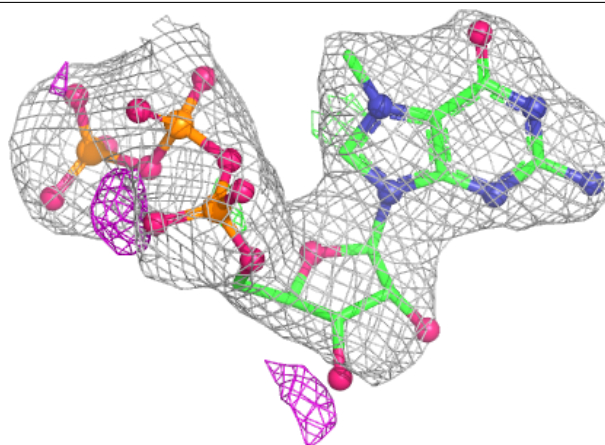
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

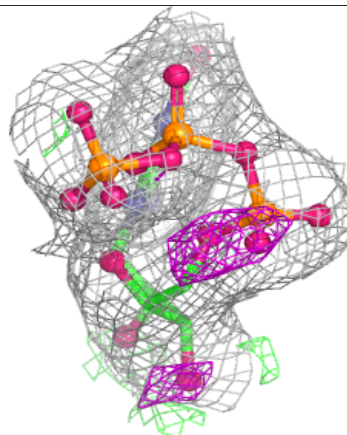
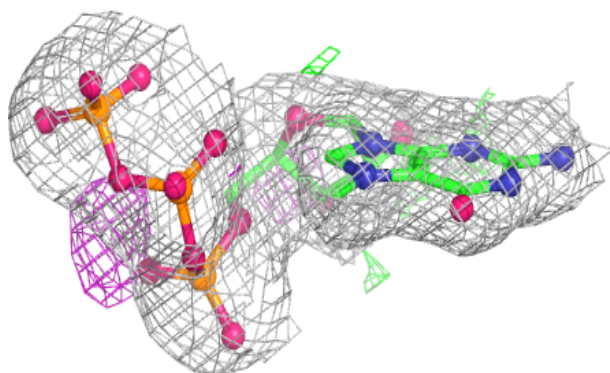
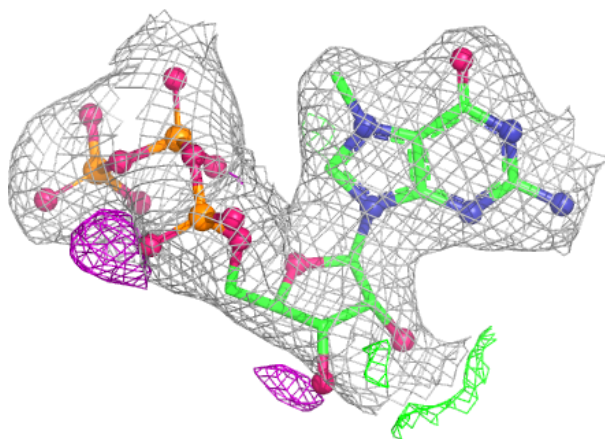
**Electron density around MGT B 801:**

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

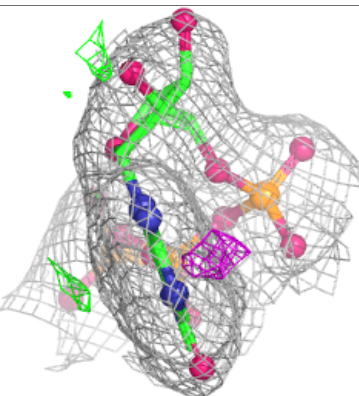
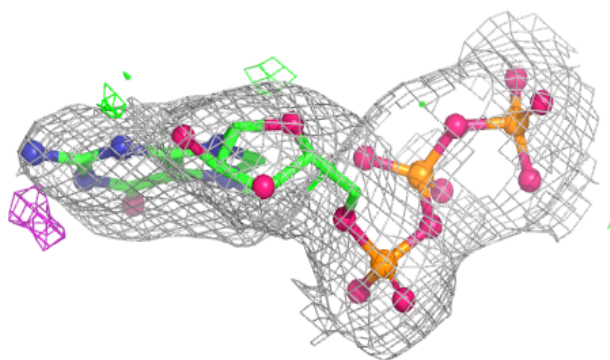
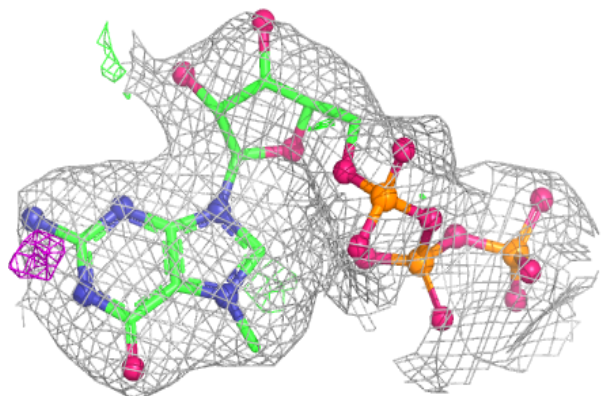


Electron density around MGT C 801:

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

**Electron density around MGT 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.