Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 04:48 AM EDT

PDB ID	:	1N78
Title	:	Crystal structure of Thermus thermophilus glutamyl-tRNA synthetase complexed with tRNA(Glu) and glutamol-AMP.
Authors	:	Sekine, S.; Nureki, O.; Dubois, D.Y.; Bernier, S.; Chenevert, R.; Lapointe, J.; Vassylyev, D.G.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2002-11-13
Resolution	:	2.10 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:

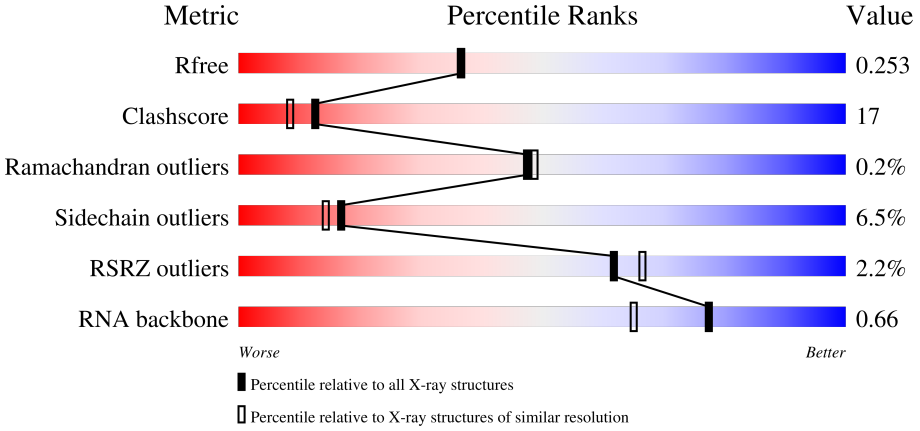
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)
RNA backbone	3102	1000 (2.54-1.66)

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	C	75	48% 37% 8% 7%
1	D	75	% 52% 28% 15% 5%
2	A	468	% 66% 31% •
2	B	468	3% 64% 33% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11637 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 RNA chain called tRNA(Glu).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	75	1597	711	284	527	75	0	0	0
1	D	75	1597	711	284	527	75	0	0	0

- Molecule 2 is a protein called Glutamyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	468	3814	2443	676	687	8	0	0	0
2	B	468	3814	2443	676	687	8	0	0	0

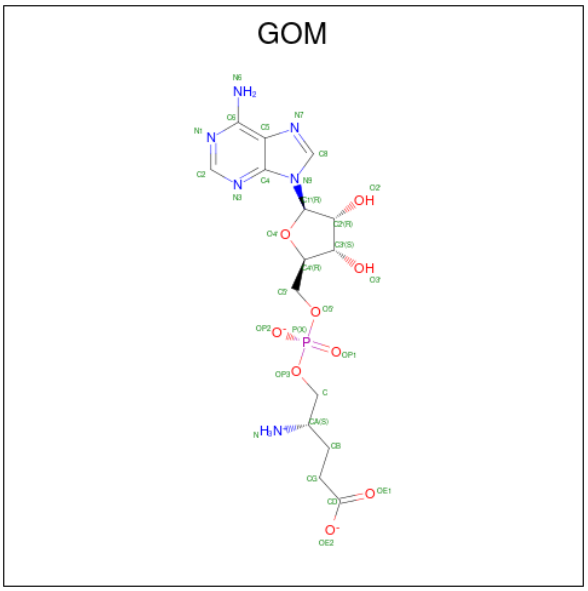
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLY	ALA	SEE REMARK 999	UNP P27000
A	75	GLY	ALA	SEE REMARK 999	UNP P27000
A	77	HIS	THR	SEE REMARK 999	UNP P27000
B	74	GLY	ALA	SEE REMARK 999	UNP P27000
B	75	GLY	ALA	SEE REMARK 999	UNP P27000
B	77	HIS	THR	SEE REMARK 999	UNP P27000

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	C	1	1	1	0	0
3	D	1	1	1	0	0

- Molecule 4 is GLUTAMOL-AMP (three-letter code: GOM) (formula: $C_{15}H_{22}N_6O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	15	6	9	1	0	0
			Total	C	N	O	P		
4	B	1	31	15	6	9	1	0	0

- Molecule 5 is water.

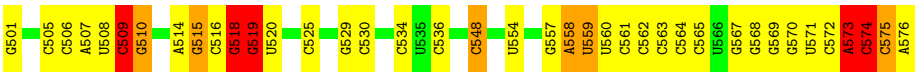
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	108	108	108	0	0
			Total	O		
5	D	122	122	122	0	0
			Total	O		
5	A	275	275	275	0	0
			Total	O		
5	B	246	246	246	0	0

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.

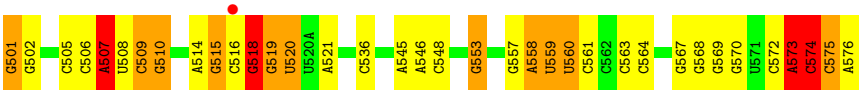
• Molecule 1: tRNA(Glu)

Chain C:



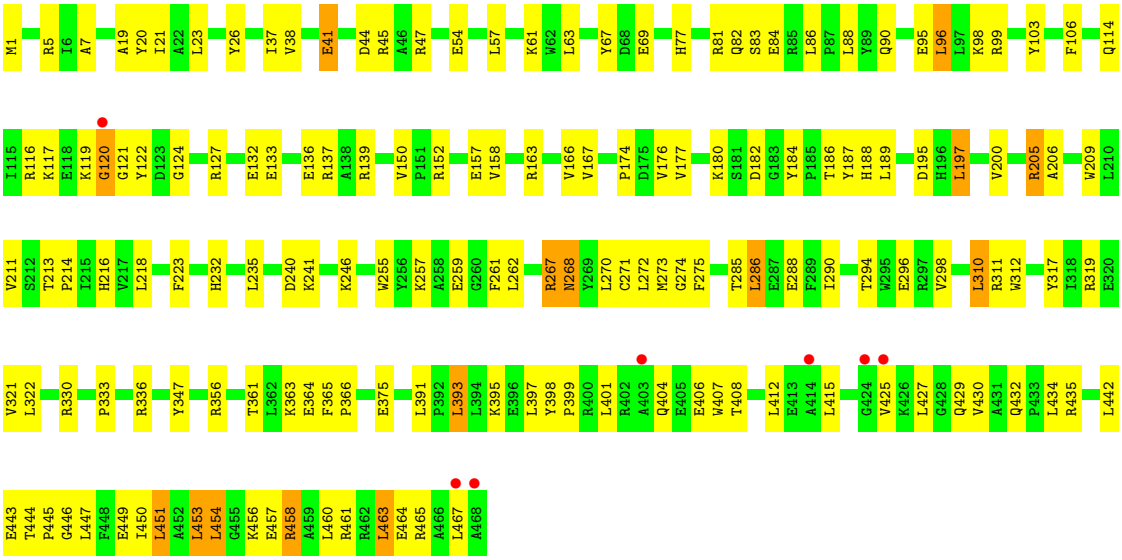
• Molecule 1: tRNA(Glu)

Chain D:



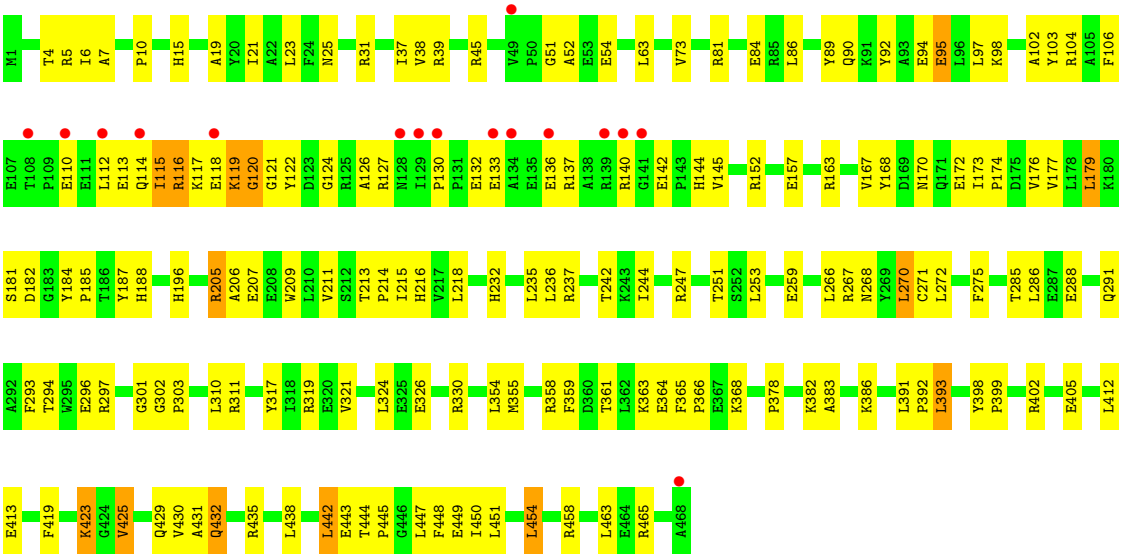
• Molecule 2: Glutamyl-tRNA synthetase

Chain A:



• Molecule 2: Glutamyl-tRNA synthetase

Chain B:


M1 T4 R5 I6 A7 P10 H15 A19 Y20 I21 A22 L23 F24 N25 R31 I37 V38 R39 R45 V49 P50 G51 A52 E53 E54 L63 V73 R81 E84 R85 L86 Y89 Q90 K91 Y92 A93 E94 E95 L96 L97 K98 A102 Y103 R104 A105 F106
E107 T108 P109 E110 E111 L112 E113 Q114 I115 R116 K117 E118 K119 G120 G121 Y122 D123 G124 R125 A126 R127 N128 I129 P130 P131 E132 E133 A134 E135 E136 R137 A138 R139 R140 G141 E142 P143 H144 V145 R152 E157 R163 V167 Y168 D169 N170 Q171 E172 I173 P174 D175 V176 V177 L178 L179 K180
S181 D182 G183 Y184 P185 T186 Y187 H188 H196 R205 A206 E207 E208 W209 L210 V211 S212 T213 P214 I215 H216 V217 L218 H232 L235 L236 R237 T242 K243 I244 R247 T251 S252 L253 E259 L266 R267 N268 Y269 L270 C271 L272 F275 T285 L286 E287 E288 Q291
A292 F293 T294 W295 E296 R297 G301 G302 P303 L310 R311 Y317 I318 R319 E320 V321 L324 E325 E326 R330 L354 M355 R358 F359 D360 T361 L362 K363 E364 F365 P366 E367 K368 P378 K382 A383 K386 L391 P392 L393 Y398 P399 R402 E405 L412
E413 F419 K423 G424 V425 Q429 V430 A431 Q432 R435 L438 L442 E443 T444 P445 G446 L447 F448 E449 I450 L451 L454 R458 L463 E464 R465 A468

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.49Å 219.87Å 135.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 2.10 49.36 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.36-2.10) 86.9 (49.36-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.259 0.211 , 0.253	Depositor DCC
R_{free} test set	4574 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11637	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: MG, GOM

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	C	0.37	1/1782 (0.1%)	0.83	8/2774 (0.3%)
1	D	0.37	1/1782 (0.1%)	0.81	7/2774 (0.3%)
2	A	0.37	0/3910	0.61	0/5293
2	B	0.36	0/3910	0.60	0/5293
All	All	0.37	2/11384 (0.0%)	0.69	15/16134 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	501	G	OP3-P	-7.08	1.52	1.61
1	D	501	G	OP3-P	-6.96	1.52	1.61

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	507	A	C2'-C3'-O3'	8.06	127.23	109.50
1	C	574	C	C2'-C3'-O3'	7.62	126.27	109.50
1	D	518	G	C2'-C3'-O3'	7.53	126.06	109.50
1	C	518	G	C2'-C3'-O3'	7.27	125.49	109.50
1	C	573	A	C2'-C3'-O3'	7.03	124.97	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	519	G	C2'-C3'-O3'	7.00	124.89	113.70
1	C	519	G	C2'-C3'-O3'	6.99	124.89	113.70
1	D	574	C	C2'-C3'-O3'	6.84	124.65	113.70
1	D	573	A	C2'-C3'-O3'	6.52	124.13	113.70
1	D	507	A	C4'-C3'-C2'	5.67	108.27	102.60
1	C	548	C	N1-C1'-C2'	5.32	120.92	114.00
1	D	518	G	C4'-C3'-C2'	5.22	107.82	102.60
1	C	501	G	OP1-P-OP2	-5.20	111.81	119.60
1	C	574	C	C4'-C3'-C2'	5.09	107.69	102.60
1	C	509	C	N1-C1'-C2'	5.01	120.51	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	515	G	Sidechain
1	D	545	A	Sidechain

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	C	1597	0	813	42	0
1	D	1597	0	813	34	0
2	A	3814	0	3818	134	0
2	B	3814	0	3818	153	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	22	3	0
4	B	31	0	22	5	0
5	A	275	0	0	13	0
5	B	246	0	0	14	0
5	C	108	0	0	3	0
5	D	122	0	0	3	0
All	All	11637	0	9306	338	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 17.

All (338) 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)
2:B:454:LEU:HD13	2:B:454:LEU:H	1.35	0.91
2:A:458:ARG:HD3	2:A:461:ARG:HH21	1.38	0.88
2:B:205:ARG:HD3	2:B:232:HIS:CE1	2.09	0.88
2:A:205:ARG:HD3	2:A:232:HIS:CE1	2.09	0.87
2:A:393:LEU:H	2:A:393:LEU:HD23	1.39	0.85
2:A:41:GLU:HG3	2:A:82:GLN:OE1	1.76	0.84
1:D:506:C:O2'	1:D:507:A:H5'	1.76	0.84
1:C:576:A:H2'	2:A:209:TRP:HH2	1.42	0.83
2:A:157:GLU:HG2	2:A:167:VAL:HG22	1.60	0.83
2:B:4:THR:HB	2:B:25:ASN:HD22	1.44	0.81
2:A:294:THR:HG22	2:A:296:GLU:H	1.46	0.81
2:A:267:ARG:HD3	5:A:1063:HOH:O	1.82	0.80
2:A:361:THR:OG1	2:A:364:GLU:HG3	1.82	0.80
2:B:435:ARG:HD3	2:B:444:THR:HG22	1.61	0.80
2:B:465:ARG:HH11	2:B:465:ARG:HB3	1.48	0.79
2:B:267:ARG:HD3	5:B:1565:HOH:O	1.84	0.78
2:B:444:THR:OG1	2:B:445:PRO:HD2	1.84	0.77
2:A:37:ILE:HD12	2:A:69:GLU:HB2	1.67	0.77
2:B:51:GLY:O	2:B:54:GLU:HG2	1.85	0.76
2:B:294:THR:HG22	2:B:297:ARG:HG2	1.67	0.75
1:C:518:G:O2'	1:C:557:G:N2	2.21	0.73
2:A:333:PRO:HA	2:A:336:ARG:NH1	2.03	0.73
2:A:454:LEU:HD13	2:A:458:ARG:HE	1.53	0.73
2:B:438:LEU:HD11	2:B:451:LEU:HD13	1.70	0.72
2:A:205:ARG:HD3	2:A:232:HIS:HE1	1.55	0.71
2:B:454:LEU:HD13	2:B:454:LEU:N	2.06	0.71
1:C:576:A:H2'	2:A:209:TRP:CH2	2.25	0.71
2:B:326:GLU:O	2:B:330:ARG:HG3	1.92	0.69
2:A:294:THR:HG22	2:A:296:GLU:N	2.07	0.69
2:A:294:THR:CG2	2:A:296:GLU:H	2.07	0.68
1:D:576:A:H5"	2:B:187:TYR:HB2	1.75	0.68
2:B:211:VAL:HG23	5:B:1009:HOH:O	1.94	0.67
1:C:575:C:H2'	1:C:576:A:O4'	1.95	0.67
2:A:401:LEU:HB3	2:A:460:LEU:HD21	1.77	0.67
2:B:235:LEU:O	2:B:237:ARG:HD3	1.95	0.67
2:B:116:ARG:O	2:B:120:GLY:HA2	1.95	0.66
2:A:319:ARG:HD2	5:A:1067:HOH:O	1.95	0.66
2:B:137:ARG:HB3	2:B:142:GLU:OE1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:365:PHE:HB3	2:A:366:PRO:HD3	1.78	0.66
2:B:294:THR:CG2	2:B:297:ARG:HG2	2.26	0.66
2:B:361:THR:OG1	2:B:364:GLU:HG3	1.96	0.65
2:A:188:HIS:HD2	2:A:216:HIS:CE1	2.13	0.65
1:D:570:G:H21	2:B:211:VAL:HG21	1.61	0.65
2:B:45:ARG:HD3	2:B:184:TYR:CE2	2.32	0.65
4:B:601:GOM:H5"	5:B:1624:HOH:O	1.96	0.64
2:B:465:ARG:HB3	2:B:465:ARG:NH1	2.12	0.64
2:A:267:ARG:HD2	2:A:286:LEU:HG	1.80	0.63
2:A:54:GLU:HG2	5:A:1584:HOH:O	1.98	0.63
2:B:285:THR:OG1	2:B:288:GLU:HG3	1.98	0.63
2:B:382:LYS:HB3	2:B:382:LYS:HZ2	1.63	0.63
2:B:382:LYS:HB3	2:B:382:LYS:NZ	2.13	0.63
1:C:534:C:O2	2:A:435:ARG:NH2	2.31	0.63
1:C:558:A:O2'	1:C:560:U:H5	1.82	0.63
2:B:237:ARG:NH1	2:B:302:GLY:HA3	2.13	0.63
2:A:458:ARG:HD3	2:A:461:ARG:NH2	2.11	0.63
2:B:398:TYR:HB3	2:B:399:PRO:HD3	1.82	0.62
4:B:601:GOM:H3'	4:B:601:GOM:HC1	1.81	0.62
1:D:520:U:H2'	1:D:521:A:H5'	1.81	0.62
2:A:444:THR:HB	2:A:445:PRO:HD2	1.81	0.62
1:C:570:G:H21	2:A:211:VAL:HG11	1.63	0.62
2:B:196:HIS:HD2	5:B:1567:HOH:O	1.82	0.62
2:A:188:HIS:HD2	2:A:216:HIS:HE1	1.46	0.62
2:B:365:PHE:HB3	2:B:366:PRO:HD3	1.82	0.62
2:B:444:THR:HG23	2:B:445:PRO:O	2.00	0.61
2:B:132:GLU:O	2:B:136:GLU:HG2	2.01	0.61
2:A:427:LEU:O	2:A:430:VAL:HG12	2.01	0.61
2:B:425:VAL:HG22	2:B:429:GLN:OE1	2.01	0.61
1:C:575:C:OP2	2:A:180:LYS:HE2	2.00	0.60
1:D:558:A:H2'	1:D:560:U:OP2	2.00	0.60
2:A:393:LEU:HD23	2:A:393:LEU:N	2.15	0.60
1:C:536:C:H4'	2:A:443:GLU:HG2	1.84	0.60
2:B:319:ARG:HD2	5:B:1023:HOH:O	2.01	0.60
2:B:435:ARG:HH11	2:B:444:THR:CG2	2.14	0.60
2:A:177:VAL:CG2	2:A:186:THR:HG21	2.32	0.60
2:A:446:GLY:O	2:A:449:GLU:HG2	2.01	0.60
2:B:90:GLN:O	2:B:94:GLU:HG3	2.01	0.60
2:B:115:ILE:HD13	2:B:116:ARG:N	2.17	0.60
2:A:41:GLU:HG2	5:A:1035:HOH:O	2.02	0.60
2:A:1:MET:HB2	5:A:1556:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:C:H5'	2:A:177:VAL:HG11	1.85	0.59
2:A:177:VAL:HG23	2:A:186:THR:HG21	1.84	0.59
1:C:529:G:H2'	1:C:530:C:C6	2.38	0.59
2:B:206:ALA:HB3	4:B:601:GOM:O2'	2.02	0.59
1:D:518:G:O2'	1:D:557:G:N2	2.35	0.59
1:D:558:A:O2'	1:D:560:U:H5	1.85	0.58
2:B:31:ARG:NH1	2:B:293:PHE:O	2.36	0.58
2:A:23:LEU:HD21	2:A:271:CYS:SG	2.43	0.58
1:D:558:A:O2'	1:D:559:U:OP1	2.19	0.58
2:A:458:ARG:CD	2:A:461:ARG:HH21	2.14	0.58
1:D:563:C:H2'	1:D:564:C:H6	1.68	0.58
1:C:563:C:H2'	1:C:564:C:C6	2.39	0.58
1:D:576:A:H2'	2:B:209:TRP:HH2	1.68	0.58
2:A:26:TYR:CE1	2:A:290:ILE:HD11	2.39	0.58
2:B:393:LEU:HD22	2:B:419:PHE:HE1	1.67	0.58
2:A:255:TRP:CZ2	2:A:259:GLU:HG3	2.39	0.57
2:B:37:ILE:HG22	2:B:38:VAL:N	2.18	0.57
1:D:558:A:H1'	5:D:1389:HOH:O	2.04	0.57
2:B:247:ARG:HB2	5:B:1025:HOH:O	2.04	0.57
2:B:188:HIS:HD2	2:B:216:HIS:CE1	2.23	0.57
2:B:104:ARG:HB3	2:B:144:HIS:HD2	1.70	0.57
1:C:505:C:O2'	2:A:163:ARG:NH1	2.38	0.57
2:A:5:ARG:NH1	4:A:600:GOM:OE2	2.35	0.57
2:A:434:LEU:HD23	2:A:447:LEU:HD21	1.88	0.56
2:B:119:LYS:H	2:B:119:LYS:HD2	1.70	0.56
2:B:311:ARG:NH1	2:B:311:ARG:HB3	2.20	0.56
2:B:425:VAL:HG22	2:B:429:GLN:CD	2.25	0.56
2:B:205:ARG:HD3	2:B:232:HIS:HE1	1.69	0.56
2:A:136:GLU:HG2	2:A:139:ARG:NH2	2.21	0.56
2:B:130:PRO:HD2	2:B:133:GLU:OE2	2.06	0.56
2:B:106:PHE:CD2	2:B:144:HIS:HB3	2.42	0.55
2:B:145:VAL:HG12	2:B:181:SER:N	2.21	0.55
1:D:574:C:O2'	1:D:575:C:OP1	2.24	0.55
1:C:518:G:H21	1:C:557:G:H2'	1.69	0.55
1:D:576:A:H2'	2:B:209:TRP:CH2	2.42	0.55
2:A:404:GLN:CG	2:A:415:LEU:HD22	2.36	0.55
2:B:19:ALA:HB2	2:B:253:LEU:HD11	1.88	0.55
2:A:240:ASP:O	2:A:241:LYS:HB2	2.07	0.55
1:C:576:A:H5"	2:A:187:TYR:HB2	1.87	0.55
2:A:19:ALA:HB1	2:A:63:LEU:CD1	2.37	0.55
2:A:213:THR:N	2:A:214:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:158:VAL:HB	2:A:166:VAL:HG23	1.87	0.55
1:C:536:C:C4'	2:A:443:GLU:HG2	2.37	0.55
2:B:157:GLU:HG2	2:B:167:VAL:HG22	1.88	0.55
2:A:188:HIS:CD2	2:A:216:HIS:HE1	2.25	0.54
2:B:267:ARG:HD2	2:B:286:LEU:HD13	1.87	0.54
2:B:116:ARG:CD	2:B:121:GLY:H	2.20	0.54
1:C:574:C:H5'	2:A:177:VAL:CG1	2.36	0.54
1:D:506:C:C2'	1:D:507:A:H5'	2.37	0.54
2:A:347:TYR:CE1	2:A:453:LEU:HD22	2.43	0.54
2:B:45:ARG:HD3	2:B:184:TYR:CZ	2.42	0.54
2:B:122:TYR:CE2	2:B:124:GLY:HA2	2.42	0.54
2:B:114:GLN:O	2:B:118:GLU:HG2	2.08	0.53
2:A:391:LEU:O	2:A:395:LYS:HG2	2.08	0.53
2:B:432:GLN:NE2	2:B:432:GLN:HA	2.23	0.53
1:D:536:C:H4'	2:B:443:GLU:HG2	1.90	0.53
2:B:393:LEU:HD22	2:B:419:PHE:CE1	2.43	0.53
1:D:575:C:H2'	1:D:576:A:O4'	2.09	0.53
2:A:21:ILE:HG13	4:A:600:GOM:H1'	1.90	0.53
2:B:247:ARG:HD3	5:B:1025:HOH:O	2.09	0.53
1:C:565:C:H1'	5:C:1363:HOH:O	2.09	0.53
2:A:460:LEU:O	2:A:464:GLU:HG3	2.08	0.53
2:A:116:ARG:HG3	2:A:121:GLY:H	1.74	0.52
2:A:114:GLN:HG3	5:A:2000:HOH:O	2.08	0.52
2:A:268:ASN:C	2:A:268:ASN:HD22	2.10	0.52
2:B:163:ARG:HG3	2:B:163:ARG:HH11	1.74	0.52
2:B:391:LEU:N	2:B:392:PRO:HD2	2.24	0.52
2:B:432:GLN:HE21	2:B:432:GLN:CA	2.22	0.52
1:D:514:A:C2'	1:D:515:G:H5'	2.39	0.52
2:B:378:PRO:HA	5:B:1300:HOH:O	2.09	0.52
2:A:150:VAL:O	2:A:152:ARG:HG3	2.09	0.52
2:B:354:LEU:HD22	2:B:449:GLU:HG3	1.91	0.52
2:B:402:ARG:HH11	2:B:402:ARG:HG2	1.75	0.52
1:C:558:A:O2'	1:C:559:U:OP1	2.24	0.52
1:D:574:C:H5'	2:B:177:VAL:HG21	1.91	0.52
2:A:195:ASP:HB3	2:A:200:VAL:CG2	2.40	0.52
2:A:445:PRO:HG2	2:A:450:ILE:HD11	1.90	0.52
1:C:509:C:H5'	1:C:510:G:OP2	2.09	0.52
2:A:205:ARG:HG3	2:A:209:TRP:CD1	2.44	0.52
2:B:454:LEU:N	2:B:454:LEU:HD22	2.24	0.52
2:B:213:THR:N	2:B:214:PRO:CD	2.73	0.52
1:D:563:C:H2'	1:D:564:C:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ALA:HA	2:B:39:ARG:O	2.09	0.52
1:C:554:U:H1'	5:C:1536:HOH:O	2.10	0.51
2:A:41:GLU:HG3	2:A:82:GLN:CD	2.31	0.51
2:A:407:TRP:CE2	2:A:456:LYS:HA	2.45	0.51
2:A:445:PRO:CG	2:A:450:ILE:HD11	2.40	0.51
2:B:205:ARG:HG3	2:B:209:TRP:CD1	2.45	0.51
1:D:576:A:N3	2:B:209:TRP:CH2	2.78	0.51
2:B:454:LEU:H	2:B:454:LEU:CD1	2.06	0.51
2:B:423:LYS:HB2	2:B:423:LYS:HZ2	1.76	0.51
2:A:5:ARG:HB3	2:A:37:ILE:HB	1.93	0.51
2:A:152:ARG:HG2	2:A:152:ARG:HH11	1.74	0.51
2:A:195:ASP:HB3	2:A:200:VAL:HG22	1.94	0.50
2:B:450:ILE:O	2:B:454:LEU:HD11	2.10	0.50
2:B:92:TYR:O	2:B:95:GLU:HB3	2.12	0.50
2:A:182:ASP:OD2	2:A:184:TYR:HB2	2.11	0.50
1:D:558:A:O2'	1:D:559:U:P	2.70	0.50
2:A:122:TYR:CE2	2:A:124:GLY:HA2	2.47	0.50
2:B:86:LEU:HD21	2:B:184:TYR:CE1	2.47	0.50
1:C:568:G:O2'	1:C:569:G:H5'	2.11	0.50
2:B:133:GLU:O	2:B:137:ARG:HG3	2.12	0.49
2:A:435:ARG:NH1	2:A:444:THR:OG1	2.44	0.49
2:B:386:LYS:NZ	2:B:432:GLN:HG2	2.28	0.49
1:D:505:C:H4'	2:B:163:ARG:HD3	1.93	0.49
2:A:261:PHE:CE2	2:A:310:LEU:HD13	2.47	0.49
2:B:413:GLU:HG3	2:B:448:PHE:CZ	2.48	0.49
2:B:168:TYR:CD2	2:B:214:PRO:HG3	2.47	0.49
2:A:133:GLU:O	2:A:137:ARG:HG3	2.12	0.49
2:A:177:VAL:HG23	2:A:186:THR:CG2	2.42	0.49
2:A:406:GLU:O	2:A:406:GLU:HG3	2.12	0.49
2:B:359:PHE:HB2	2:B:364:GLU:HB2	1.95	0.49
2:A:174:PRO:HG2	2:A:176:VAL:HG13	1.95	0.49
2:B:89:TYR:CD2	2:B:185:PRO:HG3	2.47	0.49
2:A:44:ASP:OD1	2:A:47:ARG:HG3	2.12	0.49
2:B:51:GLY:HA2	5:B:1578:HOH:O	2.12	0.49
1:C:506:C:O2'	1:C:507:A:H5'	2.12	0.49
2:A:19:ALA:HB1	2:A:63:LEU:HD11	1.95	0.49
2:B:112:LEU:O	2:B:115:ILE:HD13	2.12	0.48
2:B:119:LYS:HD2	2:B:119:LYS:N	2.28	0.48
2:A:363:LYS:HD3	5:A:1308:HOH:O	2.12	0.48
2:A:20:TYR:CE1	2:A:273:MET:HB2	2.48	0.48
2:A:96:LEU:HD13	2:A:223:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:G:H2'	1:C:568:G:H8	1.78	0.48
2:A:246:LYS:HE2	5:A:1099:HOH:O	2.14	0.48
2:A:408:THR:O	2:A:412:LEU:HD23	2.13	0.48
2:A:88:LEU:HD21	2:A:197:LEU:HD23	1.96	0.48
1:C:558:A:H1'	5:C:1315:HOH:O	2.14	0.48
2:B:206:ALA:CB	4:B:601:GOM:O2'	2.62	0.48
1:C:558:A:H2'	1:C:560:U:OP2	2.14	0.47
2:A:463:LEU:HD22	2:A:467:LEU:HG	1.95	0.47
1:C:558:A:O2'	1:C:559:U:P	2.72	0.47
2:A:271:CYS:O	2:A:275:PHE:HB3	2.14	0.47
1:C:529:G:H2'	1:C:530:C:H6	1.76	0.47
2:A:83:SER:O	2:A:86:LEU:HD13	2.13	0.47
2:A:425:VAL:HG22	2:A:429:GLN:HG3	1.96	0.47
2:B:363:LYS:O	2:B:366:PRO:HD2	2.14	0.47
2:A:363:LYS:O	2:A:366:PRO:HD2	2.15	0.47
2:B:176:VAL:HG11	2:B:215:ILE:HD13	1.96	0.47
1:D:574:C:H5'	2:B:177:VAL:CG2	2.44	0.46
2:A:398:TYR:HD1	2:A:463:LEU:HD13	1.80	0.46
2:B:6:ILE:CD1	2:B:21:ILE:HG22	2.45	0.46
1:D:576:A:H3'	2:B:187:TYR:HB2	1.97	0.46
2:B:330:ARG:HD3	5:B:1019:HOH:O	2.15	0.46
2:B:386:LYS:HE2	5:B:2076:HOH:O	2.16	0.46
2:A:404:GLN:HG3	2:A:415:LEU:HD22	1.97	0.46
2:A:330:ARG:HD3	5:A:1031:HOH:O	2.15	0.46
2:A:61:LYS:HE3	2:A:67:TYR:OH	2.15	0.46
2:A:206:ALA:HB1	2:A:235:LEU:HD13	1.98	0.46
2:B:168:TYR:CE2	2:B:214:PRO:HG3	2.51	0.46
2:B:393:LEU:HD13	2:B:430:VAL:HG22	1.97	0.46
2:A:81:ARG:HD2	2:A:84:GLU:OE2	2.16	0.46
2:A:119:LYS:NZ	5:A:1837:HOH:O	2.47	0.46
2:A:206:ALA:HB3	4:A:600:GOM:O2'	2.16	0.45
2:B:152:ARG:HG2	5:B:1640:HOH:O	2.16	0.45
2:A:106:PHE:CD1	2:A:106:PHE:N	2.84	0.45
2:A:116:ARG:O	2:A:120:GLY:HA2	2.16	0.45
2:A:257:LYS:HE3	5:A:1111:HOH:O	2.15	0.45
2:B:275:PHE:CE2	2:B:297:ARG:HB2	2.51	0.45
1:C:508:U:H6	1:C:508:U:O5'	2.00	0.45
1:D:572:C:H5'	1:D:573:A:C5'	2.46	0.45
2:B:23:LEU:HD21	2:B:271:CYS:SG	2.56	0.45
2:B:37:ILE:CG2	2:B:38:VAL:N	2.80	0.45
2:B:113:GLU:OE1	2:B:113:GLU:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:G:N2	1:C:557:G:H2'	2.31	0.45
1:D:567:G:H2'	1:D:568:G:H8	1.81	0.45
1:C:514:A:C2'	1:C:515:G:H5'	2.47	0.45
1:C:563:C:H2'	1:C:564:C:H6	1.80	0.45
1:C:519:G:N2	1:C:557:G:H1'	2.32	0.45
2:A:317:TYR:HA	2:A:321:VAL:HG23	1.99	0.45
2:A:262:LEU:HD13	2:A:322:LEU:HD11	1.99	0.45
2:B:237:ARG:HH11	2:B:302:GLY:HA3	1.82	0.45
2:B:444:THR:OG1	2:B:445:PRO:CD	2.61	0.45
2:A:454:LEU:HD13	2:A:458:ARG:NE	2.27	0.44
2:A:274:GLY:O	2:A:298:VAL:HA	2.17	0.44
2:B:432:GLN:NE2	2:B:432:GLN:CA	2.79	0.44
2:A:77:HIS:HD2	5:A:1346:HOH:O	1.99	0.44
2:B:454:LEU:H	2:B:454:LEU:HD22	1.81	0.44
1:D:501:G:H2'	1:D:502:G:C8	2.53	0.44
2:A:188:HIS:CD2	2:A:216:HIS:CE1	3.01	0.44
2:B:163:ARG:NH2	2:B:207:GLU:HG3	2.33	0.44
2:B:301:GLY:O	2:B:303:PRO:HD3	2.17	0.44
2:B:174:PRO:HG2	2:B:176:VAL:HG13	2.00	0.44
1:C:561:C:H2'	1:C:562:C:C6	2.52	0.44
1:C:573:A:O2'	1:C:574:C:H3'	2.18	0.44
2:A:174:PRO:HG2	2:A:176:VAL:CG1	2.48	0.44
2:A:397:LEU:HG	2:A:401:LEU:HD13	1.99	0.43
2:A:398:TYR:N	2:A:399:PRO:HD2	2.34	0.43
2:A:463:LEU:HD22	2:A:463:LEU:O	2.18	0.43
2:B:270:LEU:HD12	2:B:270:LEU:HA	1.89	0.43
2:A:45:ARG:HG3	2:A:45:ARG:HH11	1.84	0.43
1:C:569:G:O2'	1:C:570:G:H5'	2.19	0.43
2:B:118:GLU:HB2	2:B:119:LYS:HD2	2.00	0.43
2:B:182:ASP:OD2	2:B:184:TYR:HB2	2.18	0.43
1:D:569:G:H5"	2:B:242:THR:HA	2.01	0.43
2:A:95:GLU:O	2:A:99:ARG:HG3	2.18	0.43
2:B:152:ARG:HG2	2:B:152:ARG:HH11	1.84	0.43
2:B:454:LEU:HB2	2:B:458:ARG:HD2	2.00	0.43
1:C:525:C:H5"	2:A:312:TRP:CE2	2.54	0.43
1:C:574:C:C4'	2:A:177:VAL:HG21	2.49	0.43
2:B:244:ILE:HG12	2:B:251:THR:HG22	2.00	0.43
1:D:501:G:H2'	1:D:502:G:H8	1.84	0.43
2:A:37:ILE:HG22	2:A:38:VAL:N	2.33	0.43
2:A:38:VAL:HG11	2:A:57:LEU:HD21	2.01	0.43
1:C:519:G:C5	1:C:557:G:N2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:A:C4	2:A:209:TRP:CH2	3.07	0.42
1:D:509:C:H5'	1:D:510:G:OP2	2.20	0.42
1:D:574:C:H5	2:B:112:LEU:HD12	1.85	0.42
2:B:136:GLU:O	2:B:140:ARG:HG2	2.19	0.42
2:B:358:ARG:O	2:B:368:LYS:CE	2.68	0.42
2:B:10:PRO:HB3	2:B:52:ALA:HB3	2.01	0.42
2:A:285:THR:HG23	2:A:288:GLU:OE1	2.20	0.42
1:C:571:U:H2'	1:C:572:C:C6	2.55	0.42
1:D:521:A:H61	1:D:546:A:H2'	1.83	0.42
1:D:553:G:H2'	1:D:553:G:N3	2.35	0.42
2:A:262:LEU:HD12	2:A:317:TYR:HB3	2.00	0.42
2:B:15:HIS:HB2	5:B:1482:HOH:O	2.20	0.42
2:B:163:ARG:HG3	2:B:163:ARG:NH1	2.34	0.42
5:D:1358:HOH:O	2:B:172:GLU:HG3	2.19	0.42
2:B:86:LEU:HD21	2:B:184:TYR:CZ	2.55	0.42
2:B:170:ASN:HA	2:B:173:ILE:HD12	2.02	0.42
2:B:179:LEU:HD23	2:B:184:TYR:O	2.19	0.42
1:C:505:C:OP1	2:A:166:VAL:HG12	2.20	0.42
1:D:514:A:H2'	1:D:515:G:H5'	2.02	0.42
5:D:1539:HOH:O	2:B:188:HIS:HE1	2.03	0.42
2:A:432:GLN:HA	2:A:432:GLN:OE1	2.20	0.42
2:A:152:ARG:HG2	2:A:152:ARG:NH1	2.34	0.41
2:B:97:LEU:HD12	2:B:102:ALA:O	2.19	0.41
2:B:317:TYR:HA	2:B:321:VAL:HG23	2.02	0.41
2:B:432:GLN:HA	2:B:432:GLN:HE21	1.84	0.41
2:A:311:ARG:HB3	2:A:311:ARG:NH1	2.36	0.41
2:B:73:VAL:HG12	2:B:73:VAL:O	2.19	0.41
2:B:114:GLN:O	2:B:117:LYS:HB3	2.20	0.41
2:B:431:ALA:CB	2:B:447:LEU:HD22	2.51	0.41
2:A:7:ALA:HB1	2:A:41:GLU:OE1	2.20	0.41
2:A:361:THR:HG1	2:A:364:GLU:HG3	1.83	0.41
2:B:124:GLY:O	2:B:127:ARG:HG3	2.20	0.41
2:B:188:HIS:HD2	2:B:216:HIS:HE1	1.66	0.41
2:A:114:GLN:NE2	2:A:117:LYS:HD2	2.35	0.41
2:B:21:ILE:HD13	4:B:601:GOM:H1'	2.02	0.41
2:B:383:ALA:HA	2:B:442:LEU:HD13	2.02	0.41
2:B:435:ARG:HH11	2:B:444:THR:HG22	1.85	0.41
2:A:447:LEU:O	2:A:451:LEU:HB2	2.19	0.41
2:B:81:ARG:HB2	2:B:84:GLU:HG3	2.03	0.41
2:B:103:TYR:CE1	2:B:126:ALA:HB3	2.56	0.41
2:A:103:TYR:CZ	2:A:127:ARG:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:375:GLU:HG3	2:A:465:ARG:HH12	1.86	0.41
2:B:25:ASN:ND2	5:B:1018:HOH:O	2.52	0.41
2:B:431:ALA:HB1	2:B:447:LEU:HD22	2.02	0.41
2:B:94:GLU:O	2:B:98:LYS:HD3	2.21	0.41
2:B:110:GLU:CD	2:B:110:GLU:H	2.25	0.41
2:B:205:ARG:O	2:B:232:HIS:HA	2.22	0.40
2:A:90:GLN:HG2	5:A:1595:HOH:O	2.21	0.40
2:B:311:ARG:HH11	2:B:311:ARG:CB	2.34	0.40
2:B:450:ILE:HD13	2:B:450:ILE:HA	1.91	0.40
2:B:19:ALA:HB1	2:B:63:LEU:CD1	2.51	0.40
2:B:391:LEU:N	2:B:392:PRO:CD	2.84	0.40
2:A:163:ARG:NH2	2:A:232:HIS:O	2.53	0.40
2:B:115:ILE:HA	2:B:118:GLU:HG2	2.03	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	
2	A	466/468 (100%)	456 (98%)	9 (2%)	1 (0%)	47	49
2	B	466/468 (100%)	453 (97%)	12 (3%)	1 (0%)	47	49
All	All	932/936 (100%)	909 (98%)	21 (2%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	120	GLY
2	A	120	GLY

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	
2	A	393/393 (100%)	370 (94%)	23 (6%)	19	17
2	B	393/393 (100%)	365 (93%)	28 (7%)	14	11
All	All	786/786 (100%)	735 (94%)	51 (6%)	17	14

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	41	GLU
2	A	96	LEU
2	A	98	LYS
2	A	132	GLU
2	A	189	LEU
2	A	197	LEU
2	A	205	ARG
2	A	218	LEU
2	A	267	ARG
2	A	268	ASN
2	A	270	LEU
2	A	272	LEU
2	A	286	LEU
2	A	310	LEU
2	A	356	ARG
2	A	393	LEU
2	A	442	LEU
2	A	451	LEU
2	A	453	LEU
2	A	454	LEU
2	A	457	GLU
2	A	458	ARG
2	A	463	LEU
2	B	5	ARG
2	B	95	GLU
2	B	115	ILE
2	B	116	ARG

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Mol	Chain	Res	Type
2	B	119	LYS
2	B	179	LEU
2	B	205	ARG
2	B	218	LEU
2	B	236	LEU
2	B	259	GLU
2	B	266	LEU
2	B	268	ASN
2	B	270	LEU
2	B	272	LEU
2	B	291	GLN
2	B	296	GLU
2	B	310	LEU
2	B	324	LEU
2	B	355	MET
2	B	393	LEU
2	B	405	GLU
2	B	412	LEU
2	B	423	LYS
2	B	425	VAL
2	B	432	GLN
2	B	442	LEU
2	B	454	LEU
2	B	463	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	32	ASN
2	A	114	GLN
2	A	188	HIS
2	A	191	ASN
2	A	196	HIS
2	A	216	HIS
2	A	232	HIS
2	A	404	GLN
2	B	25	ASN
2	B	32	ASN
2	B	171	GLN
2	B	188	HIS
2	B	191	ASN
2	B	196	HIS

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Mol	Chain	Res	Type
2	B	216	HIS
2	B	232	HIS
2	B	404	GLN
2	B	432	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	11 (14%)	6 (8%)
1	D	74/75 (98%)	14 (18%)	9 (12%)
All	All	148/150 (98%)	25 (16%)	15 (10%)

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	510	G
1	C	516	C
1	C	518	G
1	C	519	G
1	C	520	U
1	C	548	C
1	C	558	A
1	C	559	U
1	C	573	A
1	C	574	C
1	C	575	C
1	D	508	U
1	D	510	G
1	D	516	C
1	D	518	G
1	D	519	G
1	D	520	U
1	D	548	C
1	D	553	G
1	D	558	A
1	D	559	U
1	D	561	C
1	D	573	A
1	D	574	C
1	D	575	C

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	509	C
1	C	518	G
1	C	519	G
1	C	558	A
1	C	573	A
1	C	574	C
1	D	507	A
1	D	509	C
1	D	515	G
1	D	518	G
1	D	519	G
1	D	558	A
1	D	560	U
1	D	573	A
1	D	574	C

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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	GOM	A	600	-	30,33,33	0.70	0	32,48,48	1.08	5 (15%)
4	GOM	B	601	-	30,33,33	0.70	0	32,48,48	1.07	4 (12%)

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
4	GOM	A	600	-	-	5/17/37/37	0/3/3/3
4	GOM	B	601	-	-	4/17/37/37	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	GOM	O3'-C3'-C4'	2.46	118.16	111.05
4	B	601	GOM	C5-C6-N6	2.31	123.86	120.35
4	A	600	GOM	C5-C6-N6	2.30	123.84	120.35
4	A	600	GOM	O4'-C1'-C2'	2.27	110.24	106.93
4	A	600	GOM	O3'-C3'-C4'	2.25	117.55	111.05
4	B	601	GOM	O4'-C1'-C2'	2.22	110.17	106.93
4	B	601	GOM	C2'-C3'-C4'	2.21	106.94	102.64
4	A	600	GOM	C2'-C3'-C4'	2.10	106.72	102.64
4	A	600	GOM	O3'-C3'-C2'	2.01	118.33	111.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	GOM	C-OP3-P-OP1
4	A	600	GOM	C-OP3-P-OP2
4	A	600	GOM	C-OP3-P-O5'
4	B	601	GOM	OP3-C-CA-N
4	B	601	GOM	OP3-C-CA-CB
4	A	600	GOM	OE1-CD-CG-CB
4	A	600	GOM	OE2-CD-CG-CB
4	B	601	GOM	OE2-CD-CG-CB
4	B	601	GOM	OE1-CD-CG-CB

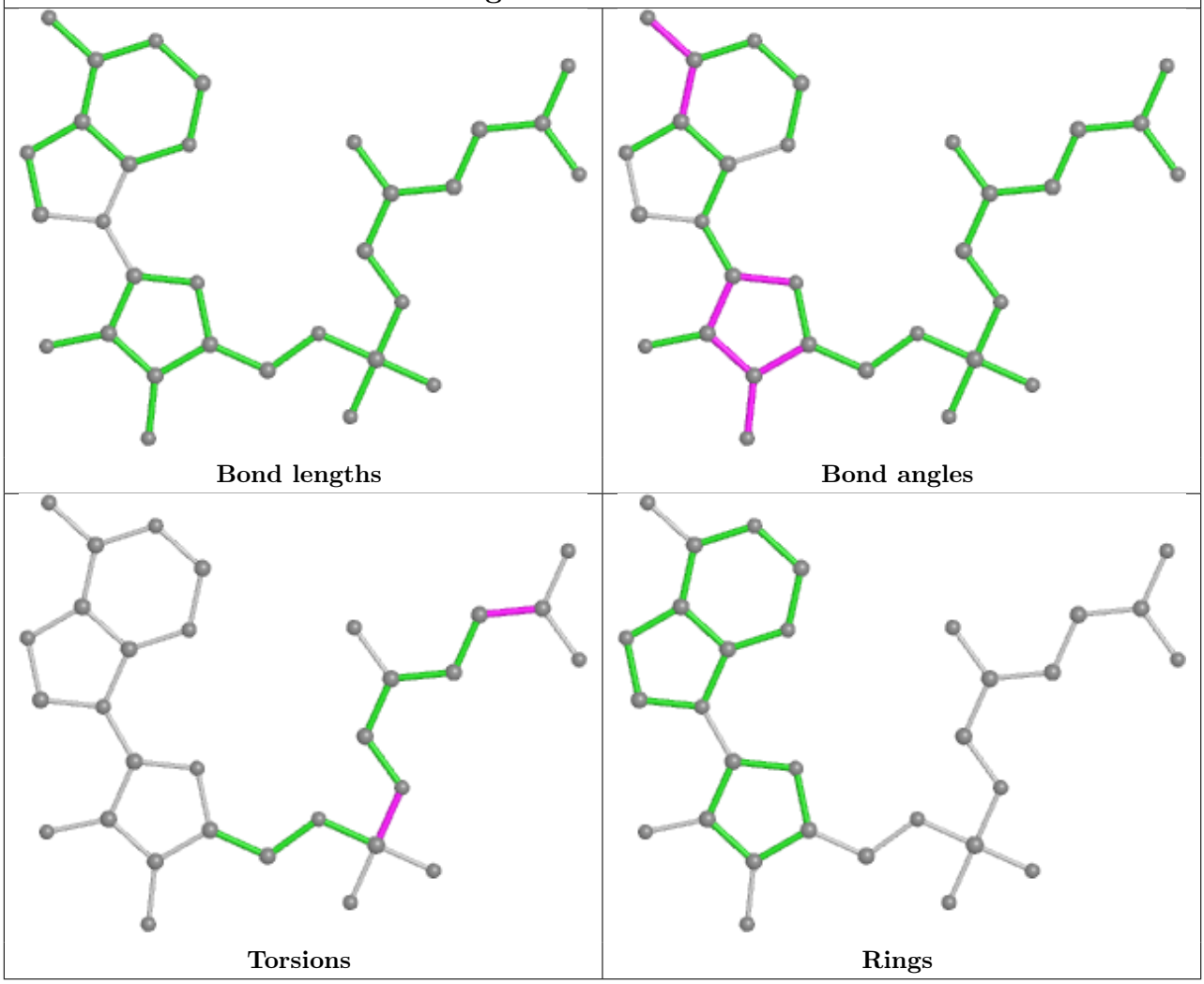
There are no ring outliers.

2 monomers are involved in 8 short contacts:

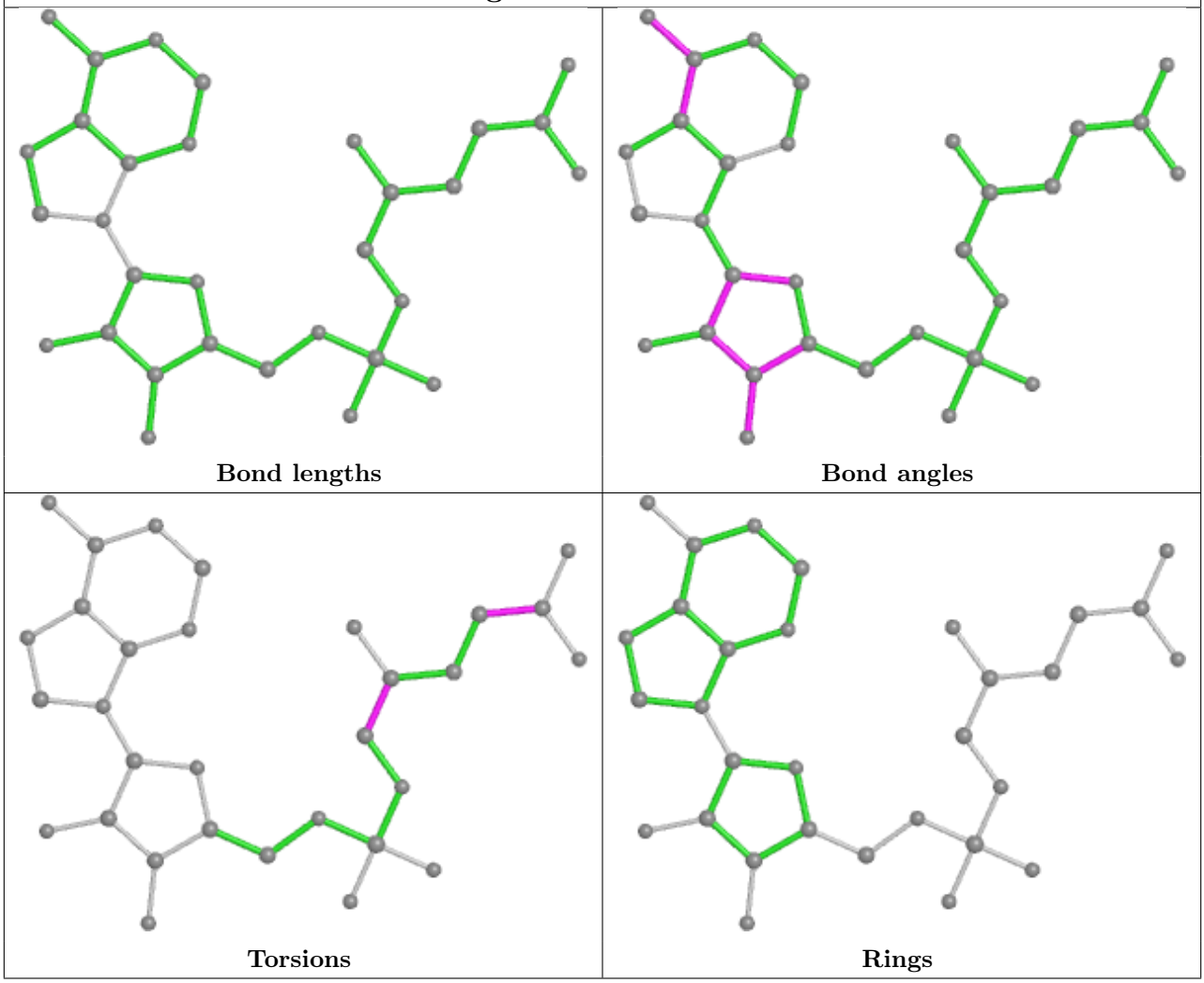
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GOM	3	0
4	B	601	GOM	5	0

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 GOM A 600



Ligand GOM B 601



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	C	75/75 (100%)	-0.60	0	100	100	23, 43, 75, 81	0
1	D	75/75 (100%)	-0.60	1 (1%)	77	80	22, 40, 77, 85	0
2	A	468/468 (100%)	-0.16	7 (1%)	73	77	14, 26, 55, 70	0
2	B	468/468 (100%)	-0.08	16 (3%)	45	51	14, 27, 66, 84	0
All	All	1086/1086 (100%)	-0.19	24 (2%)	62	66	14, 28, 68, 85	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	140	ARG	4.9
2	B	118	GLU	4.0
2	A	425	VAL	4.0
2	B	108	THR	3.5
2	B	136	GLU	3.5
2	B	128	ASN	3.1
2	B	141	GLY	3.0
2	B	139	ARG	2.9
2	A	467	LEU	2.8
2	A	424	GLY	2.7
2	B	112	LEU	2.7
2	B	129	ILE	2.6
2	B	114	GLN	2.5
2	B	130	PRO	2.4
2	B	134	ALA	2.4
2	A	403	ALA	2.4
2	A	120	GLY	2.3
2	B	468	ALA	2.3
2	B	110	GLU	2.3
2	A	468	ALA	2.3
2	B	49	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	133	GLU	2.2
1	D	516	C	2.1
2	A	414	ALA	2.1

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)

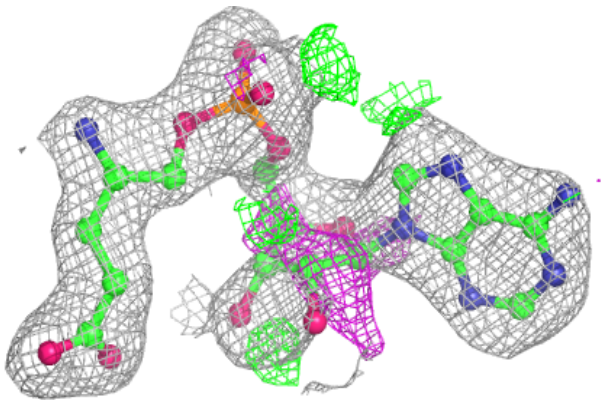
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

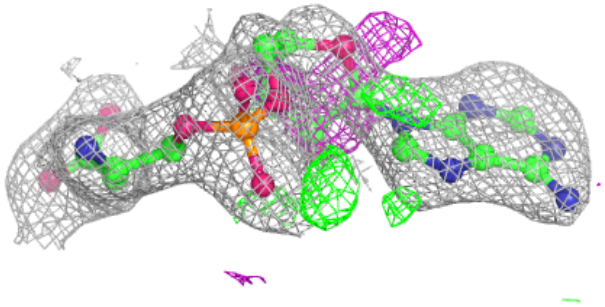
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOM	B	601	31/31	0.90	0.17	24,34,43,46	0
4	GOM	A	600	31/31	0.94	0.15	17,26,34,36	0
3	MG	D	701	1/1	0.98	0.06	33,33,33,33	0
3	MG	C	700	1/1	0.99	0.04	29,29,29,29	0

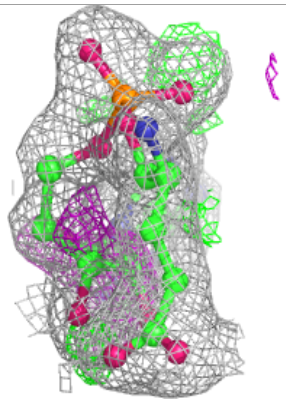
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GOM B 601:

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

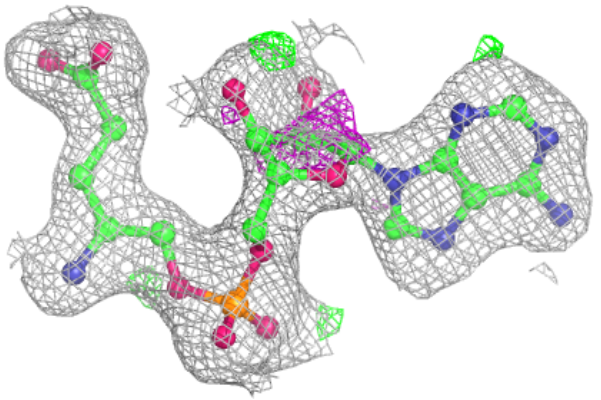


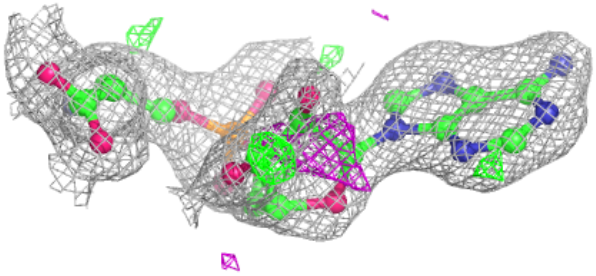


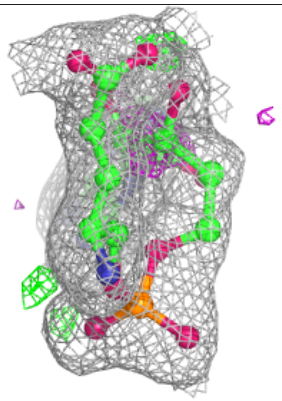


Electron density around GOM A 600:

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







6.5 Other polymers (i)

There are no such residues in this entry.