Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2024 – 04:15 AM EDT

PDB ID	:	3WQZ
Title	:	Crystal structure of Archaeoglobus fulgidus alanyl-tRNA synthetase in complex with a tRNA(Ala) variant having A3.U70
Authors	:	Naganuma, M.; Sekine, S.; Yokoyama, S.
Deposited on	:	2014-02-05
Resolution	:	3.49 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:

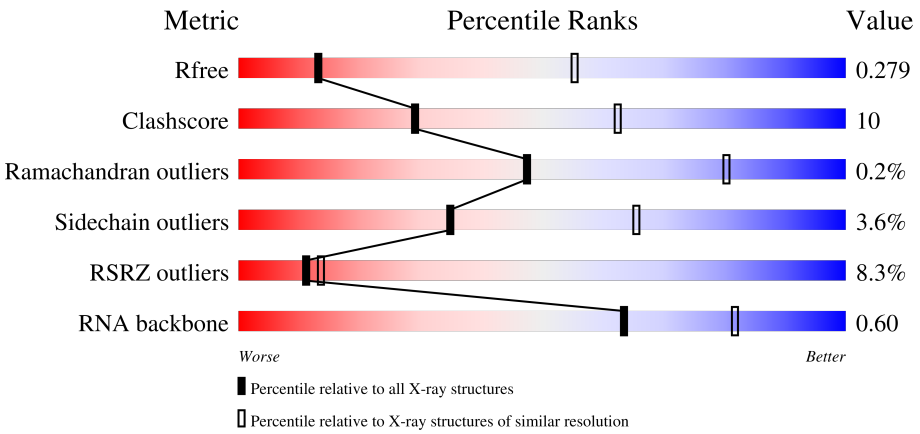
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.49 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)
RNA backbone	3102	1054 (4.00-2.96)

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

Mol	Chain	Length	Quality of chain
1	A	906	8% 74% 25% •
1	B	906	9% 75% 24% •
2	C	75	.% 53% 27% 19% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16078 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.

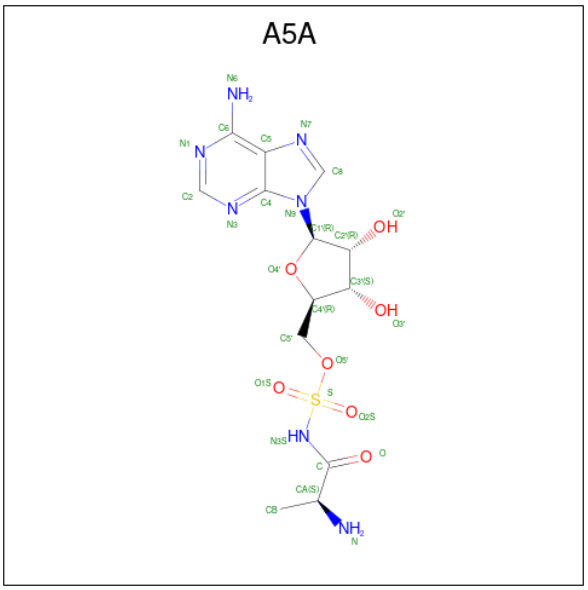
- Molecule 1 is a protein called Alanine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	905	7209	4573	1248	1357	31	0	0	0
1	B	904	7203	4571	1247	1353	32	0	0	0

- Molecule 2 is a RNA chain called RNA (75-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	75	1608	715	295	523	75	0	0	0

- Molecule 3 is '5'-O-(N-(L-ALANYL)-SULFAMOYL)ADENOSINE (three-letter code: A5A) (formula: $C_{13}H_{19}N_7O_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	28	13	7	7	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	B	1	28	13	7	7	1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

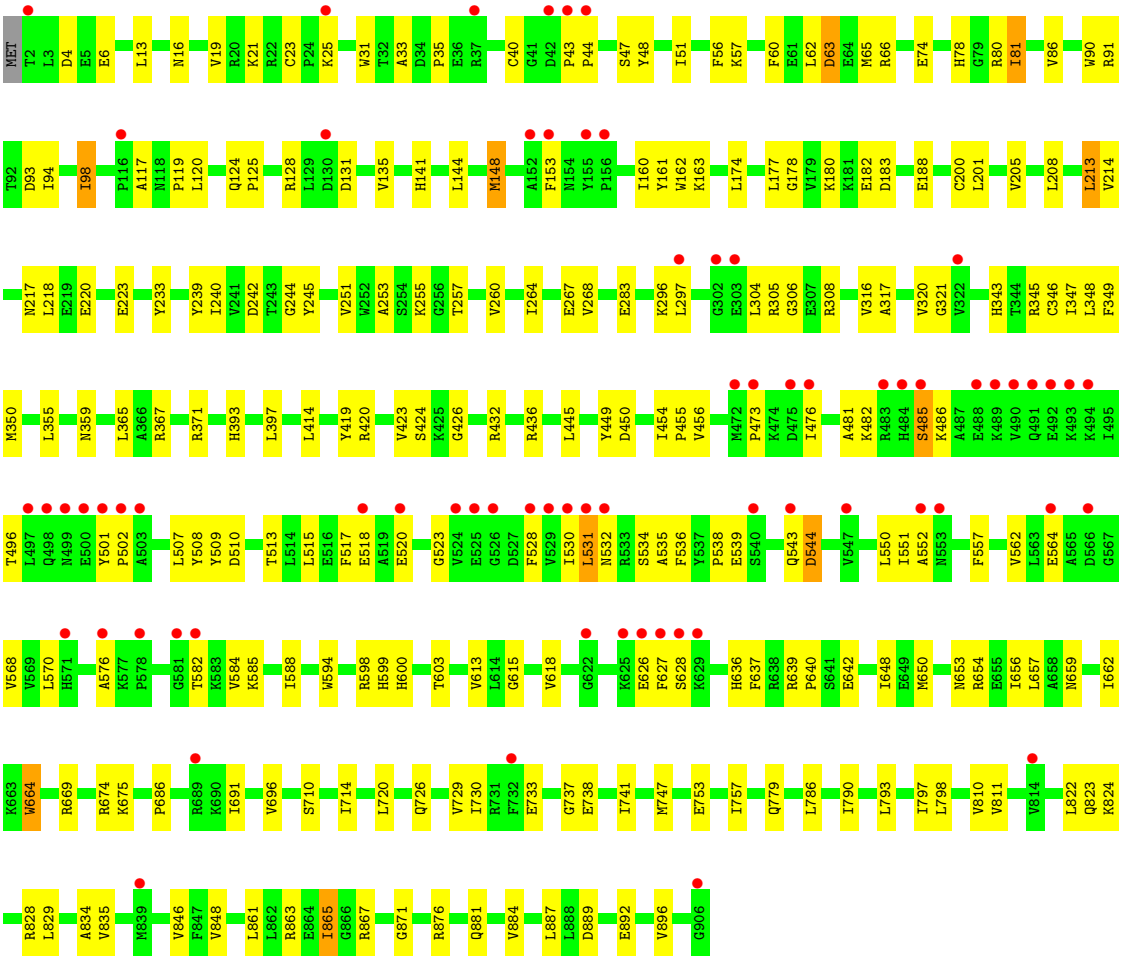
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0
			Total	Zn		
4	B	1	1	1	0	0

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.

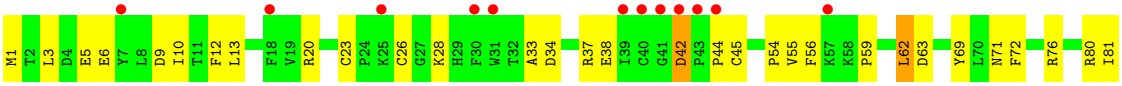
- Molecule 1: Alanine–tRNA ligase

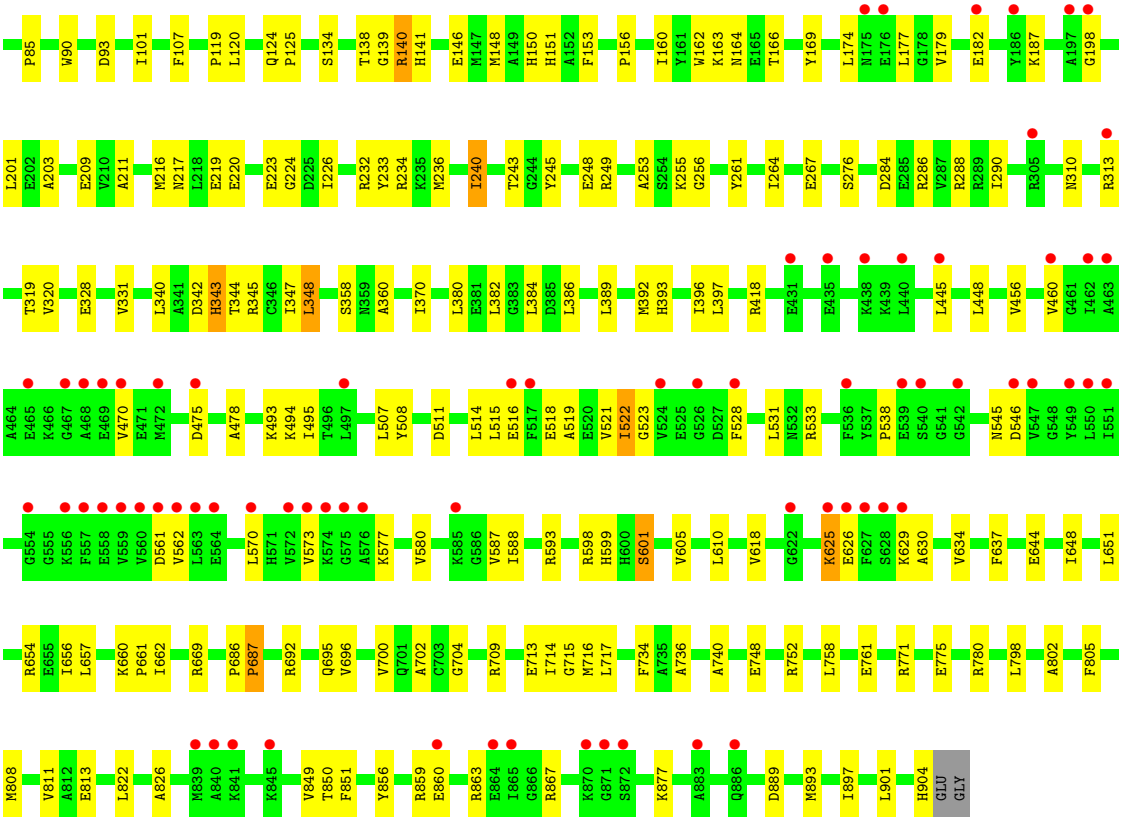
Chain A: 8% 74% 25%



- Molecule 1: Alanine–tRNA ligase

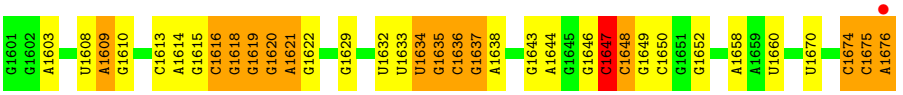
Chain B: 9% 75% 24%





- Molecule 2: RNA (75-MER)

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.61Å 169.68Å 176.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.74 – 3.49 42.95 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.74-3.49) 99.9 (42.95-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.241 , 0.277 0.245 , 0.279	Depositor DCC
R_{free} test set	1996 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	100.8	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 33.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.037 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16078	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: A5A, ZN

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	0.21	0/7347	0.39	0/9909
1	B	0.23	0/7341	0.40	0/9902
2	C	0.23	0/1797	0.76	1/2800 (0.0%)
All	All	0.22	0/16485	0.46	1/22611 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1647	C	P-O3'-C3'	5.89	126.77	119.70

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	7209	0	7200	144	0
1	B	7203	0	7203	143	0
2	C	1608	0	816	30	0
3	A	28	0	19	2	0
3	B	28	0	19	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16078	0	15257	301	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (301) 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:B:599:HIS:HD2	1:B:625:LYS:HE3	1.35	0.90
1:A:482:LYS:HA	2:C:1676:A:H61	1.38	0.86
1:B:626:GLU:HB3	1:B:629:LYS:HB2	1.63	0.80
1:A:640:PRO:HD3	1:A:730:ILE:HD13	1.67	0.75
1:A:636:HIS:HB3	1:A:730:ILE:HD12	1.69	0.74
1:B:345:ARG:HH21	1:B:397:LEU:HD21	1.53	0.72
1:B:33:ALA:HB3	1:B:182:GLU:HA	1.72	0.72
1:B:382:LEU:HG	1:B:384:LEU:H	1.53	0.72
1:A:531:LEU:HD21	1:A:534:SER:HB2	1.72	0.70
1:B:148:MET:HB2	1:B:245:TYR:HB2	1.74	0.70
1:B:138:THR:HG23	1:B:140:ARG:H	1.56	0.70
1:B:290:ILE:HD13	1:B:320:VAL:HG11	1.73	0.70
1:B:198:GLY:HA3	1:B:216:MET:HA	1.73	0.69
1:B:1:MET:HG2	1:B:226:ILE:HD11	1.74	0.69
2:C:1634:U:H4'	2:C:1635:G:O5'	1.93	0.68
2:C:1675:C:H3'	2:C:1676:A:H2'	1.76	0.67
1:B:625:LYS:HA	1:B:630:ALA:HA	1.76	0.67
1:A:509:TYR:O	1:A:664:TRP:NE1	2.28	0.67
1:A:445:LEU:HD21	1:A:456:VAL:HG13	1.77	0.66
1:A:823:GLN:NE2	2:C:1620:G:OP2	2.29	0.66
1:B:709:ARG:NH2	1:B:713:GLU:OE2	2.28	0.66
1:B:344:THR:HG21	1:B:389:LEU:HB2	1.76	0.66
1:A:669:ARG:NH2	1:A:686:PRO:O	2.29	0.65
1:B:224:GLY:HA3	1:B:232:ARG:HD2	1.76	0.65
1:B:599:HIS:CE1	1:B:630:ALA:HB1	2.32	0.65
2:C:1636:C:H1'	2:C:1637:G:OP2	1.98	0.64
1:A:876:ARG:NH1	2:C:1620:G:OP1	2.31	0.64
1:B:310:ASN:HA	1:B:313:ARG:HB2	1.79	0.64
1:A:304:LEU:HD21	1:A:308:ARG:HH21	1.62	0.63
1:A:481:ALA:O	2:C:1676:A:N6	2.31	0.63
1:B:71:ASN:OD1	1:B:80:ARG:NH2	2.26	0.62
1:B:276:SER:HB2	1:B:380:LEU:HB3	1.79	0.62
1:B:546:ASP:OD2	1:B:593:ARG:NH1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:LEU:HA	1:B:654:ARG:HE	1.65	0.62
1:B:692:ARG:HD3	1:B:704:GLY:HA2	1.81	0.62
1:B:736:ALA:HA	1:B:740:ALA:HB2	1.81	0.62
1:A:482:LYS:HA	2:C:1676:A:N6	2.12	0.62
1:B:139:GLY:HA2	1:B:261:TYR:HE1	1.63	0.62
1:B:34:ASP:HB2	1:B:182:GLU:HB2	1.83	0.61
1:A:220:GLU:OE1	2:C:1674:C:N4	2.31	0.61
1:B:219:GLU:N	1:B:234:ARG:O	2.32	0.61
1:A:515:LEU:HB3	1:A:588:ILE:HB	1.84	0.60
1:A:420:ARG:NH1	1:A:424:SER:OG	2.34	0.60
1:A:63:ASP:OD1	1:A:63:ASP:N	2.34	0.59
1:B:802:ALA:HB2	1:B:811:VAL:HB	1.83	0.59
1:A:117:ALA:H	1:A:120:LEU:HD21	1.67	0.59
1:B:717:LEU:HD11	1:B:734:PHE:HD2	1.67	0.59
1:A:656:ILE:HG22	1:A:714:ILE:HD11	1.86	0.58
1:A:220:GLU:CD	2:C:1674:C:H42	2.07	0.57
1:A:60:PHE:HB3	1:A:65:MET:HG2	1.86	0.57
1:B:508:TYR:HB2	1:B:593:ARG:HH22	1.69	0.57
1:B:826:ALA:HB1	1:B:851:PHE:HB3	1.86	0.57
1:A:544:ASP:OD1	1:A:600:HIS:NE2	2.35	0.57
1:B:37:ARG:NH2	1:B:38:GLU:O	2.38	0.57
1:A:81:ILE:HG12	1:A:120:LEU:HD22	1.87	0.57
1:A:214:VAL:HB	1:A:242:ASP:HB3	1.87	0.57
1:B:798:LEU:HD22	1:B:813:GLU:HG3	1.87	0.57
1:A:90:TRP:CD1	1:A:91:ARG:HG3	2.40	0.56
1:B:124:GLN:NE2	1:B:125:PRO:O	2.38	0.56
1:B:538:PRO:HB3	1:B:562:VAL:HG22	1.86	0.56
1:B:860:GLU:HG2	1:B:863:ARG:HH12	1.69	0.56
1:B:119:PRO:HG3	1:B:160:ILE:HG21	1.88	0.56
1:A:74:GLU:OE2	1:A:80:ARG:NH2	2.38	0.56
1:A:135:VAL:HG22	1:A:141:HIS:HB3	1.88	0.56
1:A:510:ASP:HA	1:A:664:TRP:HE1	1.69	0.56
2:C:1646:G:O2'	2:C:1648:C:OP2	2.22	0.56
1:A:33:ALA:HB3	1:A:182:GLU:HA	1.88	0.56
1:B:573:VAL:O	1:B:577:LYS:NZ	2.37	0.55
1:B:81:ILE:HD13	1:B:120:LEU:HB2	1.88	0.55
1:B:515:LEU:HG	1:B:588:ILE:HB	1.89	0.55
1:A:557:PHE:HE2	1:A:576:ALA:HB3	1.71	0.55
1:A:798:LEU:HB3	1:A:811:VAL:HG11	1.88	0.55
1:B:26:CYS:SG	1:B:28:LYS:NZ	2.74	0.55
1:A:538:PRO:HA	1:A:562:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:PHE:HE1	1:B:177:LEU:HD13	1.72	0.54
1:A:62:LEU:HD23	1:A:251:VAL:HG21	1.89	0.54
2:C:1621:A:C2	2:C:1648:C:C2	2.96	0.54
1:A:367:ARG:O	1:A:371:ARG:HG2	2.08	0.54
1:A:317:ALA:O	1:A:321:GLY:N	2.40	0.54
1:A:162:TRP:CD1	1:A:163:LYS:HG2	2.43	0.53
1:B:209:GLU:O	1:B:249:ARG:NH1	2.40	0.53
1:B:717:LEU:HD11	1:B:734:PHE:HB2	1.90	0.53
1:B:822:LEU:HD23	1:B:849:VAL:HB	1.90	0.53
1:A:473:PRO:HB3	1:A:476:ILE:HD13	1.90	0.53
2:C:1609:A:O2'	2:C:1610:G:N7	2.41	0.53
1:A:520:GLU:OE2	1:A:532:ASN:ND2	2.41	0.53
1:B:150:HIS:HE1	1:B:166:THR:HG21	1.74	0.53
1:B:599:HIS:CD2	1:B:625:LYS:HE3	2.27	0.52
1:A:283:GLU:N	1:A:283:GLU:OE1	2.42	0.52
1:A:539:GLU:HB2	1:A:543:GLN:O	2.09	0.52
1:B:610:LEU:HD23	1:B:648:ILE:HD12	1.91	0.52
1:B:340:LEU:HD11	1:B:386:LEU:HD21	1.92	0.52
1:B:460:VAL:HG13	1:B:470:VAL:HG11	1.92	0.52
1:A:726:GLN:HG2	1:A:729:VAL:HB	1.92	0.51
1:A:78:HIS:HA	1:A:119:PRO:HG2	1.92	0.51
1:A:642:GLU:OE2	1:B:752:ARG:NH2	2.43	0.51
1:B:328:GLU:HA	1:B:331:VAL:HG22	1.92	0.51
1:B:531:LEU:HD23	1:B:533:ARG:H	1.74	0.51
1:B:445:LEU:HD13	1:B:456:VAL:HG13	1.93	0.51
2:C:1616:C:O2'	2:C:1618:G:OP2	2.25	0.51
1:B:808:MET:HE2	1:B:901:LEU:HD21	1.92	0.51
1:A:13:LEU:HD13	1:A:31:TRP:CD2	2.46	0.50
1:A:686:PRO:HG2	1:A:691:ILE:HD12	1.93	0.50
1:B:10:ILE:HG13	1:B:12:PHE:H	1.76	0.50
1:A:823:GLN:HG3	1:A:881:GLN:HE21	1.75	0.50
1:B:343:HIS:O	1:B:347:ILE:HG12	2.12	0.50
1:B:59:PRO:HB3	1:B:255:LYS:HA	1.94	0.50
1:B:69:TYR:CE2	1:B:148:MET:HB3	2.47	0.50
2:C:1647:C:H2'	2:C:1650:C:OP1	2.11	0.50
1:B:493:LYS:NZ	1:B:494:LYS:O	2.45	0.49
1:A:829:LEU:HB3	1:A:834:ALA:HB3	1.94	0.49
3:A:1001:A5A:O5'	3:A:1001:A5A:H8	2.11	0.49
1:A:810:VAL:HG12	1:A:835:VAL:HB	1.94	0.49
2:C:1632:U:H2'	2:C:1633:U:O4'	2.11	0.49
1:A:31:TRP:NE1	1:A:188:GLU:OE1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:VAL:HG11	1:A:865:ILE:HD11	1.95	0.49
1:B:358:SER:OG	1:B:360:ALA:O	2.27	0.49
1:A:538:PRO:HG2	1:A:564:GLU:HB3	1.95	0.48
1:A:260:VAL:O	1:A:264:ILE:HG12	2.12	0.48
1:B:644:GLU:O	1:B:648:ILE:HG12	2.14	0.48
1:A:824:LYS:HE3	1:A:828:ARG:HH22	1.77	0.48
1:B:651:LEU:HB2	1:B:654:ARG:HH21	1.78	0.48
1:A:25:LYS:HE3	1:A:43:PRO:HD3	1.94	0.48
1:A:846:VAL:HG21	1:A:887:LEU:HD23	1.95	0.48
1:B:85:PRO:HG2	1:B:90:TRP:HZ3	1.76	0.48
1:A:432:ARG:HB3	1:A:436:ARG:HH12	1.79	0.48
1:B:599:HIS:CE1	1:B:630:ALA:CB	2.96	0.48
1:A:871:GLY:HA3	1:A:884:VAL:HG22	1.96	0.48
1:B:601:SER:HB3	1:B:714:ILE:HD11	1.95	0.48
1:A:543:GLN:HG2	1:A:626:GLU:HA	1.96	0.48
1:B:162:TRP:CD1	1:B:163:LYS:HG2	2.49	0.48
1:B:150:HIS:CE1	1:B:243:THR:HG21	2.48	0.48
1:A:346:CYS:O	1:A:350:MET:HG3	2.14	0.47
1:A:657:LEU:HD13	1:B:598:ARG:HH12	1.79	0.47
1:A:793:LEU:O	1:A:797:ILE:HG12	2.14	0.47
1:B:601:SER:O	1:B:605:VAL:HG23	2.14	0.47
1:A:6:GLU:OE2	1:A:217:ASN:ND2	2.47	0.47
1:A:650:MET:O	1:A:654:ARG:HG2	2.14	0.47
1:B:148:MET:N	1:B:245:TYR:O	2.47	0.47
1:B:545:ASN:ND2	1:B:561:ASP:OD1	2.42	0.47
1:A:343:HIS:O	1:A:347:ILE:HG12	2.13	0.47
2:C:1675:C:H5'	2:C:1676:A:H2'	1.97	0.47
1:A:508:TYR:HB3	1:A:535:ALA:HA	1.96	0.47
1:A:613:VAL:HG11	1:A:648:ILE:HG13	1.97	0.47
1:A:753:GLU:O	1:A:757:ILE:HG12	2.14	0.47
1:B:519:ALA:HB3	1:B:531:LEU:HD21	1.97	0.47
1:B:203:ALA:HB3	1:B:211:ALA:HB3	1.97	0.47
1:A:93:ASP:OD1	1:A:94:ILE:N	2.46	0.47
1:A:162:TRP:CG	1:A:163:LYS:N	2.82	0.47
1:A:674:ARG:HG3	1:A:675:LYS:HG3	1.96	0.47
1:B:56:PHE:HE2	1:B:253:ALA:HB3	1.80	0.47
2:C:1633:U:H2'	2:C:1634:U:H5'	1.97	0.47
1:B:669:ARG:NH1	1:B:686:PRO:O	2.48	0.46
2:C:1608:U:H4'	2:C:1648:C:H4'	1.97	0.46
1:A:255:LYS:HB3	1:A:257:THR:HG23	1.97	0.46
1:B:805:PHE:HD2	1:B:901:LEU:HD23	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LYS:NZ	1:A:183:ASP:OD2	2.39	0.46
1:B:522:ILE:HA	1:B:580:VAL:HG23	1.97	0.46
1:B:516:GLU:HG2	1:B:587:VAL:HA	1.97	0.46
1:A:304:LEU:HD21	1:A:308:ARG:HD2	1.97	0.46
1:A:485:SER:HB3	2:C:1676:A:H2	1.81	0.46
1:A:720:LEU:N	1:A:733:GLU:O	2.45	0.46
1:B:138:THR:HG21	1:B:141:HIS:ND1	2.30	0.46
1:B:867:ARG:HA	1:B:867:ARG:HD3	1.66	0.46
1:A:297:LEU:HD13	1:A:316:VAL:HB	1.98	0.46
1:B:125:PRO:HA	1:B:146:GLU:HA	1.97	0.46
1:A:98:ILE:HG22	1:A:128:ARG:HG2	1.97	0.46
1:B:656:ILE:HD12	1:B:714:ILE:HB	1.97	0.46
1:A:86:VAL:HG11	1:A:349:PHE:HB3	1.98	0.45
1:A:432:ARG:HB3	1:A:436:ARG:NH1	2.31	0.45
1:A:551:ILE:HG12	1:A:552:ALA:H	1.81	0.45
1:B:223:GLU:HB3	1:B:234:ARG:HD3	1.97	0.45
1:A:43:PRO:HA	1:A:44:PRO:HA	1.64	0.45
1:B:493:LYS:HZ2	1:B:495:ILE:HG12	1.80	0.45
1:A:160:ILE:HG22	1:A:161:TYR:HD1	1.81	0.45
1:B:217:ASN:O	1:B:236:MET:HG2	2.16	0.45
1:B:521:VAL:HG12	1:B:523:GLY:H	1.81	0.45
1:A:786:LEU:O	1:A:790:ILE:HG12	2.17	0.45
1:B:55:VAL:HG22	1:B:179:VAL:HG22	1.99	0.45
1:B:859:ARG:HH21	1:B:877:LYS:HG3	1.82	0.45
1:A:450:ASP:O	2:C:1670:U:O2'	2.26	0.45
1:A:518:GLU:HA	1:A:585:LYS:HD2	1.98	0.45
1:A:530:ILE:HD12	1:A:531:LEU:H	1.82	0.45
1:A:594:TRP:HB3	1:A:598:ARG:NH1	2.31	0.45
1:A:889:ASP:HB3	1:A:892:GLU:HG3	1.98	0.45
1:B:101:ILE:HD13	1:B:151:HIS:CD2	2.52	0.45
1:B:511:ASP:HB3	1:B:514:LEU:HG	1.98	0.45
1:B:856:TYR:CE2	1:B:904:HIS:HB2	2.52	0.45
1:B:717:LEU:HD11	1:B:734:PHE:CD2	2.48	0.44
1:B:686:PRO:HG3	1:B:702:ALA:HB1	1.99	0.44
1:A:741:ILE:HG12	1:B:716:MET:HE1	2.00	0.44
1:B:72:PHE:O	1:B:76:ARG:HG2	2.18	0.44
1:B:662:ILE:HG23	1:B:696:VAL:HG22	1.99	0.44
1:A:599:HIS:O	1:A:603:THR:OG1	2.24	0.44
1:A:653:ASN:O	1:A:656:ILE:HG12	2.18	0.44
1:A:367:ARG:HH11	1:A:371:ARG:NH2	2.16	0.44
1:A:420:ARG:HA	1:A:423:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:GLN:OE1	2:C:1619:G:O2'	2.33	0.44
1:B:758:LEU:O	2:C:1647:C:N4	2.51	0.44
1:A:568:VAL:HG12	1:A:570:LEU:HD23	2.00	0.44
1:B:56:PHE:CD1	1:B:177:LEU:HB3	2.52	0.44
1:A:659:ASN:OD1	1:A:710:SER:HB2	2.17	0.43
1:B:348:LEU:HD12	1:B:393:HIS:HB3	2.00	0.43
1:A:19:VAL:HG13	1:A:21:LYS:HD3	2.00	0.43
1:B:893:MET:O	1:B:897:ILE:HG12	2.19	0.43
1:A:371:ARG:HD2	1:A:419:TYR:CD2	2.53	0.43
1:A:639:ARG:HA	1:A:640:PRO:HD3	1.85	0.43
1:B:10:ILE:HG12	1:B:13:LEU:HG	1.99	0.43
1:B:28:LYS:HE2	1:B:187:LYS:HD2	1.99	0.43
1:B:618:VAL:HG13	1:B:634:VAL:HB	2.00	0.43
1:B:662:ILE:HA	1:B:695:GLN:O	2.18	0.43
1:B:771:ARG:NH1	1:B:775:GLU:OE2	2.51	0.43
2:C:1674:C:H3'	2:C:1675:C:H5"	2.00	0.43
1:A:6:GLU:O	1:A:163:LYS:NZ	2.39	0.43
1:B:56:PHE:HD1	1:B:177:LEU:HB3	1.83	0.43
2:C:1643:G:H2'	2:C:1644:A:C8	2.54	0.43
1:A:153:PHE:CD2	1:A:240:ILE:HD12	2.54	0.43
1:A:201:LEU:HB2	1:A:213:LEU:HD11	1.99	0.43
1:A:267:GLU:CD	1:A:267:GLU:H	2.22	0.43
1:B:516:GLU:HG2	1:B:587:VAL:HG22	2.01	0.43
1:B:657:LEU:HD12	1:B:657:LEU:HA	1.91	0.43
1:B:859:ARG:H	1:B:859:ARG:HG2	1.64	0.43
1:B:124:GLN:HA	1:B:125:PRO:HD3	1.86	0.43
1:B:134:SER:O	1:B:138:THR:HG22	2.19	0.43
1:A:51:ILE:HD12	1:A:296:LYS:HA	2.01	0.43
1:A:449:TYR:CD1	1:A:455:PRO:HA	2.53	0.43
1:A:56:PHE:HE2	1:A:253:ALA:HB3	1.83	0.43
1:B:10:ILE:HD12	1:B:164:ASN:HA	2.01	0.43
1:A:268:VAL:HG21	1:A:393:HIS:CE1	2.54	0.42
1:B:507:LEU:HD11	1:B:533:ARG:HG2	2.00	0.42
1:B:656:ILE:HG21	1:B:715:GLY:O	2.20	0.42
1:A:552:ALA:HA	1:A:584:VAL:HB	2.01	0.42
1:B:54:PRO:HG3	1:B:256:GLY:HA3	2.01	0.42
1:B:811:VAL:HG13	1:B:851:PHE:HZ	1.84	0.42
1:B:220:GLU:HA	1:B:233:TYR:HA	2.01	0.42
2:C:1636:C:HO2'	2:C:1637:G:P	2.42	0.42
1:A:244:GLY:HA3	3:A:1001:A5A:HB1	2.01	0.42
1:A:359:ASN:OD1	1:A:726:GLN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLN:HB3	1:A:544:ASP:H	1.59	0.42
1:A:218:LEU:HB3	1:A:233:TYR:HB3	2.01	0.42
1:A:305:ARG:NH1	1:A:306:GLY:O	2.53	0.42
1:A:486:LYS:HB3	1:A:486:LYS:HE2	1.81	0.42
1:A:426:GLY:HA3	1:A:454:ILE:HD11	2.01	0.42
2:C:1636:C:O2'	2:C:1637:G:OP1	2.33	0.42
1:A:57:LYS:HE2	1:A:178:GLY:HA2	2.02	0.42
1:A:345:ARG:HB2	1:A:393:HIS:CE1	2.55	0.42
1:A:615:GLY:O	1:A:618:VAL:HG22	2.20	0.42
1:A:81:ILE:H	1:A:81:ILE:HG13	1.72	0.42
1:A:863:ARG:O	1:A:867:ARG:HG2	2.19	0.42
1:A:536:PHE:CZ	1:A:588:ILE:HG13	2.55	0.41
1:B:475:ASP:HB2	1:B:478:ALA:HB3	2.02	0.41
1:B:860:GLU:HG2	1:B:863:ARG:NH1	2.34	0.41
1:A:47:SER:HB2	1:A:296:LYS:O	2.20	0.41
1:A:66:ARG:HA	1:A:148:MET:HE1	2.02	0.41
1:A:501:TYR:CE2	1:A:523:GLY:HA3	2.55	0.41
1:A:550:LEU:N	1:A:557:PHE:O	2.53	0.41
1:A:737:GLY:O	1:A:741:ILE:HG13	2.21	0.41
1:A:501:TYR:HA	1:A:502:PRO:HD3	1.74	0.41
1:A:662:ILE:HG23	1:A:696:VAL:HA	2.02	0.41
1:A:510:ASP:HA	1:A:664:TRP:NE1	2.34	0.41
1:B:107:PHE:HE2	1:B:687:PRO:HA	1.86	0.41
1:B:267:GLU:HB2	1:B:396:ILE:HD11	2.02	0.41
1:B:284:ASP:O	1:B:288:ARG:HG3	2.21	0.41
1:B:286:ARG:O	1:B:290:ILE:HG12	2.21	0.41
1:B:386:LEU:HD23	1:B:386:LEU:HA	1.90	0.41
1:A:432:ARG:NH2	2:C:1614:A:OP1	2.54	0.41
1:B:418:ARG:NH2	1:B:637:PHE:O	2.40	0.41
2:C:1636:C:O2'	2:C:1637:G:P	2.79	0.41
1:A:564:GLU:HA	1:A:570:LEU:HG	2.02	0.41
1:A:738:GLU:HA	1:A:741:ILE:HD12	2.02	0.41
1:B:695:GLN:HG2	1:B:700:VAL:HG22	2.02	0.41
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.82	0.41
1:A:345:ARG:HE	1:A:397:LEU:HD21	1.84	0.41
1:B:660:LYS:HA	1:B:661:PRO:HD3	1.94	0.41
1:B:717:LEU:HA	1:B:717:LEU:HD12	1.75	0.41
1:A:25:LYS:HD3	1:A:25:LYS:HA	1.78	0.41
1:A:48:TYR:HE1	1:A:208:LEU:HD13	1.86	0.41
1:A:316:VAL:O	1:A:320:VAL:HG22	2.21	0.41
1:A:865:ILE:HG22	1:A:896:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ASP:HB3	1:B:44:PRO:HD2	2.03	0.41
1:B:248:GLU:HG3	1:B:264:ILE:HD13	2.03	0.41
1:B:528:PHE:CG	1:B:570:LEU:HD23	2.55	0.41
1:B:630:ALA:HB3	1:B:734:PHE:O	2.21	0.41
1:A:414:LEU:HD23	1:A:637:PHE:HB2	2.02	0.41
1:A:747:MET:SD	1:B:748:GLU:HG2	2.60	0.41
1:B:23:CYS:SG	1:B:26:CYS:HB3	2.61	0.41
1:A:124:GLN:NE2	1:A:125:PRO:O	2.54	0.40
1:A:148:MET:HG3	1:A:245:TYR:O	2.21	0.40
1:A:627:PHE:O	1:A:628:SER:OG	2.31	0.40
1:A:779:GLN:HE22	1:B:780:ARG:NH1	2.19	0.40
1:B:3:LEU:O	1:B:6:GLU:HG2	2.21	0.40
2:C:1675:C:H5'	2:C:1676:A:C2'	2.51	0.40
1:B:5:GLU:O	1:B:9:ASP:N	2.49	0.40
1:B:56:PHE:CE1	1:B:177:LEU:HD13	2.54	0.40
1:B:856:TYR:HE2	1:B:904:HIS:HB2	1.85	0.40
1:A:657:LEU:HD13	1:B:598:ARG:NH1	2.36	0.40
1:B:62:LEU:HD12	1:B:63:ASP:N	2.37	0.40
1:B:889:ASP:O	1:B:893:MET:HG3	2.21	0.40
1:B:153:PHE:CD2	1:B:240:ILE:HD13	2.56	0.40
3:B:1001:A5A:O5'	3:B:1001:A5A:H8	2.21	0.40
1:B:493:LYS:NZ	1:B:495:ILE:HG12	2.36	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	903/906 (100%)	863 (96%)	39 (4%)	1 (0%)	51	84
1	B	902/906 (100%)	864 (96%)	36 (4%)	2 (0%)	47	80
All	All	1805/1812 (100%)	1727 (96%)	75 (4%)	3 (0%)	47	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	PRO
1	A	35	PRO
1	B	687	PRO

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	766/767 (100%)	734 (96%)	32 (4%)	30	61
1	B	766/767 (100%)	743 (97%)	23 (3%)	41	70
All	All	1532/1534 (100%)	1477 (96%)	55 (4%)	35	65

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

Mol	Chain	Res	Type
1	A	4	ASP
1	A	16	ASN
1	A	23	CYS
1	A	40	CYS
1	A	63	ASP
1	A	81	ILE
1	A	98	ILE
1	A	131	ASP
1	A	144	LEU
1	A	148	MET
1	A	174	LEU
1	A	200	CYS
1	A	205	VAL
1	A	213	LEU
1	A	223	GLU
1	A	239	TYR
1	A	348	LEU
1	A	355	LEU
1	A	365	LEU
1	A	485	SER

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Mol	Chain	Res	Type
1	A	496	THR
1	A	507	LEU
1	A	513	THR
1	A	517	PHE
1	A	528	PHE
1	A	531	LEU
1	A	544	ASP
1	A	582	THR
1	A	664	TRP
1	A	822	LEU
1	A	861	LEU
1	A	865	ILE
1	B	20	ARG
1	B	42	ASP
1	B	45	CYS
1	B	62	LEU
1	B	93	ASP
1	B	140	ARG
1	B	169	TYR
1	B	174	LEU
1	B	201	LEU
1	B	240	ILE
1	B	319	THR
1	B	342	ASP
1	B	343	HIS
1	B	348	LEU
1	B	370	ILE
1	B	392	MET
1	B	448	LEU
1	B	518	GLU
1	B	522	ILE
1	B	601	SER
1	B	625	LYS
1	B	761	GLU
1	B	850	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	604	HIS
1	B	150	HIS
1	B	596	HIS

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Mol	Chain	Res	Type
1	B	599	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	74/75 (98%)	24 (32%)	5 (6%)

All (24) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	1603	A
2	C	1609	A
2	C	1613	C
2	C	1615	G
2	C	1616	C
2	C	1618	G
2	C	1619	G
2	C	1620	G
2	C	1621	A
2	C	1622	G
2	C	1629	G
2	C	1635	G
2	C	1636	C
2	C	1637	G
2	C	1638	A
2	C	1647	C
2	C	1648	C
2	C	1649	G
2	C	1652	G
2	C	1658	A
2	C	1660	U
2	C	1674	C
2	C	1675	C
2	C	1676	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	1616	C
2	C	1621	A
2	C	1634	U

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Mol	Chain	Res	Type
2	C	1636	C
2	C	1647	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	$\#\|Z\| > 2$
3	A5A	B	1001	-	26,30,30	2.71	12 (46%)	30,45,45	2.29	9 (30%)
3	A5A	A	1001	-	26,30,30	2.73	12 (46%)	30,45,45	2.26	8 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A5A	B	1001	-	-	3/14/35/35	0/3/3/3
3	A5A	A	1001	-	-	5/14/35/35	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	A5A	O1S-S	5.81	1.47	1.42
3	B	1001	A5A	O1S-S	5.79	1.47	1.42
3	B	1001	A5A	O5'-S	-5.76	1.47	1.59
3	A	1001	A5A	O5'-S	-5.70	1.47	1.59
3	B	1001	A5A	C2'-C1'	-4.40	1.47	1.53
3	A	1001	A5A	C2'-C1'	-4.33	1.47	1.53
3	A	1001	A5A	C-N3S	3.82	1.44	1.37
3	A	1001	A5A	O-C	-3.78	1.15	1.23
3	A	1001	A5A	C2'-C3'	-3.77	1.43	1.53
3	B	1001	A5A	C2'-C3'	-3.76	1.43	1.53
3	B	1001	A5A	O-C	-3.73	1.16	1.23
3	B	1001	A5A	C-N3S	3.65	1.44	1.37
3	A	1001	A5A	O2S-S	3.64	1.45	1.42
3	B	1001	A5A	O2S-S	3.58	1.45	1.42
3	A	1001	A5A	C6-N6	3.55	1.47	1.34
3	B	1001	A5A	C6-N6	3.53	1.46	1.34
3	A	1001	A5A	S-N3S	3.13	1.65	1.59
3	B	1001	A5A	S-N3S	2.92	1.65	1.59
3	A	1001	A5A	C3'-C4'	-2.91	1.45	1.53
3	B	1001	A5A	C3'-C4'	-2.88	1.45	1.53
3	A	1001	A5A	CA-N	-2.40	1.40	1.48
3	B	1001	A5A	CA-N	-2.40	1.40	1.48
3	A	1001	A5A	C2-N3	2.32	1.35	1.32
3	B	1001	A5A	C2-N3	2.23	1.35	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	A5A	O2S-S-O1S	-7.75	108.69	120.76
3	B	1001	A5A	O2S-S-O1S	-7.15	109.62	120.76
3	B	1001	A5A	N3-C2-N1	-5.62	119.89	128.68
3	A	1001	A5A	N3-C2-N1	-5.46	120.14	128.68
3	A	1001	A5A	O5'-C5'-C4'	4.59	116.19	107.62
3	B	1001	A5A	O5'-C5'-C4'	4.21	115.47	107.62
3	B	1001	A5A	C-N3S-S	-3.07	119.64	124.61
3	A	1001	A5A	C4-C5-N7	-2.77	106.51	109.40
3	B	1001	A5A	C4-C5-N7	-2.74	106.55	109.40
3	B	1001	A5A	CA-C-N3S	2.62	119.89	114.34
3	B	1001	A5A	C3'-C2'-C1'	2.56	104.83	100.98
3	A	1001	A5A	C3'-C2'-C1'	2.36	104.53	100.98
3	A	1001	A5A	CA-C-N3S	2.33	119.27	114.34
3	B	1001	A5A	C2-N1-C6	2.32	122.72	118.75
3	B	1001	A5A	C2'-C3'-C4'	2.32	107.14	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	A5A	C2'-C3'-C4'	2.16	106.83	102.64
3	A	1001	A5A	C2-N1-C6	2.12	122.38	118.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	A5A	C-N3S-S-O2S
3	A	1001	A5A	C5'-O5'-S-N3S
3	A	1001	A5A	C5'-O5'-S-O2S
3	A	1001	A5A	C3'-C4'-C5'-O5'
3	B	1001	A5A	C5'-O5'-S-N3S
3	A	1001	A5A	C5'-O5'-S-O1S
3	B	1001	A5A	C5'-O5'-S-O2S
3	B	1001	A5A	C5'-O5'-S-O1S

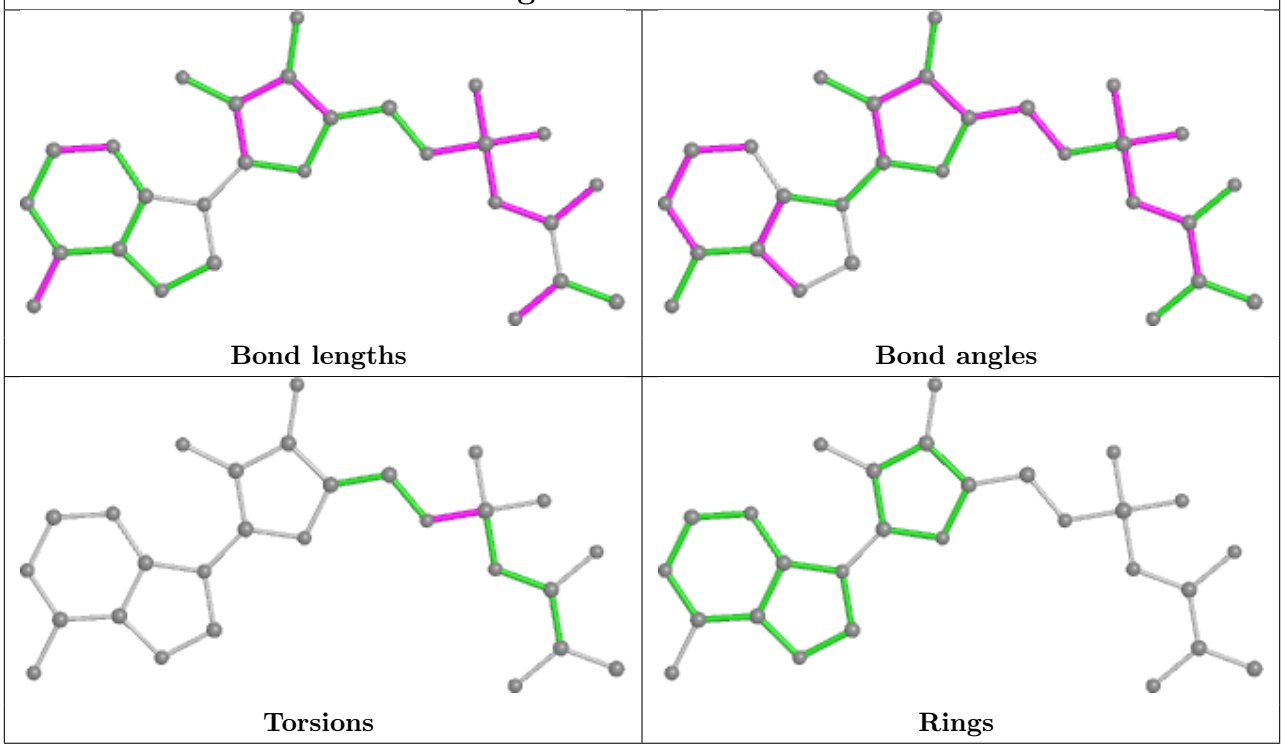
There are no ring outliers.

2 monomers are involved in 3 short contacts:

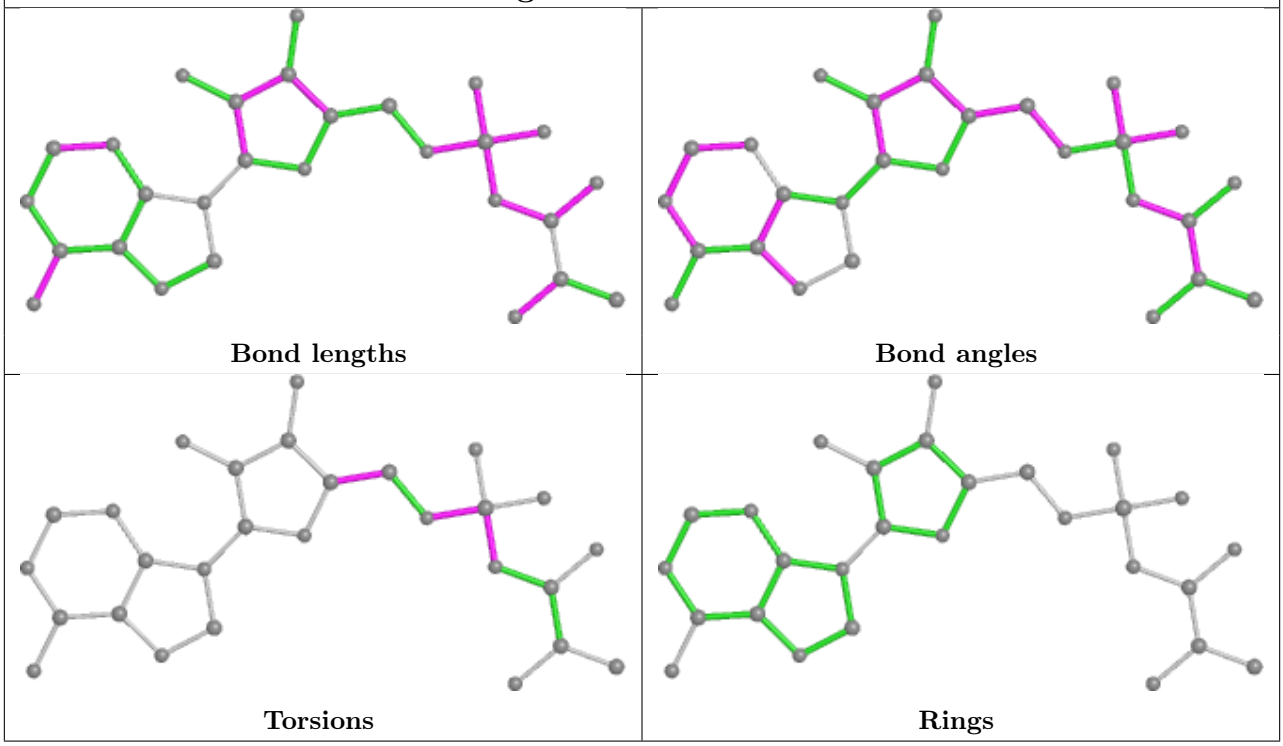
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	A5A	1	0
3	A	1001	A5A	2	0

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

Ligand A5A B 1001



Ligand A5A A 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	905/906 (99%)	0.50	70 (7%) 13 15	45, 111, 199, 233	0
1	B	904/906 (99%)	0.48	85 (9%) 8 10	49, 122, 194, 246	0
2	C	75/75 (100%)	0.23	1 (1%) 77 73	59, 90, 162, 213	0
All	All	1884/1887 (99%)	0.48	156 (8%) 11 13	45, 116, 197, 246	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	628	SER	12.8
1	B	41	GLY	12.6
1	A	502	PRO	8.2
1	A	628	SER	7.8
1	A	627	PHE	7.8
1	A	626	GLU	7.4
1	A	581	GLY	7.2
1	B	629	LYS	6.7
1	B	561	ASP	6.6
1	B	560	VAL	6.4
1	B	42	ASP	6.0
1	A	503	ALA	5.9
1	A	582	THR	5.9
1	B	40	CYS	5.9
1	B	197	ALA	5.3
1	B	558	GLU	5.2
1	B	627	PHE	5.2
1	B	570	LEU	5.2
1	A	906	GLY	5.1
1	A	490	VAL	5.0
1	A	491	GLN	5.0
1	A	497	LEU	4.9
1	A	494	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	524	VAL	4.8
1	A	529	VAL	4.8
1	B	572	VAL	4.7
1	A	528	PHE	4.6
1	A	492	GLU	4.5
1	B	564	GLU	4.5
1	B	626	GLU	4.5
1	B	44	PRO	4.5
1	B	872	SER	4.4
1	B	539	GLU	4.4
1	A	475	ASP	4.3
1	B	625	LYS	4.3
1	A	499	ASN	4.3
1	A	498	GLN	4.2
1	A	42	ASP	4.2
1	B	563	LEU	4.2
1	A	43	PRO	4.1
1	B	547	VAL	4.0
1	B	39	ILE	4.0
1	A	302	GLY	3.9
1	B	549	TYR	3.8
1	B	573	VAL	3.8
1	A	488	GLU	3.8
1	A	493	LYS	3.8
1	A	156	PRO	3.7
1	B	467	GLY	3.7
1	B	554	GLY	3.6
1	B	470	VAL	3.6
1	A	552	ALA	3.6
1	B	556	LYS	3.5
1	A	564	GLU	3.5
1	A	484	HIS	3.5
1	A	501	TYR	3.4
1	B	557	PHE	3.4
1	B	497	LEU	3.3
1	B	43	PRO	3.3
1	A	526	GLY	3.2
1	B	559	VAL	3.2
1	B	550	LEU	3.2
1	B	871	GLY	3.1
1	B	546	ASP	3.1
1	A	629	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	524	VAL	3.1
1	B	860	GLU	3.0
1	B	839	MET	3.0
1	A	116	PRO	3.0
1	B	526	GLY	3.0
1	B	576	ALA	3.0
1	B	175	ASN	3.0
1	A	814	VAL	2.9
1	B	528	PHE	2.9
1	B	465	GLU	2.9
1	B	574	LYS	2.9
1	B	870	LYS	2.9
1	B	435	GLU	2.9
1	A	483	ARG	2.8
1	B	883	ALA	2.8
1	B	575	GLY	2.8
1	A	578	PRO	2.8
1	A	625	LYS	2.8
1	A	500	GLU	2.8
1	B	542	GLY	2.7
1	B	622	GLY	2.7
1	A	489	LYS	2.7
1	B	305	ARG	2.7
1	B	886	GLN	2.7
1	A	520	GLU	2.7
1	B	25	LYS	2.7
1	A	518	GLU	2.7
1	A	532	ASN	2.7
1	A	303	GLU	2.7
1	B	841	LYS	2.6
1	A	155	TYR	2.6
1	B	517	PHE	2.6
1	B	431	GLU	2.6
1	B	460	VAL	2.6
1	B	840	ALA	2.5
2	C	1676	A	2.5
1	B	313	ARG	2.5
1	A	525	GLU	2.5
1	B	864	GLU	2.5
1	A	566	ASP	2.5
1	B	31	TRP	2.5
1	A	297	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	198	GLY	2.4
1	A	472	MET	2.4
1	A	540	SER	2.4
1	B	472	MET	2.4
1	A	485	SER	2.4
1	A	531	LEU	2.4
1	A	553	ASN	2.4
1	B	186	TYR	2.4
1	B	462	ILE	2.4
1	A	689	ARG	2.4
1	B	540	SER	2.3
1	A	543	GLN	2.3
1	A	476	ILE	2.3
1	B	438	LYS	2.3
1	A	547	VAL	2.3
1	B	57	LYS	2.3
1	B	536	PHE	2.3
1	A	25	LYS	2.2
1	A	2	THR	2.2
1	A	37	ARG	2.2
1	A	576	ALA	2.2
1	A	839	MET	2.2
1	A	152	ALA	2.2
1	A	732	PHE	2.2
1	A	44	PRO	2.2
1	B	475	ASP	2.2
1	B	440	LEU	2.2
1	B	562	VAL	2.2
1	B	551	ILE	2.1
1	B	845	LYS	2.1
1	B	585	LYS	2.1
1	B	7	TYR	2.1
1	A	622	GLY	2.1
1	B	468	ALA	2.1
1	B	516	GLU	2.1
1	B	30	PHE	2.1
1	A	473	PRO	2.1
1	B	176	GLU	2.1
1	A	322	VAL	2.0
1	A	153	PHE	2.0
1	A	130	ASP	2.0
1	B	182	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	469	GLU	2.0
1	B	445	LEU	2.0
1	B	18	PHE	2.0
1	A	571	HIS	2.0
1	B	865	ILE	2.0
1	A	530	ILE	2.0
1	B	463	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

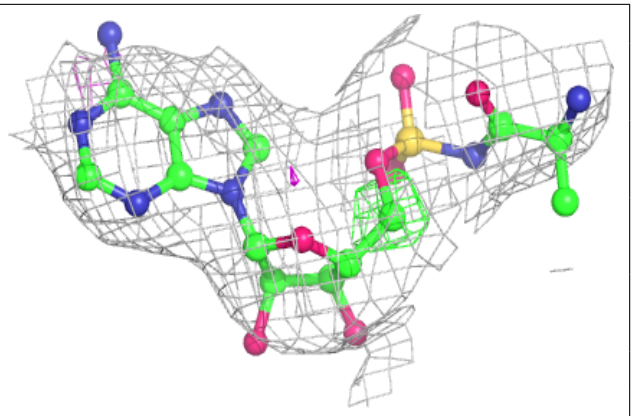
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

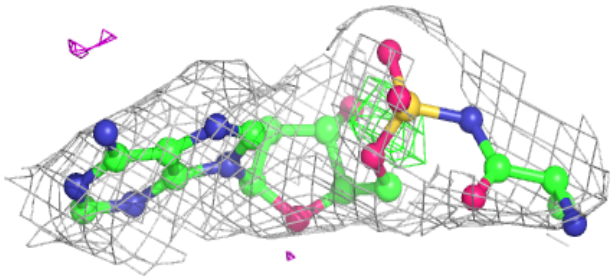
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	A5A	B	1001	28/28	0.90	0.36	86,117,135,148	0
4	ZN	A	1002	1/1	0.92	0.14	119,119,119,119	0
4	ZN	B	1002	1/1	0.92	0.22	109,109,109,109	0
3	A5A	A	1001	28/28	0.93	0.33	94,107,119,123	0

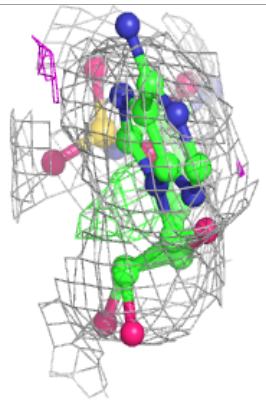
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A5A B 1001:

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

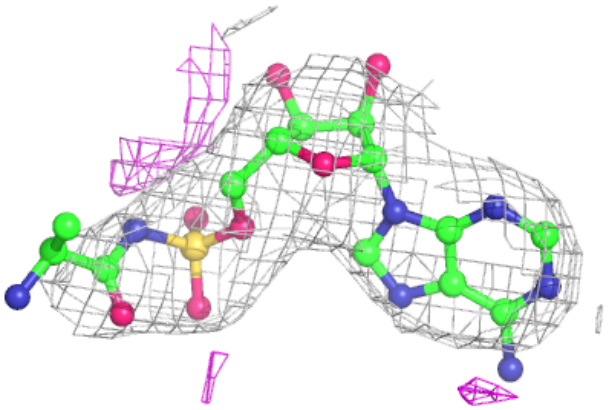


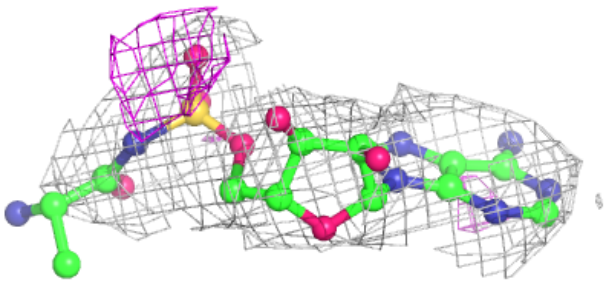


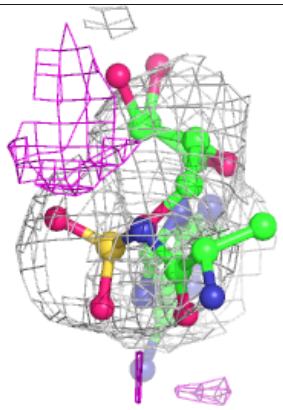


Electron density around A5A A 1001:

$2mF_o$-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.