



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 06:27 AM UTC

PDB ID : 9L8V / pdb_00009l8v
Title : PyrN C-terminl domain in complex with L-glutamyl-sulfamoyl-adenosine (GSA)
Authors : Du, Y.L.; Zhao, G.
Deposited on : 2024-12-28
Resolution : 2.23 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

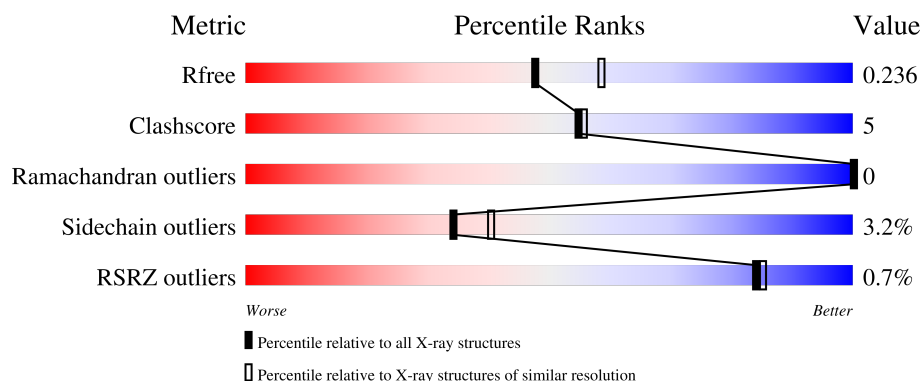
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	546	% 86% 11% ..
1	B	546	% 86% 11% .
1	B00Z	546	% 95% ..
1	D	546	% 81% 15% ..

2 Entry composition [i](#)

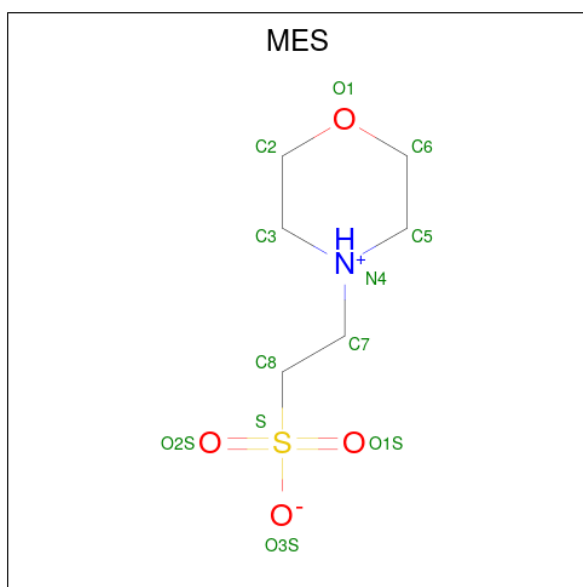
There are 5 unique types of molecules in this entry. The entry contains 17498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Methionine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4095	2594	728	754	19			
1	B	531	Total	C	N	O	S	0	0	0
			4088	2590	728	751	19			
1	D	532	Total	C	N	O	S	0	0	0
			4088	2590	729	750	19			
1	B00Z	533	Total	C	N	O	S	0	0	0
			4094	2594	731	750	19			

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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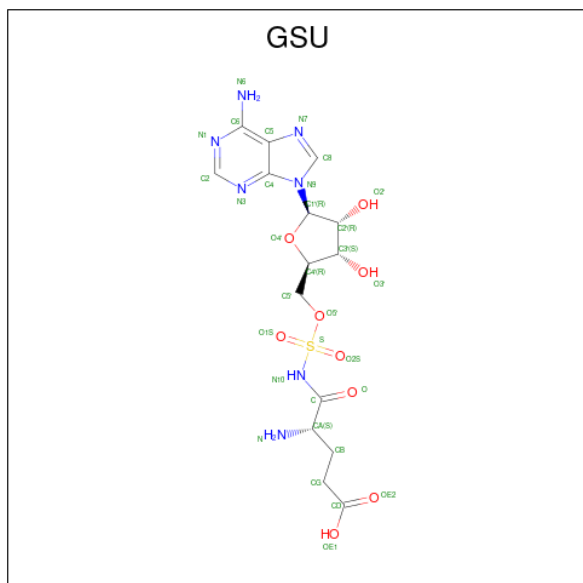
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B00Z	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B00Z	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		
3	B00Z	2	Total	Zn	0	0
			2	2		

- Molecule 4 is O5'-(L-GLUTAMYL-SULFAMOYL)-ADENOSINE (CCD ID: GSU) (formula: C₁₅H₂₁N₇O₉S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			32	15	7	9	1		
4	B	1	Total	C	N	O	S	0	0
			32	15	7	9	1		
4	D	1	Total	C	N	O	S	0	0
			32	15	7	9	1		
4	B00Z	1	Total	C	N	O	S	0	0
			32	15	7	9	1		

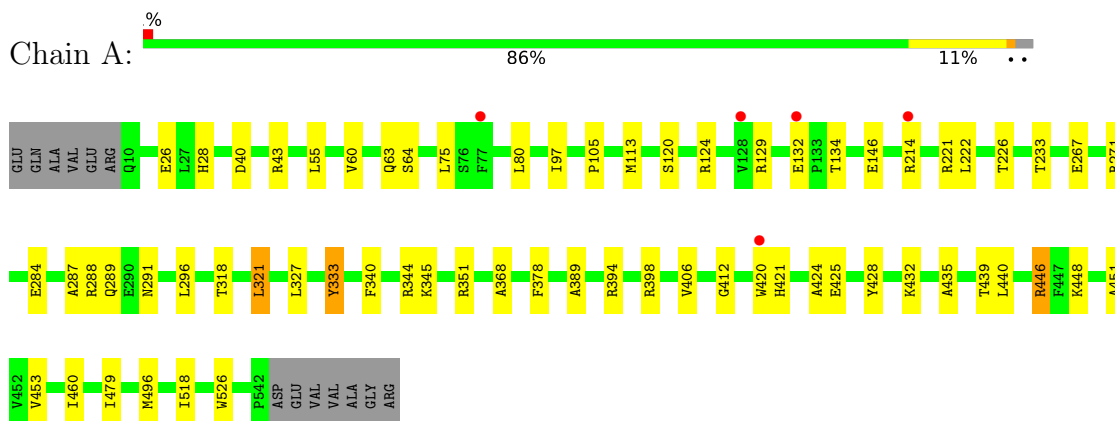
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	200	Total	O	0	0
			200	200		
5	B	228	Total	O	0	0
			228	228		
5	D	222	Total	O	0	0
			222	222		
5	B00Z	251	Total	O	0	0
			251	251		

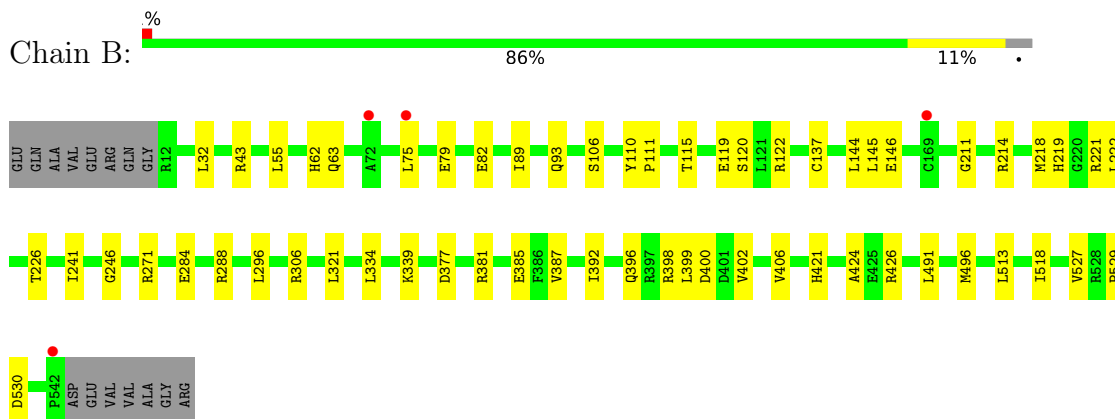
3 Residue-property plots

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.

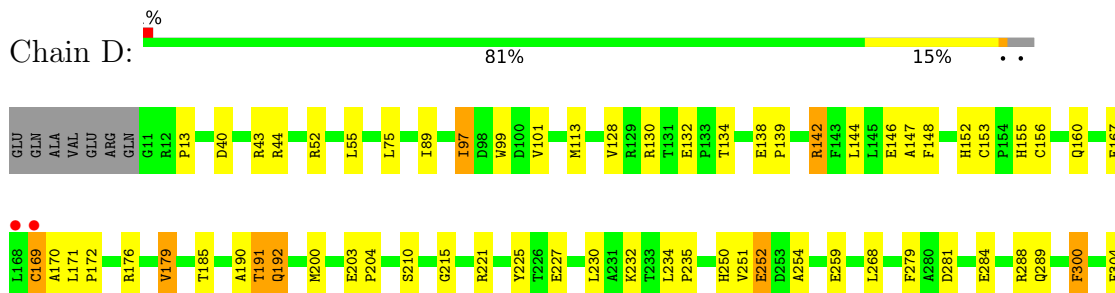
• Molecule 1: Methionine-tRNA ligase

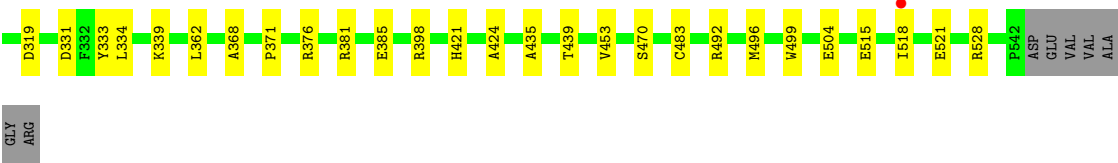


• Molecule 1: Methionine-tRNA ligase



• Molecule 1: Methionine-tRNA ligase





● Molecule 1: Methionine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.01Å 243.81Å 100.62Å 90.00° 99.04° 90.00°	Depositor
Resolution (Å)	33.12 – 2.23 33.12 – 2.23	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.12-2.23) 99.9 (33.12-2.23)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.187 , 0.237 0.189 , 0.236	Depositor DCC
R_{free} test set	2000 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17498	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, ZN, GSU

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	0.38	0/4203	0.53	1/5726 (0.0%)
1	B	0.40	0/4196	0.53	1/5716 (0.0%)
1	B00Z	0.43	1/4202 (0.0%)	0.61	4/5724 (0.1%)
1	D	0.61	0/4196	0.63	3/5716 (0.1%)
All	All	0.47	1/16797 (0.0%)	0.57	9/22882 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B00Z	291	ASN	C-O	6.56	1.26	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B00Z	179	VAL	N-CA-C	9.86	119.69	110.42
1	B00Z	255	SER	N-CA-C	-6.56	98.57	109.46
1	B	377	ASP	N-CA-C	6.31	119.75	109.59
1	D	170	ALA	N-CA-C	-5.73	105.59	113.56
1	B00Z	254	ALA	N-CA-C	5.66	119.05	109.76
1	D	169	CYS	CB-CA-C	-5.59	102.06	110.90
1	D	190	ALA	N-CA-C	5.57	119.31	109.96
1	A	318	THR	N-CA-C	5.48	117.40	109.07
1	B00Z	377	ASP	N-CA-C	5.08	117.77	109.59

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	4095	0	3958	36	0
1	B	4088	0	3958	32	0
1	B00Z	4094	0	0	0	0
1	D	4088	0	3957	47	0
2	A	12	0	12	3	0
2	B	36	0	36	3	0
2	B00Z	24	0	0	0	0
2	D	24	0	24	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	B00Z	2	0	0	0	0
3	D	2	0	0	0	0
4	A	32	0	19	0	0
4	B	32	0	19	0	0
4	B00Z	32	0	0	0	0
4	D	32	0	19	0	0
5	A	200	0	0	1	0
5	B	228	0	0	2	0
5	B00Z	251	0	0	0	0
5	D	222	0	0	1	0
All	All	17498	0	12002	117	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 5.

All (117) 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:D:152:HIS:HB2	1:D:179:VAL:HG22	1.58	0.86
1:D:172:PRO:HB2	1:D:235:PRO:HG3	1.63	0.81
1:D:528:ARG:HH11	1:D:528:ARG:HG3	1.54	0.71
1:D:492:ARG:NE	1:D:515:GLU:OE2	2.21	0.69
1:B:284:GLU:OE2	1:B:288:ARG:NH1	2.25	0.67
1:D:250:HIS:CD2	1:D:252:GLU:HG2	2.33	0.63
1:D:250:HIS:ND1	1:D:259:GLU:OE2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:HIS:HD2	1:B:424:ALA:H	1.48	0.62
1:D:156:CYS:HB3	1:D:169:CYS:SG	2.40	0.62
1:B:119:GLU:OE1	1:B:122:ARG:NH2	2.34	0.61
1:D:155:HIS:HB2	1:D:169:CYS:SG	2.40	0.61
1:D:421:HIS:CD2	1:D:424:ALA:H	2.19	0.60
1:A:368:ALA:HB2	1:A:453:VAL:HG11	1.84	0.59
1:A:26:GLU:OE1	1:A:351:ARG:HD3	2.03	0.59
1:D:496:MET:HB2	1:D:518:ILE:HG21	1.84	0.59
1:A:284:GLU:OE2	1:A:288:ARG:NH1	2.34	0.59
1:D:152:HIS:HB2	1:D:179:VAL:CG2	2.31	0.59
1:D:284:GLU:O	1:D:288:ARG:HG3	2.02	0.59
1:A:526:TRP:CD1	2:A:601:MES:H81	2.38	0.58
1:A:496:MET:HB2	1:A:518:ILE:HG21	1.86	0.56
1:D:101:VAL:HG21	1:D:279:PHE:HB2	1.87	0.56
1:B:513:LEU:HD22	1:B:527:VAL:HG21	1.88	0.54
1:D:421:HIS:HD2	1:D:424:ALA:H	1.55	0.54
1:A:435:ALA:O	1:A:439:THR:HG23	2.07	0.54
1:D:528:ARG:HG3	1:D:528:ARG:NH1	2.22	0.52
1:B:62:HIS:CD2	1:B:246:GLY:HA2	2.45	0.52
1:B:211:GLY:HA2	1:B:214:ARG:NH1	2.24	0.52
1:B:399:LEU:HD23	1:B:491:LEU:HD13	1.91	0.51
1:D:230:LEU:HD23	1:D:234:LEU:HD21	1.92	0.51
1:B:334:LEU:HA	1:B:339:LYS:HA	1.93	0.51
1:D:435:ALA:O	1:D:439:THR:HG23	2.11	0.51
1:B:89:ILE:O	1:B:93:GLN:HG3	2.12	0.50
1:A:267:GLU:O	1:A:271:ARG:HG3	2.12	0.50
1:B:75:LEU:HD12	1:B:79:GLU:HG2	1.94	0.50
1:A:440:LEU:HD13	1:A:446:ARG:NH2	2.27	0.50
1:A:291:ASN:ND2	5:A:705:HOH:O	2.30	0.50
1:D:439:THR:HG21	1:D:521:GLU:C	2.37	0.49
1:B:82:GLU:OE2	1:B:106:SER:OG	2.29	0.49
1:A:526:TRP:NE1	2:A:601:MES:H52	2.27	0.48
1:B:381:ARG:O	1:B:385:GLU:HG3	2.13	0.48
1:D:138:GLU:HB2	1:D:139:PRO:HD3	1.95	0.48
1:A:421:HIS:HD2	1:A:424:ALA:H	1.61	0.48
1:A:428:TYR:CE2	1:A:432:LYS:HE2	2.48	0.48
1:B:421:HIS:HB2	2:B:601:MES:O3S	2.13	0.47
1:A:287:ALA:HB1	1:A:321:LEU:HB3	1.95	0.47
1:A:26:GLU:CD	1:A:351:ARG:HH11	2.21	0.47
1:A:120:SER:O	1:A:124:ARG:HG3	2.14	0.47
1:A:421:HIS:CD2	1:A:424:ALA:H	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:GLN:NE2	1:B:400:ASP:OD1	2.48	0.47
1:B:496:MET:HB2	1:B:518:ILE:HG21	1.95	0.47
1:A:75:LEU:HD12	1:A:80:LEU:HD12	1.96	0.47
1:B:421:HIS:CD2	1:B:424:ALA:H	2.31	0.47
1:D:203:GLU:HB3	1:D:204:PRO:HD3	1.97	0.47
1:D:40:ASP:HB2	1:D:97:ILE:HG23	1.96	0.46
1:D:44:ARG:HB3	1:D:499:TRP:CZ3	2.50	0.46
1:B:387:VAL:HG12	1:B:392:ILE:HD12	1.96	0.46
1:D:288:ARG:NH2	1:D:319:ASP:OD1	2.49	0.46
2:B:602:MES:H51	2:B:602:MES:H81	1.61	0.45
1:D:43:ARG:HD3	1:D:55:LEU:HB2	1.98	0.45
1:D:251:VAL:HG12	1:D:254:ALA:HB2	1.98	0.45
1:B:63:GLN:HE21	1:B:271:ARG:HH22	1.65	0.45
1:D:470:SER:HB2	1:D:483:CYS:HB3	1.99	0.45
1:D:259:GLU:HG3	5:D:881:HOH:O	2.16	0.45
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.74	0.44
1:B:402:VAL:O	1:B:406:VAL:HG23	2.17	0.44
1:A:28:HIS:CE1	1:A:340:PHE:HB3	2.52	0.44
1:D:334:LEU:HA	1:D:339:LYS:HA	1.99	0.44
1:D:381:ARG:HG3	1:D:385:GLU:OE2	2.18	0.44
1:A:64:SER:HB3	1:A:146:GLU:CD	2.43	0.44
1:B:222:LEU:O	1:B:226:THR:HG23	2.18	0.44
1:B:43:ARG:HD3	1:B:55:LEU:HB2	2.00	0.44
1:D:169:CYS:C	1:D:171:LEU:H	2.26	0.44
1:D:132:GLU:O	1:D:134:THR:HG23	2.18	0.44
1:D:169:CYS:C	1:D:171:LEU:N	2.76	0.43
1:A:526:TRP:HE1	2:A:601:MES:H52	1.83	0.43
1:B:115:THR:O	1:B:119:GLU:HG2	2.19	0.43
2:D:601:MES:H81	2:D:601:MES:H31	1.64	0.43
1:D:172:PRO:HB2	1:D:235:PRO:CG	2.43	0.43
1:A:113:MET:HE2	1:A:113:MET:HB2	1.92	0.43
1:B:219:HIS:CE1	1:B:221:ARG:HB3	2.54	0.43
1:A:63:GLN:NE2	1:A:271:ARG:HH12	2.17	0.42
1:A:460:ILE:HD13	1:A:460:ILE:HA	1.82	0.42
1:B:110:TYR:HB3	1:B:111:PRO:HD3	2.02	0.42
1:D:225:TYR:OH	1:D:304:PHE:HB2	2.19	0.42
1:D:113:MET:HE2	1:D:113:MET:HB2	1.93	0.42
1:A:296:LEU:HD12	1:A:327:LEU:HD22	2.02	0.42
1:B:426:ARG:HD2	5:B:756:HOH:O	2.20	0.42
1:B:529:PRO:O	1:B:530:ASP:HB2	2.20	0.42
1:D:191:THR:OG1	1:D:192:GLN:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:PRO:HA	1:D:376:ARG:HG3	2.01	0.42
1:B:398:ARG:NH1	5:B:722:HOH:O	2.53	0.42
1:A:333:TYR:CE2	1:A:378:PHE:HB2	2.55	0.42
1:A:221:ARG:HH11	1:A:221:ARG:HG3	1.84	0.41
1:B:137:CYS:HB2	1:B:144:LEU:HD11	2.02	0.41
1:D:284:GLU:OE2	1:D:288:ARG:NH1	2.53	0.41
1:A:448:LYS:HG2	1:A:451:ALA:H	1.86	0.41
1:B:218:MET:HB2	1:B:222:LEU:HD23	2.02	0.41
1:A:60:VAL:HA	1:A:105:PRO:HA	2.02	0.41
1:A:214:ARG:HH12	2:B:601:MES:H22	1.86	0.41
1:D:89:ILE:HG23	1:D:99:TRP:HH2	1.85	0.41
1:D:368:ALA:HB2	1:D:453:VAL:HG11	2.03	0.41
1:A:389:ALA:O	1:A:394:ARG:HG3	2.20	0.41
1:D:146:GLU:HB3	1:D:147:ALA:H	1.68	0.41
1:D:215:GLY:HA2	2:D:601:MES:H62	2.03	0.41
1:D:221:ARG:HG2	1:D:300:PHE:HE2	1.86	0.41
1:A:40:ASP:HB2	1:A:97:ILE:HG23	2.03	0.41
1:D:160:GLN:O	1:D:167:GLU:HG2	2.21	0.41
1:D:496:MET:HB2	1:D:518:ILE:CG2	2.49	0.41
1:A:43:ARG:HD3	1:A:55:LEU:HB2	2.03	0.40
1:A:222:LEU:O	1:A:226:THR:HG23	2.22	0.40
1:A:406:VAL:HG12	1:A:412:GLY:HA2	2.04	0.40
1:A:344:ARG:NH1	1:A:344:ARG:HG2	2.36	0.40
1:A:420:TRP:CE3	1:A:425:GLU:OE2	2.75	0.40
1:B:145:LEU:HB2	1:B:241:ILE:HD11	2.04	0.40
1:B:296:LEU:HD13	1:B:306:ARG:HD2	2.04	0.40
1:D:13:PRO:HD3	1:D:52:ARG:NH2	2.36	0.40
1:D:142:ARG:HD2	1:D:148:PHE:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	531/546 (97%)	519 (98%)	12 (2%)	0	100	100
1	B	529/546 (97%)	516 (98%)	13 (2%)	0	100	100
1	B00Z	531/546 (97%)	523 (98%)	8 (2%)	0	100	100
1	D	530/546 (97%)	517 (98%)	13 (2%)	0	100	100
All	All	2121/2184 (97%)	2075 (98%)	46 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	409/420 (97%)	398 (97%)	11 (3%)	39	47
1	B	409/420 (97%)	406 (99%)	3 (1%)	76	81
1	B00Z	408/420 (97%)	396 (97%)	12 (3%)	37	44
1	D	408/420 (97%)	382 (94%)	26 (6%)	16	14
All	All	1634/1680 (97%)	1582 (97%)	52 (3%)	34	40

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ARG
1	A	132	GLU
1	A	134	THR
1	A	233	THR
1	A	289	GLN
1	A	321	LEU
1	A	333	TYR
1	A	345	LYS
1	A	398	ARG
1	A	446	ARG
1	A	479	ILE
1	B	32	LEU
1	B	120	SER

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Mol	Chain	Res	Type
1	B	146	GLU
1	D	75	LEU
1	D	97	ILE
1	D	128	VAL
1	D	130	ARG
1	D	142	ARG
1	D	144	LEU
1	D	153	CYS
1	D	176	ARG
1	D	179	VAL
1	D	185	THR
1	D	191	THR
1	D	192	GLN
1	D	200	MET
1	D	210	SER
1	D	227	GLU
1	D	232	LYS
1	D	252	GLU
1	D	268	LEU
1	D	281	ASP
1	D	289	GLN
1	D	300	PHE
1	D	331	ASP
1	D	333	TYR
1	D	362	LEU
1	D	398	ARG
1	D	504	GLU
1	B00Z	60	VAL
1	B00Z	63	GLN
1	B00Z	67	SER
1	B00Z	131	THR
1	B00Z	321	LEU
1	B00Z	333	TYR
1	B00Z	339	LYS
1	B00Z	362	LEU
1	B00Z	376	ARG
1	B00Z	381	ARG
1	B00Z	421	HIS
1	B00Z	474	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	160	GLN
1	A	250	HIS
1	A	352	GLN
1	A	421	HIS
1	B	63	GLN
1	B	160	GLN
1	B	421	HIS
1	D	62	HIS
1	D	78	HIS
1	D	152	HIS
1	D	160	GLN
1	D	421	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](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	MES	B	603	-	12,12,12	1.95	1 (8%)	15,16,16	2.03	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	D	601	-	12,12,12	2.54	1 (8%)	15,16,16	2.27	6 (40%)
2	MES	B00Z	602	-	12,12,12	1.87	1 (8%)	15,16,16	2.46	4 (26%)
2	MES	B00Z	601	-	12,12,12	2.16	1 (8%)	15,16,16	2.68	7 (46%)
4	GSU	D	605	-	34,34,34	7.03	15 (44%)	47,50,50	2.20	13 (27%)
4	GSU	A	604	-	34,34,34	6.83	16 (47%)	47,50,50	2.26	12 (25%)
4	GSU	B	606	-	34,34,34	6.99	15 (44%)	47,50,50	2.45	12 (25%)
2	MES	B	602	-	12,12,12	2.12	1 (8%)	15,16,16	2.30	5 (33%)
2	MES	A	601	-	12,12,12	2.09	1 (8%)	15,16,16	1.55	2 (13%)
4	GSU	B00Z	605	-	34,34,34	6.84	15 (44%)	47,50,50	2.36	14 (29%)
2	MES	D	602	-	12,12,12	2.21	1 (8%)	15,16,16	1.90	2 (13%)
2	MES	B	601	-	12,12,12	2.09	1 (8%)	15,16,16	1.93	3 (20%)

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	MES	B	603	-	-	4/6/14/14	0/1/1/1
2	MES	D	601	-	-	4/6/14/14	0/1/1/1
2	MES	B00Z	602	-	-	4/6/14/14	0/1/1/1
2	MES	B00Z	601	-	-	1/6/14/14	0/1/1/1
4	GSU	D	605	-	-	1/23/40/40	0/3/3/3
4	GSU	A	604	-	-	3/23/40/40	0/3/3/3
4	GSU	B	606	-	-	1/23/40/40	0/3/3/3
2	MES	B	602	-	-	4/6/14/14	0/1/1/1
2	MES	A	601	-	-	1/6/14/14	0/1/1/1
4	GSU	B00Z	605	-	-	5/23/40/40	0/3/3/3
2	MES	D	602	-	-	5/6/14/14	0/1/1/1
2	MES	B	601	-	-	1/6/14/14	0/1/1/1

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	605	GSU	O1S-S	27.08	1.66	1.42
4	B	606	GSU	O1S-S	26.87	1.66	1.42
4	B00Z	605	GSU	O1S-S	26.79	1.65	1.42
4	A	604	GSU	O1S-S	25.47	1.64	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	605	GSU	O2S-S	24.95	1.64	1.42
4	B	606	GSU	O2S-S	24.64	1.64	1.42
4	A	604	GSU	O2S-S	24.61	1.64	1.42
4	B00Z	605	GSU	O2S-S	23.29	1.62	1.42
4	B	606	GSU	C3'-C4'	-9.11	1.29	1.53
4	A	604	GSU	C3'-C4'	-8.92	1.30	1.53
4	B00Z	605	GSU	C3'-C4'	-8.65	1.31	1.53
4	D	605	GSU	C3'-C4'	-8.63	1.31	1.53
2	D	601	MES	C8-S	-8.55	1.65	1.77
2	D	602	MES	C8-S	-7.29	1.67	1.77
4	B	606	GSU	O4'-C4'	7.24	1.61	1.45
2	B00Z	601	MES	C8-S	-7.15	1.67	1.77
4	B00Z	605	GSU	O4'-C4'	7.14	1.60	1.45
2	B	602	MES	C8-S	-7.13	1.67	1.77
4	A	604	GSU	O4'-C4'	7.02	1.60	1.45
4	B00Z	605	GSU	C-N10	7.00	1.50	1.37
4	B	606	GSU	C-N10	6.91	1.50	1.37
4	D	605	GSU	O4'-C4'	6.90	1.60	1.45
4	A	604	GSU	C-N10	6.89	1.50	1.37
2	B	601	MES	C8-S	-6.84	1.68	1.77
2	A	601	MES	C8-S	-6.84	1.68	1.77
4	D	605	GSU	C-N10	6.39	1.49	1.37
2	B	603	MES	C8-S	-6.30	1.68	1.77
2	B00Z	602	MES	C8-S	-5.96	1.69	1.77
4	B	606	GSU	S-N10	5.60	1.69	1.59
4	D	605	GSU	O4'-C1'	-5.15	1.30	1.42
4	B00Z	605	GSU	S-N10	5.02	1.68	1.59
4	D	605	GSU	S-N10	4.92	1.67	1.59
4	B00Z	605	GSU	O4'-C1'	-4.89	1.30	1.42
4	D	605	GSU	C6-N6	4.85	1.46	1.34
4	A	604	GSU	O4'-C1'	-4.79	1.30	1.42
4	B	606	GSU	O4'-C1'	-4.73	1.31	1.42
4	A	604	GSU	S-N10	4.72	1.67	1.59
4	B00Z	605	GSU	C6-N6	4.56	1.45	1.34
4	B	606	GSU	C6-N6	4.26	1.45	1.34
4	A	604	GSU	O5'-S	4.11	1.68	1.60
4	A	604	GSU	C6-N6	4.10	1.44	1.34
4	D	605	GSU	C8-N9	-3.89	1.30	1.37
4	B00Z	605	GSU	C8-N9	-3.85	1.31	1.37
4	B00Z	605	GSU	O5'-S	3.81	1.67	1.60
4	A	604	GSU	C8-N9	-3.67	1.31	1.37
4	A	604	GSU	C4-N9	-3.56	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	605	GSU	C4-N9	-3.49	1.30	1.37
4	B	606	GSU	C8-N9	-3.43	1.31	1.37
4	B	606	GSU	O5'-S	3.39	1.66	1.60
4	B00Z	605	GSU	O-C	-3.34	1.17	1.23
4	B00Z	605	GSU	C4-N9	-3.28	1.30	1.37
4	D	605	GSU	O3'-C3'	3.19	1.50	1.43
4	D	605	GSU	O5'-S	3.12	1.66	1.60
4	A	604	GSU	O3'-C3'	3.12	1.50	1.43
4	B00Z	605	GSU	O2'-C2'	-3.08	1.35	1.43
4	B	606	GSU	O3'-C3'	3.07	1.50	1.43
4	A	604	GSU	O2'-C2'	-3.03	1.35	1.43
4	B	606	GSU	O2'-C2'	-2.83	1.35	1.43
4	B	606	GSU	C4-N9	-2.79	1.31	1.37
4	B00Z	605	GSU	O3'-C3'	2.78	1.49	1.43
4	D	605	GSU	O2'-C2'	-2.72	1.36	1.43
4	D	605	GSU	C5-N7	-2.61	1.34	1.39
4	B	606	GSU	O-C	-2.55	1.18	1.23
4	A	604	GSU	C5-N7	-2.50	1.34	1.39
4	D	605	GSU	O-C	-2.44	1.18	1.23
4	A	604	GSU	C2-N3	-2.43	1.29	1.33
4	A	604	GSU	O-C	-2.26	1.19	1.23
4	B	606	GSU	C5-N7	-2.18	1.35	1.39
4	B00Z	605	GSU	C5-N7	-2.04	1.35	1.39

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	606	GSU	O2S-S-O1S	-9.68	106.35	120.85
4	B00Z	605	GSU	O2S-S-O1S	-7.69	109.33	120.85
4	A	604	GSU	O2S-S-O1S	-7.40	109.78	120.85
4	D	605	GSU	O2S-S-O1S	-6.42	111.24	120.85
2	B00Z	602	MES	O2S-S-C8	6.31	116.27	106.73
4	B00Z	605	GSU	C4-N9-C8	5.94	111.97	105.74
2	D	602	MES	C5-N4-C3	5.56	120.83	108.84
4	B	606	GSU	C5-C4-N3	-5.47	119.18	126.72
2	D	601	MES	C5-N4-C3	5.40	120.47	108.84
4	D	605	GSU	C5-C4-N3	-5.20	119.56	126.72
4	B00Z	605	GSU	N3-C4-N9	5.01	135.69	127.17
4	B	606	GSU	N3-C4-N9	5.00	135.66	127.17
4	A	604	GSU	C5-C4-N3	-4.92	119.94	126.72
2	B00Z	601	MES	C5-N4-C3	4.91	119.41	108.84
4	D	605	GSU	N3-C4-N9	4.87	135.45	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B00Z	602	MES	C5-N4-C3	4.84	119.26	108.84
2	B00Z	601	MES	O1S-S-C8	4.79	113.96	106.73
4	D	605	GSU	C4-N9-C8	4.76	110.73	105.74
4	B00Z	605	GSU	N1-C2-N3	-4.69	121.49	128.58
4	A	604	GSU	C4-N9-C8	4.63	110.60	105.74
2	B	601	MES	C5-N4-C3	4.60	118.74	108.84
4	A	604	GSU	N3-C4-N9	4.58	134.96	127.17
2	B	602	MES	O2S-S-C8	4.53	113.58	106.73
4	B00Z	605	GSU	C5-C4-N3	-4.52	120.49	126.72
2	B	602	MES	C5-N4-C3	4.41	118.34	108.84
4	B	606	GSU	C4-N9-C8	4.39	110.35	105.74
2	B00Z	601	MES	C6-C5-N4	-4.27	103.62	110.12
4	B	606	GSU	C2-N3-C4	4.22	122.14	111.83
2	B	603	MES	C5-N4-C3	4.19	117.87	108.84
4	A	604	GSU	N1-C2-N3	-4.17	122.26	128.58
4	A	604	GSU	C2-N3-C4	4.15	121.97	111.83
4	B	606	GSU	N1-C2-N3	-4.14	122.31	128.58
2	A	601	MES	C5-N4-C3	4.14	117.75	108.84
4	B00Z	605	GSU	C2-N3-C4	4.09	121.83	111.83
2	B	602	MES	C6-C5-N4	-3.98	104.08	110.12
2	B	601	MES	O3S-S-C8	3.87	113.58	106.00
4	D	605	GSU	C2-N3-C4	3.72	120.92	111.83
4	D	605	GSU	N1-C2-N3	-3.65	123.06	128.58
2	D	601	MES	O1S-S-C8	3.60	112.17	106.73
4	D	605	GSU	O5'-S-N10	3.45	114.62	105.69
2	B	603	MES	O1S-S-C8	3.43	111.91	106.73
2	B	603	MES	C7-N4-C3	3.42	120.36	111.24
2	D	601	MES	O2S-S-C8	3.20	111.56	106.73
4	A	604	GSU	O5'-S-N10	3.17	113.90	105.69
4	B00Z	605	GSU	N9-C8-N7	-3.10	109.53	113.94
2	B00Z	601	MES	C2-C3-N4	-3.10	105.41	110.12
2	B	601	MES	O1S-S-C8	3.09	111.40	106.73
2	B00Z	601	MES	C7-N4-C3	2.97	119.16	111.24
4	B	606	GSU	C6-C5-N7	2.96	137.80	132.09
2	B00Z	602	MES	C7-N4-C5	2.90	118.98	111.24
4	A	604	GSU	C6-C5-N7	2.86	137.60	132.09
4	B	606	GSU	O5'-S-N10	2.84	113.05	105.69
2	B00Z	601	MES	C7-N4-C5	2.71	118.46	111.24
2	B	603	MES	O2S-S-C8	2.65	110.74	106.73
4	B00Z	605	GSU	C6-C5-N7	2.65	137.19	132.09
4	B	606	GSU	N9-C8-N7	-2.64	110.19	113.94
4	D	605	GSU	C-N10-S	-2.63	114.44	124.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	606	GSU	C4-C5-N7	-2.63	107.57	110.58
4	A	604	GSU	N9-C8-N7	-2.63	110.20	113.94
4	D	605	GSU	N9-C8-N7	-2.56	110.30	113.94
2	B	602	MES	O1S-S-C8	2.47	110.46	106.73
4	D	605	GSU	OE1-CD-CG	2.43	121.67	114.00
4	B	606	GSU	C5-C6-N1	2.41	123.62	117.51
4	B00Z	605	GSU	C5-C6-N1	2.38	123.55	117.51
2	D	601	MES	C7-N4-C3	2.37	117.55	111.24
2	B	602	MES	C7-N4-C5	2.36	117.52	111.24
2	D	601	MES	C6-C5-N4	-2.33	106.58	110.12
4	A	604	GSU	C5-C6-N1	2.32	123.40	117.51
4	B00Z	605	GSU	C6-C5-C4	-2.30	114.03	117.18
4	D	605	GSU	O-C-CA	2.30	125.12	120.28
4	D	605	GSU	C4-C5-N7	-2.27	107.99	110.58
4	B00Z	605	GSU	CG-CB-CA	-2.26	108.67	113.86
2	B00Z	601	MES	O3S-S-O1S	-2.24	105.79	111.40
2	D	601	MES	C8-C7-N4	-2.24	103.89	112.36
2	A	601	MES	C7-N4-C5	2.24	117.20	111.24
4	B00Z	605	GSU	C5-C6-N6	-2.23	117.75	123.29
4	B00Z	605	GSU	C4-N9-C1'	-2.20	121.48	126.63
2	B00Z	602	MES	O2S-S-O1S	-2.20	106.67	113.82
4	A	604	GSU	C6-C5-C4	-2.15	114.24	117.18
4	D	605	GSU	C6-C5-N7	2.13	136.19	132.09
4	A	604	GSU	C4-C5-N7	-2.12	108.16	110.58
4	B	606	GSU	C5-N7-C8	2.09	106.74	103.45
4	B00Z	605	GSU	O5'-S-N10	2.08	111.06	105.69
2	D	602	MES	O2S-S-C8	2.03	109.79	106.73

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	MES	C8-C7-N4-C5
2	B	602	MES	C8-C7-N4-C5
2	B	602	MES	C7-C8-S-O1S
2	B	602	MES	C7-C8-S-O2S
2	B	602	MES	C7-C8-S-O3S
2	B	603	MES	C8-C7-N4-C3
2	B	603	MES	C7-C8-S-O1S
2	B	603	MES	C7-C8-S-O2S
2	D	601	MES	C8-C7-N4-C3
2	B00Z	602	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
2	D	601	MES	C7-C8-S-O3S
2	D	602	MES	C7-C8-S-O3S
2	B	603	MES	C7-C8-S-O3S
2	B00Z	602	MES	C7-C8-S-O3S
2	B	601	MES	C8-C7-N4-C5
2	D	602	MES	C8-C7-N4-C5
2	B00Z	601	MES	C8-C7-N4-C3
2	B00Z	602	MES	C8-C7-N4-C3
2	D	601	MES	C7-C8-S-O1S
2	D	601	MES	C7-C8-S-O2S
2	D	602	MES	C7-C8-S-O1S
2	D	602	MES	C7-C8-S-O2S
2	B00Z	602	MES	C7-C8-S-O2S
4	A	604	GSU	C5'-O5'-S-N10
4	B	606	GSU	C5'-O5'-S-N10
4	B00Z	605	GSU	C5'-O5'-S-N10
2	D	602	MES	C8-C7-N4-C3
4	A	604	GSU	O-C-CA-N
4	A	604	GSU	N10-C-CA-N
4	B00Z	605	GSU	O-C-CA-N
4	B00Z	605	GSU	N10-C-CA-N
4	D	605	GSU	C5'-O5'-S-N10
4	B00Z	605	GSU	OE2-CD-CG-CB
4	B00Z	605	GSU	OE1-CD-CG-CB

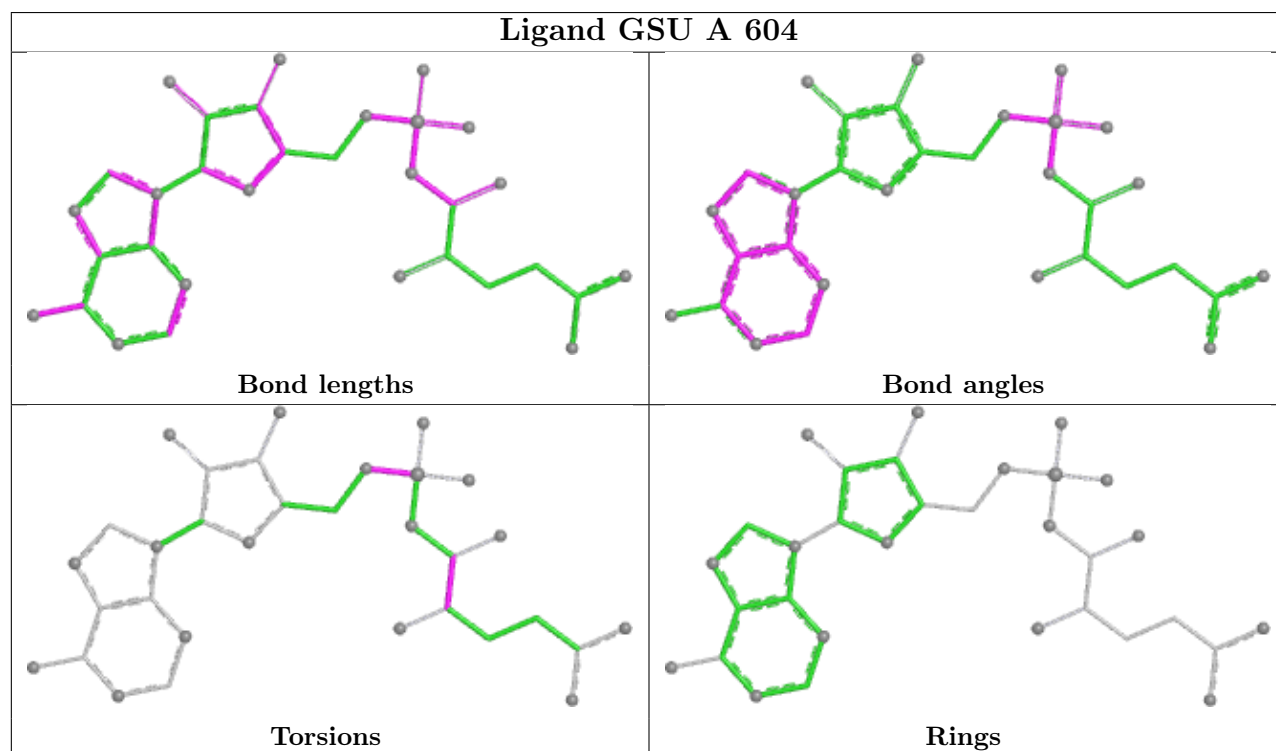
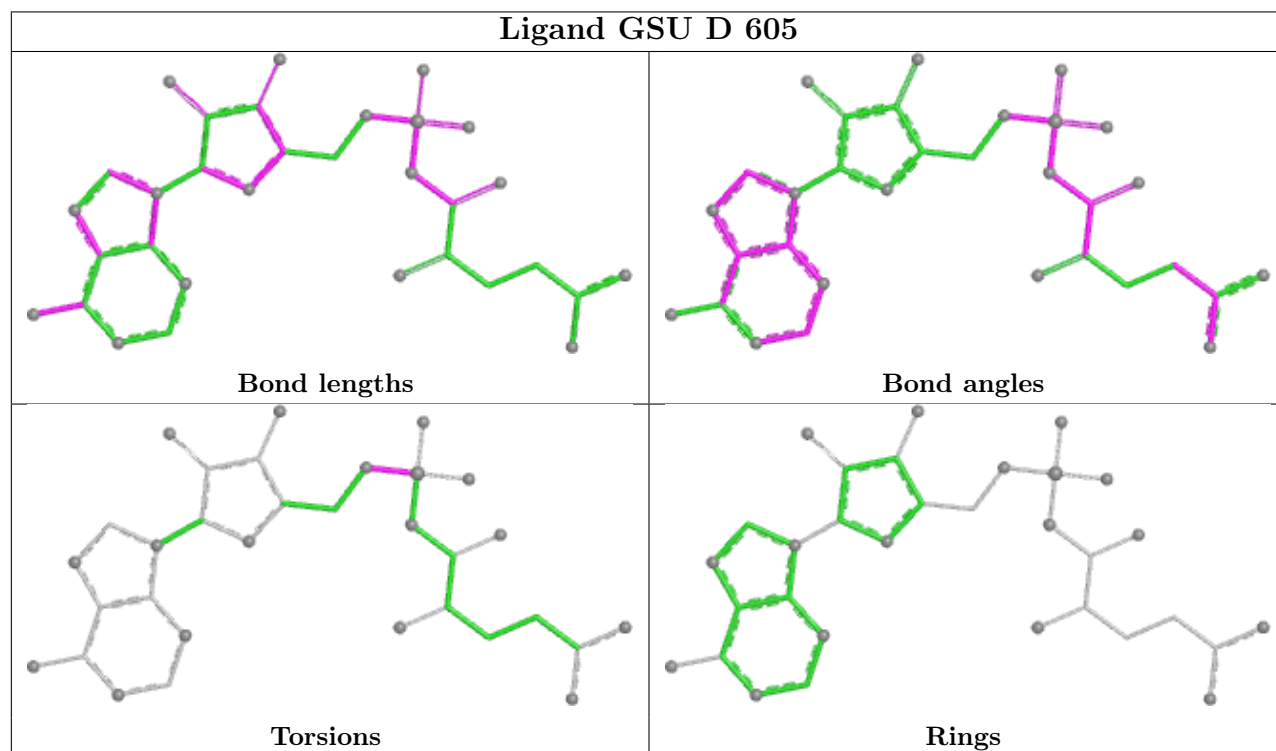
There are no ring outliers.

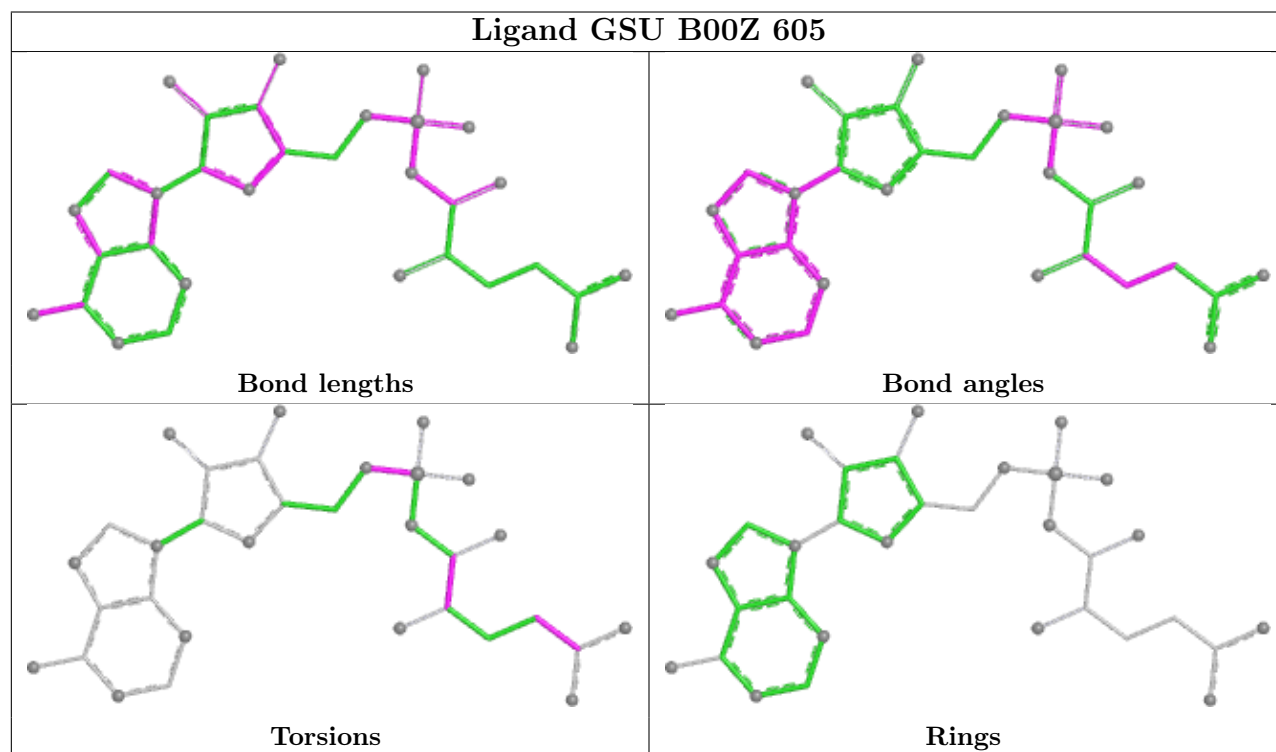
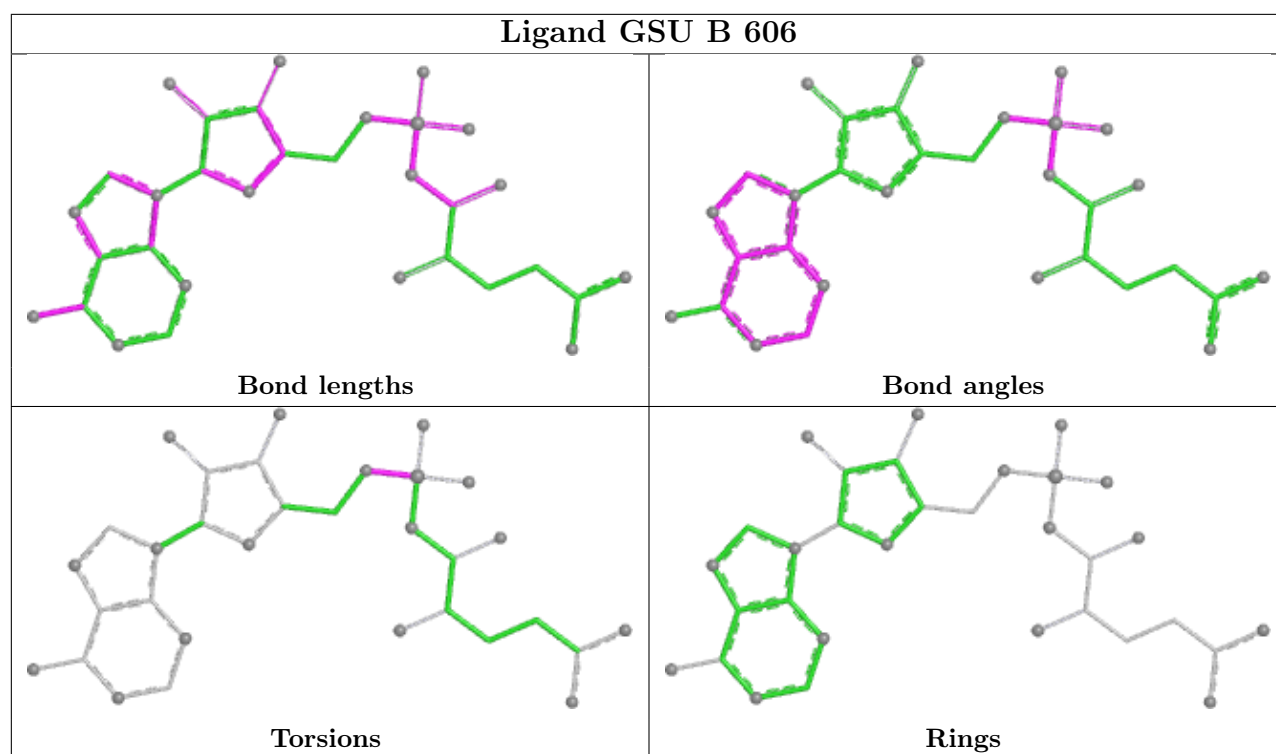
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	MES	2	0
2	B	602	MES	1	0
2	A	601	MES	3	0
2	B	601	MES	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 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 ⓘ

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	533/546 (97%)	0.02	5 (0%) 81 82	29, 39, 51, 61	0
1	B	531/546 (97%)	-0.12	4 (0%) 82 84	27, 36, 52, 69	0
1	B00Z	533/546 (97%)	-0.20	3 (0%) 85 87	24, 34, 50, 61	0
1	D	532/546 (97%)	-0.08	3 (0%) 85 87	24, 36, 57, 67	0
All	All	2129/2184 (97%)	-0.09	15 (0%) 84 85	24, 37, 53, 69	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	168	LEU	3.0
1	D	169	CYS	2.8
1	B00Z	168	LEU	2.5
1	B	72	ALA	2.3
1	A	420	TRP	2.3
1	A	77	PHE	2.2
1	A	132	GLU	2.2
1	B00Z	167	GLU	2.2
1	D	518	ILE	2.2
1	A	214	ARG	2.2
1	B	542	PRO	2.2
1	B00Z	253	ASP	2.1
1	B	169	CYS	2.1
1	A	128	VAL	2.1
1	B	75	LEU	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

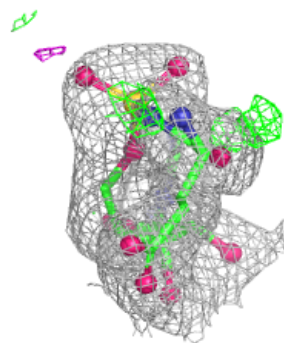
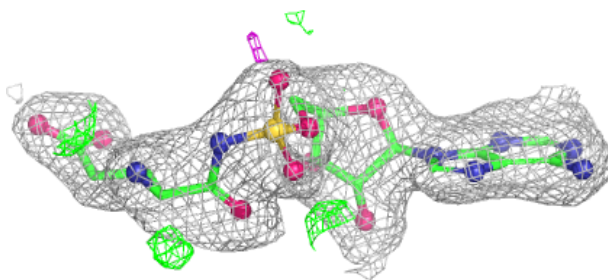
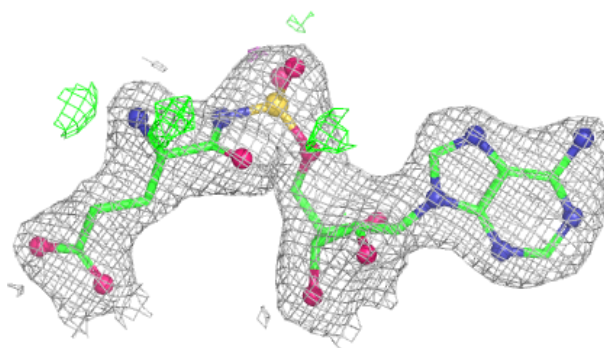
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MES	D	602	12/12	0.79	0.15	50,57,65,74	0
2	MES	B00Z	602	12/12	0.82	0.15	42,50,56,61	0
2	MES	B	602	12/12	0.91	0.11	38,43,48,51	0
2	MES	D	601	12/12	0.92	0.11	43,47,53,54	0
2	MES	B	601	12/12	0.93	0.11	42,48,52,53	0
2	MES	B	603	12/12	0.94	0.08	40,45,49,51	0
2	MES	A	601	12/12	0.94	0.10	44,47,53,53	0
2	MES	B00Z	601	12/12	0.95	0.10	34,42,48,49	0
3	ZN	D	604	1/1	0.95	0.06	70,70,70,70	0
4	GSU	B	606	32/32	0.96	0.07	30,36,38,39	0
4	GSU	B00Z	605	32/32	0.96	0.07	27,32,36,39	0
4	GSU	D	605	32/32	0.97	0.06	29,32,35,37	0
4	GSU	A	604	32/32	0.97	0.06	28,32,37,38	0
3	ZN	A	602	1/1	0.98	0.04	45,45,45,45	0
3	ZN	B00Z	604	1/1	0.98	0.03	51,51,51,51	0
3	ZN	B	605	1/1	0.98	0.03	45,45,45,45	0
3	ZN	D	603	1/1	0.99	0.03	65,65,65,65	0
3	ZN	B	604	1/1	0.99	0.02	29,29,29,29	0
3	ZN	B00Z	603	1/1	0.99	0.04	40,40,40,40	0
3	ZN	A	603	1/1	0.99	0.02	45,45,45,45	0

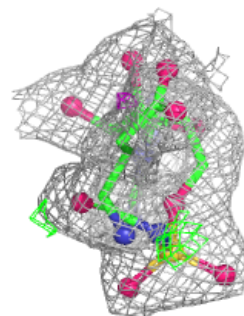
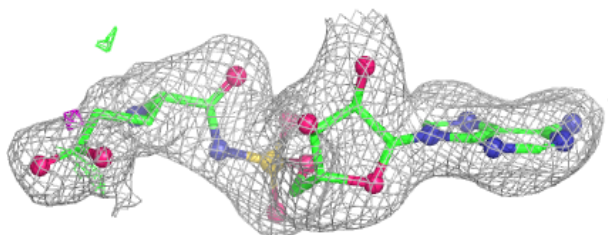
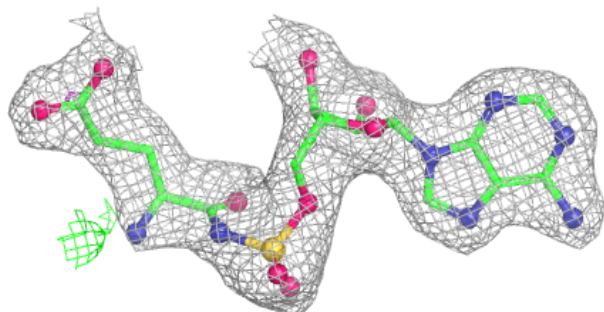
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GSU B 606:

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

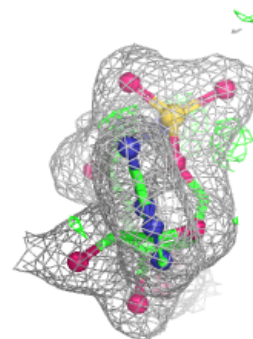
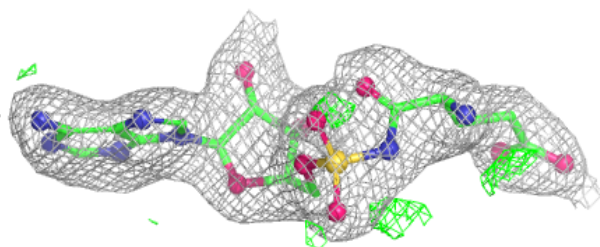
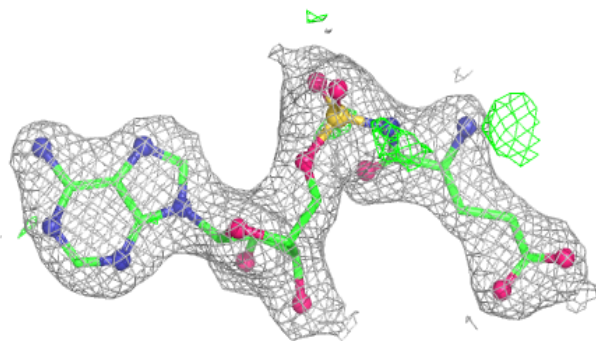
**Electron density around GSU B00Z 605:**

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

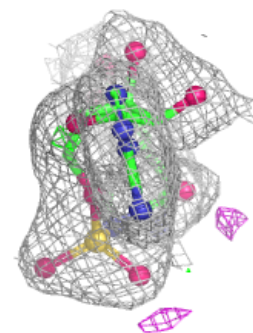
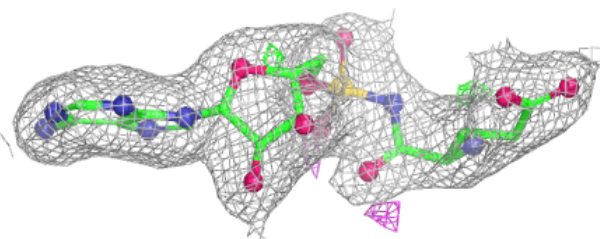
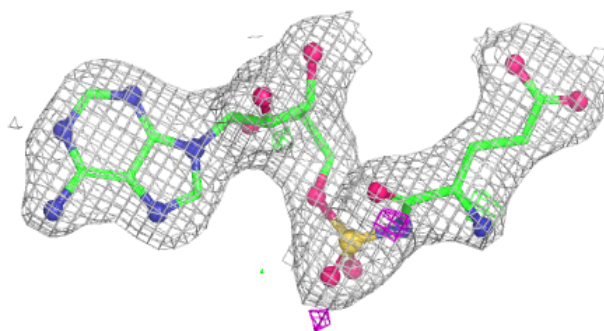


Electron density around GSU D 605:

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

**Electron density around GSU A 604:**

$2mF_o-DF_c$ (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.