Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:13 am BST

PDB ID	:	3WQY
Title	:	Crystal structure of Archaeoglobus fulgidus alanyl-tRNA synthetase in complex with wild-type tRNA(Ala) having G3.U70
Authors	:	Naganuma, M.; Sekine, S.; Yokoyama, S.
Deposited on	:	2014-02-05
Resolution	:	3.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

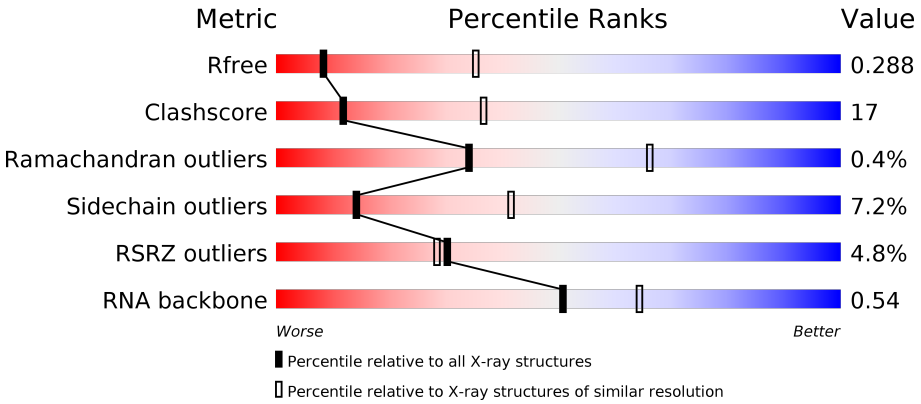
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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 on 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	5% 63% 34% ·
1	B	906	4% 60% 36% ·
2	C	75	% 51% 36% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	C	1701	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16096 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.

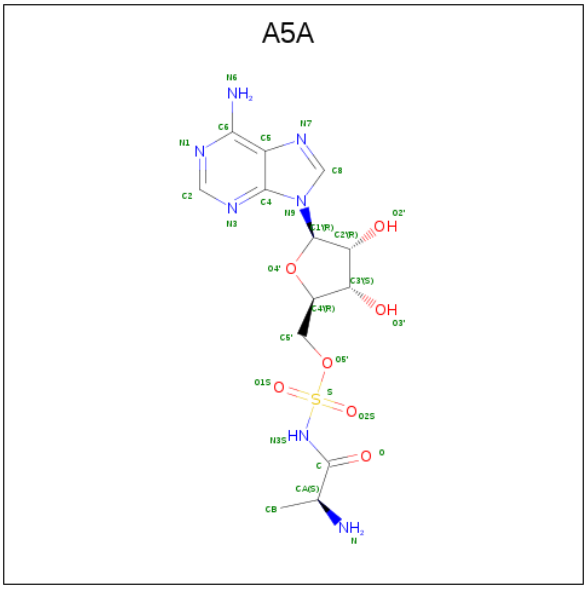
- Molecule 1 is a protein called Alanine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	905	Total	C	N	O	S	0	0	0
			7209	4573	1248	1357	31			
1	B	905	Total	C	N	O	S	0	0	0
			7212	4576	1248	1356	32			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	75	Total	C	N	O	P	0	0	0
			1609	715	295	524	75			

- 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
3	A	1	Total	C	N	O	S	0	0
			28	13	7	7	1		

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total	Mg	0	0
			3	3		

- Molecule 5 is water.

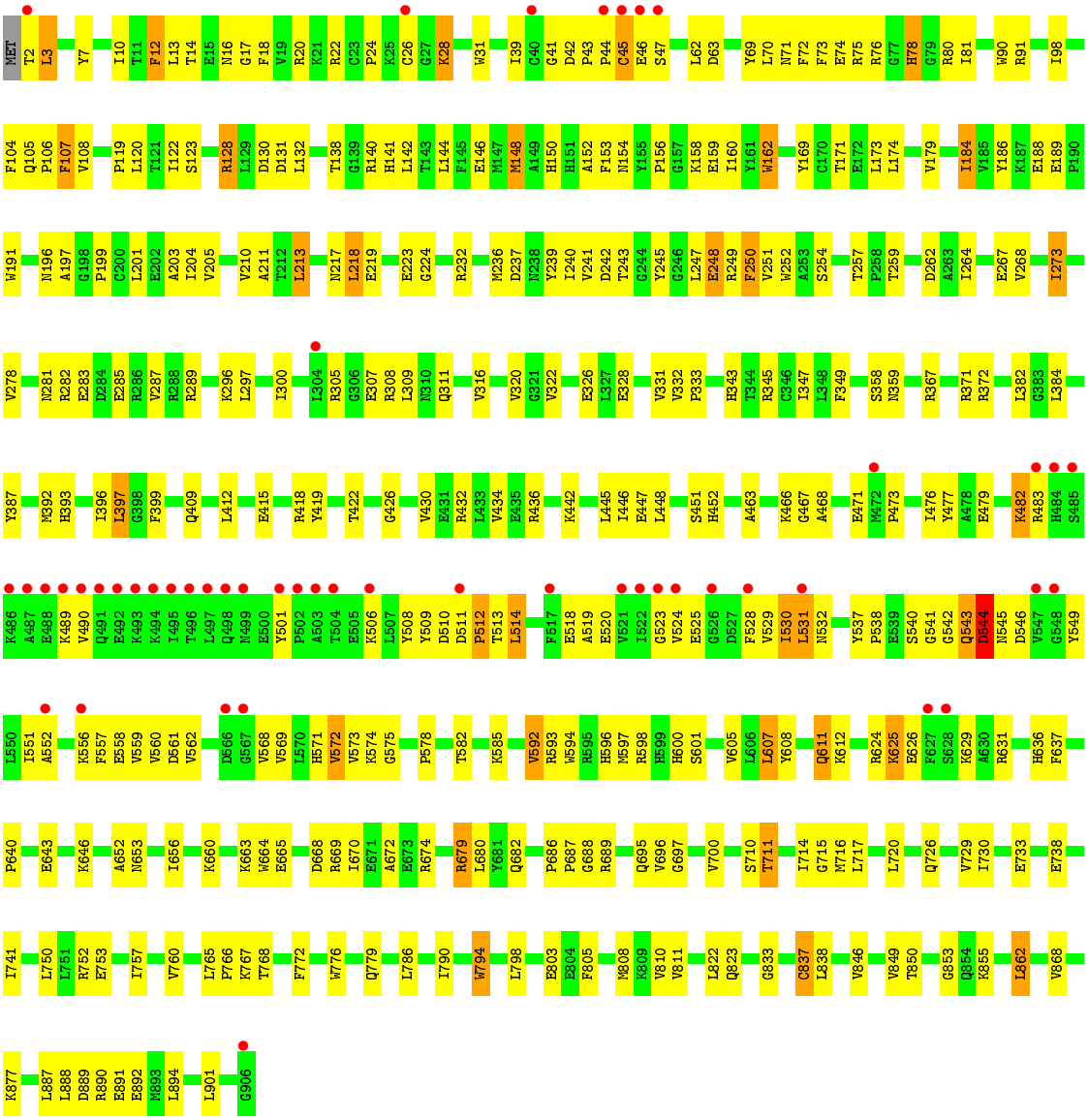
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	B	5	Total	O	0	0
			5	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

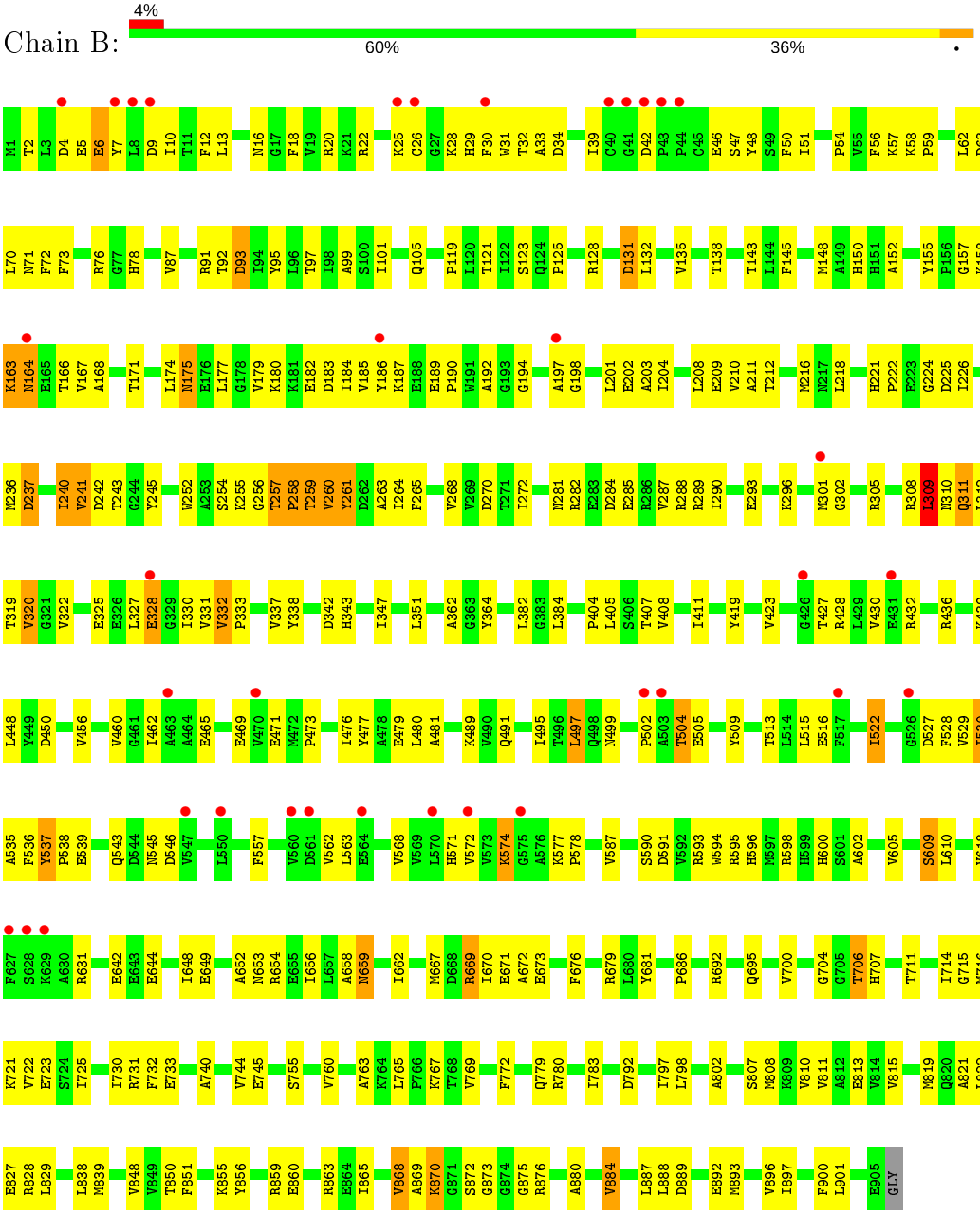
- Molecule 1: Alanine–tRNA ligase

Chain A:



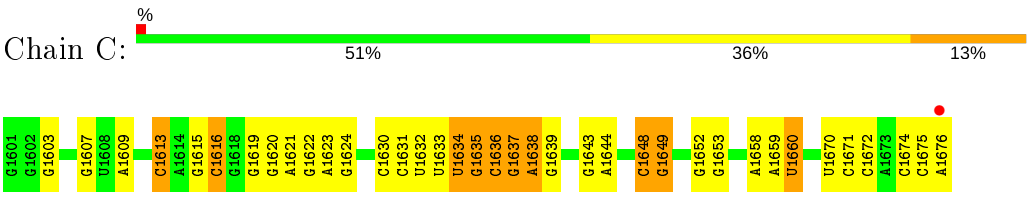
- Molecule 1: Alanine–tRNA ligase

Chain B:



- 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	99.74Å 169.84Å 175.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.77 – 3.30 41.76 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.77-3.30) 99.5 (41.76-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.250 , 0.289 0.254 , 0.288	Depositor DCC
R_{free} test set	2329 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	75.9	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.069 for -h,l,k	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16096	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A5A, MG

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	0.27	0/7347	0.47	0/9909
1	B	0.31	0/7350	0.50	1/9914 (0.0%)
2	C	0.26	0/1798	0.83	0/2802
All	All	0.29	0/16495	0.54	1/22625 (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})
1	B	309	LEU	CA-CB-CG	5.77	128.56	115.30

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	7209	0	7201	250	0
1	B	7212	0	7210	267	0
2	C	1609	0	816	34	0
3	A	28	0	19	5	0
3	B	28	0	19	0	0
4	C	3	0	0	0	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	0	0
All	All	16096	0	15265	542	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 (542) 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:C:1636:C:H1'	2:C:1637:G:OP2	1.47	1.11
1:B:10:ILE:HG22	1:B:164:ASN:HD22	1.12	1.06
1:B:18:PHE:HB3	1:B:31:TRP:HE1	1.27	0.96
2:C:1637:G:H2'	2:C:1638:A:O4'	1.67	0.95
1:B:20:ARG:HE	1:B:31:TRP:HZ3	1.11	0.94
1:B:18:PHE:HB3	1:B:31:TRP:NE1	1.83	0.94
1:B:257:THR:HG22	1:B:258:PRO:HD2	1.50	0.92
1:B:305:ARG:HA	1:B:309:LEU:HD23	1.54	0.90
2:C:1634:U:C4	2:C:1636:C:C5	2.60	0.90
2:C:1636:C:C1'	2:C:1637:G:OP2	2.23	0.86
1:B:10:ILE:HG22	1:B:164:ASN:ND2	1.92	0.84
2:C:1636:C:H4'	2:C:1637:G:O5'	1.79	0.83
1:B:31:TRP:HB3	1:B:186:TYR:HB2	1.63	0.80
1:A:322:VAL:HG13	1:A:326:GLU:HB3	1.61	0.80
1:B:658:ALA:O	1:B:659:ASN:ND2	2.11	0.79
1:B:224:GLY:HA3	1:B:232:ARG:HB3	1.66	0.78
1:B:237:ASP:N	1:B:237:ASP:OD1	2.17	0.78
1:A:224:GLY:HA3	1:A:232:ARG:HB3	1.63	0.78
1:B:20:ARG:HB3	1:B:31:TRP:CZ3	2.18	0.77
1:A:28:LYS:HE2	1:A:188:GLU:HB2	1.65	0.77
1:B:18:PHE:CB	1:B:31:TRP:HE1	2.00	0.75
1:A:72:PHE:O	1:A:76:ARG:NH1	2.20	0.74
1:B:654:ARG:NH1	1:B:654:ARG:O	2.21	0.73
1:B:255:LYS:HD3	1:B:263:ALA:HB1	1.72	0.72
1:B:9:ASP:OD2	1:B:163:LYS:NZ	2.20	0.71
1:B:32:THR:HG22	1:B:185:VAL:HG12	1.71	0.71
1:B:218:LEU:HB2	1:B:233:TYR:CZ	2.26	0.71
1:A:43:PRO:HG2	1:A:308:ARG:HH12	1.55	0.71
1:A:669:ARG:NH2	1:A:688:GLY:O	2.24	0.71
1:A:669:ARG:NH1	1:A:686:PRO:O	2.24	0.70
1:A:132:LEU:HD21	1:A:372:ARG:CZ	2.21	0.70
2:C:1638:A:H2'	2:C:1639:G:C8	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HD23	1:B:477:TYR:HB3	1.72	0.70
1:A:624:ARG:HD2	1:A:631:ARG:HH21	1.57	0.69
1:A:551:ILE:HG22	1:A:556:LYS:HG3	1.74	0.69
1:B:535:ALA:O	1:B:593:ARG:NH2	2.25	0.69
1:B:9:ASP:OD1	1:B:10:ILE:HG23	1.92	0.69
1:B:711:THR:O	1:B:714:ILE:HG13	1.93	0.69
1:A:640:PRO:HD3	1:A:730:ILE:HD13	1.75	0.69
1:B:473:PRO:HG2	1:B:476:ILE:HG22	1.74	0.69
1:B:539:GLU:HB2	1:B:545:ASN:HD21	1.57	0.69
2:C:1633:U:H3	2:C:1636:C:N4	1.91	0.69
1:A:76:ARG:HD3	1:A:169:TYR:CE1	2.28	0.68
1:B:477:TYR:HA	1:B:480:LEU:HG	1.74	0.68
1:A:71:ASN:OD1	1:A:72:PHE:N	2.27	0.68
1:A:543:GLN:HB3	1:A:626:GLU:HA	1.74	0.67
1:A:273:ILE:HG13	1:A:278:VAL:HG21	1.76	0.67
1:A:752:ARG:NH1	1:B:642:GLU:OE1	2.27	0.67
1:A:39:ILE:HG13	1:A:45:CYS:HB3	1.75	0.67
1:B:203:ALA:HB3	1:B:211:ALA:HB3	1.76	0.67
2:C:1634:U:N3	2:C:1636:C:C5	2.62	0.67
1:B:33:ALA:HB3	1:B:182:GLU:HA	1.76	0.66
2:C:1638:A:H2'	2:C:1639:G:H8	1.61	0.66
1:A:223:GLU:O	1:A:232:ARG:NH2	2.26	0.66
1:A:71:ASN:HA	1:A:74:GLU:HB2	1.77	0.66
1:A:540:SER:OG	1:A:541:GLY:N	2.28	0.66
2:C:1636:C:C4'	2:C:1637:G:O5'	2.45	0.65
1:B:197:ALA:HB3	1:B:233:TYR:CE2	2.31	0.65
1:B:810:VAL:HG11	1:B:901:LEU:HD11	1.78	0.65
1:B:105:GLN:HE22	1:B:194:GLY:HA3	1.61	0.65
1:A:367:ARG:HD3	1:A:371:ARG:HH21	1.62	0.65
1:B:598:ARG:HA	1:B:714:ILE:HG22	1.78	0.64
1:A:442:LYS:HD2	1:A:476:ILE:HD13	1.78	0.64
1:A:289:ARG:NH2	1:A:320:VAL:O	2.28	0.64
1:B:252:TRP:CE3	1:B:260:VAL:HA	2.33	0.64
1:A:837:CYS:HB3	1:A:850:THR:HG22	1.80	0.64
1:B:224:GLY:O	1:B:232:ARG:NH2	2.29	0.63
1:A:62:LEU:HD23	1:A:251:VAL:HG21	1.78	0.63
1:B:4:ASP:HA	1:B:7:TYR:CE2	2.33	0.63
1:A:546:ASP:OD2	1:A:593:ARG:NH1	2.31	0.63
1:B:610:LEU:HD23	1:B:648:ILE:HD12	1.80	0.63
1:A:660:LYS:HD2	1:A:697:GLY:HA3	1.80	0.62
1:A:543:GLN:N	1:A:625:LYS:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:LEU:HG	1:B:384:LEU:H	1.64	0.62
1:A:624:ARG:HB2	1:A:631:ARG:HE	1.64	0.62
1:A:509:TYR:O	1:A:664:TRP:NE1	2.31	0.61
1:A:668:ASP:HB2	1:A:689:ARG:HH12	1.64	0.61
1:A:549:TYR:HD1	1:A:558:GLU:HA	1.65	0.61
1:A:889:ASP:OD1	1:A:890:ARG:N	2.34	0.60
1:A:152:ALA:H	1:A:241:VAL:HG22	1.65	0.60
1:B:839:MET:HG2	1:B:848:VAL:HG22	1.83	0.60
1:A:105:GLN:HE21	1:A:196:ASN:HD22	1.49	0.60
1:B:546:ASP:OD2	1:B:593:ARG:NH2	2.25	0.60
1:A:119:PRO:HD3	1:A:160:ILE:HG21	1.84	0.60
1:B:432:ARG:O	1:B:436:ARG:HB2	2.01	0.60
1:B:18:PHE:CE1	1:B:33:ALA:HB2	2.37	0.60
1:B:644:GLU:O	1:B:648:ILE:HG12	2.02	0.60
1:B:706:THR:O	1:B:707:HIS:ND1	2.35	0.60
1:B:162:TRP:CE3	1:B:162:TRP:HA	2.36	0.60
1:B:865:ILE:HG12	1:B:896:VAL:HG21	1.84	0.60
1:B:889:ASP:OD1	1:B:892:GLU:N	2.33	0.59
1:B:216:MET:HG3	1:B:240:ILE:HG23	1.83	0.59
1:B:54:PRO:HG3	1:B:256:GLY:HA3	1.83	0.59
1:B:131:ASP:N	1:B:131:ASP:OD1	2.34	0.59
1:B:480:LEU:HD12	1:B:481:ALA:N	2.18	0.59
1:B:9:ASP:OD1	1:B:10:ILE:N	2.36	0.59
1:A:201:LEU:HB2	1:A:213:LEU:HD11	1.83	0.59
1:B:308:ARG:NH1	1:B:311:GLN:OE1	2.36	0.58
1:B:309:LEU:HD12	1:B:310:ASN:N	2.19	0.58
1:A:512:PRO:HB2	1:A:597:MET:HE1	1.85	0.58
1:B:439:LYS:HG3	1:B:469:GLU:HB3	1.84	0.58
1:A:12:PHE:HA	1:A:16:ASN:HD22	1.69	0.58
1:B:10:ILE:HB	1:B:164:ASN:HB3	1.83	0.58
1:A:358:SER:O	1:A:367:ARG:NE	2.36	0.58
1:B:47:SER:OG	1:B:296:LYS:O	2.21	0.58
2:C:1623:A:H2'	2:C:1624:G:C8	2.38	0.58
1:A:47:SER:HB3	1:A:300:ILE:HG12	1.86	0.58
1:A:262:ASP:OD2	1:A:282:ARG:NH2	2.37	0.57
1:B:824:LYS:O	1:B:828:ARG:NH1	2.37	0.57
1:B:596:HIS:O	1:B:600:HIS:ND1	2.27	0.57
1:A:90:TRP:CD1	1:A:91:ARG:HG3	2.39	0.57
1:B:51:ILE:HD11	1:B:296:LYS:HG2	1.86	0.57
1:B:532:ASN:OD1	1:B:533:ARG:N	2.38	0.57
1:A:150:HIS:HE1	1:A:245:TYR:HE2	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:GLU:OE2	1:B:212:THR:OG1	2.20	0.57
1:B:5:GLU:N	1:B:5:GLU:OE1	2.38	0.56
1:B:504:THR:HG21	1:B:568:VAL:HA	1.87	0.56
1:B:93:ASP:N	1:B:93:ASP:OD1	2.38	0.56
1:A:328:GLU:HA	1:A:331:VAL:HB	1.88	0.56
1:B:539:GLU:HB2	1:B:545:ASN:ND2	2.21	0.56
1:B:427:THR:O	1:B:430:VAL:HG12	2.06	0.56
1:A:81:ILE:HD12	1:A:120:LEU:HD22	1.88	0.56
1:A:203:ALA:HB3	1:A:211:ALA:HB3	1.88	0.56
1:A:218:LEU:HA	1:A:236:MET:HG3	1.88	0.56
1:B:39:ILE:HD11	1:B:46:GLU:HG2	1.88	0.56
1:B:471:GLU:HG2	1:B:471:GLU:O	2.06	0.56
1:B:62:LEU:H	1:B:62:LEU:HD12	1.70	0.55
1:A:716:MET:HE2	1:B:716:MET:HB2	1.88	0.55
1:B:495:ILE:HG23	1:B:497:LEU:HD13	1.89	0.55
1:A:13:LEU:HD13	1:A:31:TRP:CD2	2.42	0.55
1:A:594:TRP:HB3	1:A:598:ARG:NH1	2.22	0.55
1:B:430:VAL:HG13	1:B:462:ILE:HG21	1.88	0.55
1:B:162:TRP:HE3	1:B:162:TRP:HA	1.71	0.55
1:B:218:LEU:HB2	1:B:233:TYR:CE2	2.42	0.55
1:B:504:THR:OG1	1:B:505:GLU:N	2.37	0.55
1:B:12:PHE:HA	1:B:16:ASN:HB2	1.88	0.55
1:B:439:LYS:NZ	1:B:441:GLU:OE1	2.35	0.55
1:A:63:ASP:N	1:A:63:ASP:OD1	2.39	0.55
1:A:726:GLN:HG2	1:A:729:VAL:HB	1.89	0.55
1:B:875:GLY:HA3	1:B:880:ALA:HA	1.87	0.54
2:C:1634:U:C4	2:C:1636:C:C4	2.96	0.54
2:C:1635:G:O2'	2:C:1637:G:N2	2.40	0.54
1:A:850:THR:HG23	1:A:862:LEU:HD12	1.88	0.54
1:A:98:ILE:O	1:A:128:ARG:NE	2.40	0.54
1:A:542:GLY:HA3	1:A:625:LYS:H	1.72	0.54
1:A:822:LEU:HB3	1:A:849:VAL:HG21	1.89	0.54
1:B:91:ARG:HH12	1:B:105:GLN:HE21	1.56	0.54
1:B:489:LYS:HB2	1:B:491:GLN:OE1	2.07	0.54
1:A:367:ARG:HD3	1:A:371:ARG:NH2	2.22	0.54
1:B:221:HIS:CG	1:B:222:PRO:HD2	2.42	0.54
1:B:20:ARG:HB3	1:B:31:TRP:CE3	2.42	0.54
1:B:516:GLU:N	1:B:516:GLU:OE1	2.41	0.54
1:B:808:MET:HE1	1:B:856:TYR:CE1	2.43	0.54
1:A:150:HIS:CD2	1:A:243:THR:HG21	2.42	0.54
1:A:397:LEU:HB3	1:A:399:PHE:HD1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:TYR:CZ	1:A:612:LYS:HD2	2.43	0.54
1:A:506:LYS:HD3	1:A:508:TYR:CE2	2.43	0.54
1:A:636:HIS:HB3	1:A:730:ILE:HD12	1.88	0.54
1:A:552:ALA:HB1	1:A:582:THR:HG21	1.90	0.54
1:A:73:PHE:HD1	1:A:78:HIS:HE2	1.56	0.54
1:A:81:ILE:O	1:A:122:ILE:HD13	2.08	0.53
1:A:561:ASP:O	1:A:572:VAL:HG13	2.09	0.53
1:A:798:LEU:HB3	1:A:811:VAL:HG21	1.91	0.53
1:B:73:PHE:HA	1:B:76:ARG:HB2	1.90	0.53
1:A:573:VAL:HG12	1:A:575:GLY:H	1.73	0.53
1:A:150:HIS:HE1	1:A:245:TYR:CE2	2.27	0.53
1:A:545:ASN:HD21	1:A:561:ASP:HA	1.73	0.53
1:B:197:ALA:N	1:B:233:TYR:OH	2.42	0.53
1:A:596:HIS:O	1:A:600:HIS:ND1	2.41	0.53
1:B:312:LEU:O	1:B:316:VAL:HG12	2.09	0.53
1:B:91:ARG:NH1	1:B:105:GLN:HE21	2.07	0.53
1:A:451:SER:O	1:A:452:HIS:ND1	2.42	0.53
1:B:56:PHE:HD1	1:B:177:LEU:HB3	1.74	0.53
1:B:180:LYS:HG3	1:B:183:ASP:H	1.73	0.53
1:A:560:VAL:HG11	1:A:574:LYS:HE2	1.91	0.53
1:B:138:THR:HG22	1:B:302:GLY:HA3	1.90	0.52
1:B:872:SER:OG	1:B:873:GLY:N	2.43	0.52
1:A:307:GLU:OE1	1:A:311:GLN:NE2	2.42	0.52
1:B:543:GLN:HG3	1:B:625:LYS:H	1.72	0.52
1:A:779:GLN:OE1	1:B:780:ARG:NH1	2.42	0.52
1:A:142:LEU:HD12	1:A:248:GLU:HG3	1.90	0.52
1:A:562:VAL:HG12	1:A:571:HIS:HA	1.90	0.52
1:B:187:LYS:HZ1	1:B:189:GLU:HB2	1.75	0.52
1:B:537:TYR:OH	1:B:704:GLY:O	2.24	0.52
1:B:536:PHE:CG	1:B:571:HIS:HE1	2.28	0.52
1:B:128:ARG:HH12	1:B:145:PHE:HZ	1.57	0.52
1:B:166:THR:HG21	1:B:241:VAL:HG21	1.92	0.52
1:B:667:MET:HG2	1:B:672:ALA:HB2	1.92	0.52
1:A:476:ILE:HG13	1:A:479:GLU:HB2	1.91	0.52
1:A:188:GLU:O	1:A:189:GLU:HG2	2.10	0.52
1:A:434:VAL:HG11	1:A:466:LYS:HD2	1.92	0.52
1:B:293:GLU:HG2	1:B:320:VAL:HG13	1.92	0.52
1:B:529:VAL:N	1:B:571:HIS:O	2.36	0.52
2:C:1637:G:H2'	2:C:1638:A:C4'	2.39	0.51
1:A:150:HIS:CE1	1:A:245:TYR:HE2	2.28	0.51
1:B:78:HIS:HA	1:B:119:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:825:LEU:HD12	1:B:826:ALA:N	2.25	0.51
1:B:839:MET:HE1	1:B:888:LEU:HB3	1.92	0.51
1:A:422:THR:OG1	2:C:1670:U:OP1	2.20	0.51
1:A:501:TYR:CE2	1:A:523:GLY:HA3	2.46	0.51
1:B:316:VAL:O	1:B:319:THR:HG22	2.10	0.51
1:B:618:VAL:O	1:B:679:ARG:NH1	2.36	0.51
2:C:1671:C:H2'	2:C:1672:C:C6	2.46	0.51
1:B:185:VAL:HG23	1:B:204:ILE:HB	1.93	0.51
1:A:508:TYR:HH	1:A:537:TYR:HD1	1.59	0.51
1:B:591:ASP:HA	1:B:594:TRP:HB2	1.93	0.51
1:B:591:ASP:O	1:B:595:ARG:HG2	2.11	0.51
1:A:482:LYS:HG3	1:A:483:ARG:N	2.26	0.51
1:B:155:TYR:O	1:B:157:GLY:N	2.44	0.51
2:C:1670:U:H2'	2:C:1671:C:C6	2.46	0.51
1:B:22:ARG:HD2	1:B:29:HIS:CE1	2.46	0.51
1:B:528:PHE:HD1	1:B:572:VAL:HG22	1.75	0.51
1:A:530:ILE:HD13	1:A:568:VAL:HG13	1.92	0.50
1:B:4:ASP:HA	1:B:7:TYR:HE2	1.76	0.50
1:A:359:ASN:OD1	1:A:726:GLN:HB2	2.11	0.50
1:B:91:ARG:NH2	1:B:93:ASP:OD2	2.32	0.50
1:B:869:ALA:O	1:B:870:LYS:HB2	2.11	0.50
2:C:1615:G:H5'	2:C:1616:C:OP2	2.10	0.50
1:B:99:ALA:HB3	1:B:101:ILE:HG22	1.93	0.50
1:A:107:PHE:HD1	1:A:108:VAL:HG23	1.76	0.50
1:A:247:LEU:HA	1:A:250:PHE:HB2	1.93	0.50
1:B:59:PRO:HB3	1:B:255:LYS:HA	1.94	0.50
1:B:529:VAL:O	1:B:571:HIS:N	2.42	0.50
1:A:62:LEU:HD21	1:A:264:ILE:HD12	1.94	0.50
1:B:148:MET:HB2	1:B:245:TYR:HB2	1.94	0.50
1:A:13:LEU:HD13	1:A:31:TRP:CE2	2.47	0.49
1:A:524:VAL:HG13	1:A:529:VAL:HG12	1.93	0.49
1:B:301:MET:HB3	1:B:312:LEU:HD12	1.94	0.49
1:B:860:GLU:HG2	1:B:863:ARG:HH12	1.77	0.49
2:C:1623:A:H2'	2:C:1624:G:H8	1.76	0.49
1:A:47:SER:HB3	1:A:300:ILE:CD1	2.42	0.49
1:A:663:LYS:HG2	1:A:665:GLU:OE1	2.13	0.49
1:A:805:PHE:CD1	1:A:901:LEU:HD23	2.47	0.49
1:B:101:ILE:O	1:B:105:GLN:HG2	2.13	0.49
1:B:135:VAL:HG21	1:B:143:THR:HG23	1.94	0.49
1:B:656:ILE:HD12	1:B:714:ILE:HD11	1.94	0.49
1:A:540:SER:H	1:A:544:ASP:HB3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:HD23	1:A:571:HIS:HE2	1.77	0.49
1:B:63:ASP:N	1:B:63:ASP:OD1	2.45	0.49
1:A:162:TRP:CE3	1:A:162:TRP:HA	2.46	0.49
1:A:343:HIS:O	1:A:347:ILE:HG12	2.13	0.49
1:A:418:ARG:NH2	1:A:637:PHE:O	2.46	0.49
1:B:202:GLU:HG2	1:B:212:THR:HG23	1.94	0.49
1:B:327:LEU:O	1:B:331:VAL:HG22	2.12	0.49
1:B:649:GLU:OE2	1:B:718:LYS:NZ	2.34	0.49
2:C:1607:G:HO2'	2:C:1649:G:H8	1.57	0.49
1:A:162:TRP:HE3	1:A:162:TRP:HA	1.78	0.49
1:B:189:GLU:HG2	1:B:190:PRO:HD2	1.94	0.49
1:A:463:ALA:O	1:A:467:GLY:N	2.45	0.49
1:A:518:GLU:HG2	1:A:585:LYS:HE2	1.93	0.49
1:A:670:ILE:O	1:A:674:ARG:HG3	2.13	0.49
1:B:859:ARG:HH11	1:B:876:ARG:HA	1.78	0.49
1:B:252:TRP:CD2	1:B:260:VAL:HA	2.48	0.49
1:A:138:THR:HG21	1:A:141:HIS:ND1	2.29	0.48
1:A:392:MET:O	1:A:396:ILE:HG12	2.13	0.48
1:A:471:GLU:O	1:A:473:PRO:HD3	2.13	0.48
1:A:196:ASN:OD1	1:A:219:GLU:HG2	2.13	0.48
1:B:31:TRP:N	1:B:186:TYR:O	2.45	0.48
1:B:528:PHE:CD1	1:B:572:VAL:HG22	2.46	0.48
1:B:343:HIS:O	1:B:347:ILE:HG12	2.13	0.48
1:B:332:VAL:HG12	1:B:333:PRO:HD3	1.96	0.48
1:B:364:TYR:OH	1:B:450:ASP:OD1	2.23	0.48
1:A:252:TRP:NE1	1:A:257:THR:O	2.33	0.48
1:A:760:VAL:HG21	1:A:768:THR:HG21	1.94	0.48
1:A:217:ASN:HA	1:A:239:TYR:CD1	2.48	0.48
1:B:829:LEU:HD13	1:B:851:PHE:CZ	2.48	0.48
1:B:225:ASP:OD1	1:B:226:ILE:N	2.47	0.48
1:A:543:GLN:HE21	1:A:596:HIS:HE1	1.62	0.48
1:B:150:HIS:NE2	1:B:243:THR:HG21	2.29	0.48
1:B:56:PHE:CD1	1:B:177:LEU:HB3	2.48	0.48
1:A:594:TRP:O	1:A:598:ARG:HG3	2.14	0.47
1:B:721:LYS:HB2	1:B:733:GLU:HB2	1.96	0.47
1:A:7:TYR:O	1:A:10:ILE:HG12	2.14	0.47
1:A:130:ASP:OD1	1:A:131:ASP:N	2.47	0.47
1:B:192:ALA:HA	1:B:197:ALA:HB2	1.94	0.47
1:A:463:ALA:O	1:A:468:ALA:N	2.47	0.47
1:B:2:THR:O	1:B:6:GLU:OE2	2.32	0.47
1:B:325:GLU:HA	1:B:328:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:ASP:OD1	1:B:828:ARG:NE	2.47	0.47
1:B:57:LYS:HG2	1:B:177:LEU:O	2.13	0.47
1:A:153:PHE:HD1	1:A:240:ILE:HD12	1.80	0.47
1:A:652:ALA:O	1:A:656:ILE:HG13	2.14	0.47
1:B:821:ALA:O	1:B:825:LEU:HG	2.14	0.47
1:B:850:THR:OG1	1:B:880:ALA:HB3	2.14	0.47
1:A:446:ILE:HG13	1:A:447:GLU:N	2.29	0.47
1:A:557:PHE:HE2	1:A:578:PRO:HB3	1.80	0.47
1:B:473:PRO:O	1:B:476:ILE:HG23	2.13	0.47
1:B:4:ASP:OD1	1:B:7:TYR:HE2	1.97	0.47
1:A:191:TRP:CZ2	3:A:1001:A5A:N	2.67	0.47
1:A:382:LEU:HG	1:A:384:LEU:H	1.80	0.47
1:A:790:ILE:HG22	1:A:794:TRP:HD1	1.80	0.47
1:B:725:ILE:HD11	1:B:731:ARG:HB2	1.97	0.47
1:A:426:GLY:O	1:A:430:VAL:HG23	2.15	0.47
1:A:846:VAL:HG11	1:A:887:LEU:HD23	1.96	0.47
1:A:656:ILE:HD13	1:A:715:GLY:O	2.15	0.47
1:B:208:LEU:O	1:B:210:VAL:HG23	2.15	0.47
1:B:69:TYR:CE2	1:B:148:MET:HB3	2.49	0.47
1:B:167:VAL:HG13	1:B:186:TYR:HE2	1.80	0.47
1:A:217:ASN:HA	1:A:239:TYR:HD1	1.80	0.47
1:A:371:ARG:HH11	1:A:419:TYR:HD1	1.63	0.46
1:A:652:ALA:HB1	1:A:717:LEU:HD23	1.97	0.46
1:B:152:ALA:HB1	1:B:160:ILE:HD13	1.98	0.46
1:B:522:ILE:HG13	1:B:522:ILE:O	2.15	0.46
1:B:531:LEU:HD13	1:B:571:HIS:CD2	2.51	0.46
1:B:860:GLU:HG2	1:B:863:ARG:NH1	2.30	0.46
1:B:839:MET:HE3	1:B:887:LEU:HD12	1.97	0.46
1:A:285:GLU:OE1	1:A:289:ARG:HD3	2.16	0.46
1:A:598:ARG:HG2	1:A:714:ILE:HA	1.97	0.46
1:A:753:GLU:O	1:A:757:ILE:HG12	2.15	0.46
1:B:527:ASP:OD2	1:B:574:LYS:HD2	2.16	0.46
1:B:656:ILE:HG21	1:B:715:GLY:O	2.16	0.46
2:C:1658:A:H1'	2:C:1660:U:OP2	2.15	0.46
1:A:22:ARG:NH2	1:A:26:CYS:SG	2.89	0.46
1:B:281:ASN:O	1:B:287:VAL:HG21	2.15	0.46
2:C:1671:C:H2'	2:C:1672:C:H6	1.81	0.46
1:A:73:PHE:HD1	1:A:78:HIS:NE2	2.14	0.46
1:A:855:LYS:O	1:A:877:LYS:NZ	2.39	0.46
1:B:557:PHE:CG	1:B:578:PRO:HG3	2.51	0.46
1:B:624:ARG:HB2	1:B:631:ARG:HE	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1636:C:C1'	2:C:1637:G:P	3.04	0.46
1:A:432:ARG:NH1	2:C:1613:C:H4'	2.29	0.46
1:A:672:ALA:HB1	1:A:680:LEU:HD11	1.97	0.46
1:A:716:MET:SD	1:A:716:MET:N	2.89	0.46
1:B:78:HIS:CD2	1:B:119:PRO:HB2	2.51	0.46
1:A:332:VAL:HB	1:A:333:PRO:HD3	1.98	0.46
1:A:345:ARG:HE	1:A:397:LEU:HD11	1.81	0.46
1:A:543:GLN:O	1:A:545:ASN:HB2	2.16	0.46
1:B:192:ALA:HA	1:B:197:ALA:CB	2.46	0.46
1:B:309:LEU:HD13	1:B:313:ARG:HH11	1.79	0.46
1:A:242:ASP:CG	3:A:1001:A5A:HB3	2.35	0.46
1:A:267:GLU:H	1:A:267:GLU:CD	2.18	0.46
1:A:174:LEU:CD2	1:A:184:ILE:HD12	2.46	0.46
1:A:20:ARG:HB2	1:A:31:TRP:CZ3	2.51	0.46
1:A:297:LEU:HD12	1:A:316:VAL:HB	1.97	0.46
1:A:551:ILE:HG13	1:A:585:LYS:O	2.15	0.46
1:B:179:VAL:HG23	1:B:184:ILE:HD11	1.98	0.46
1:A:646:LYS:HE2	1:B:745:GLU:OE1	2.16	0.46
1:B:765:LEU:O	1:B:769:VAL:HG23	2.16	0.46
1:A:150:HIS:CE1	1:A:245:TYR:CE2	3.03	0.45
1:B:802:ALA:HB2	1:B:811:VAL:HB	1.98	0.45
1:A:786:LEU:O	1:A:790:ILE:HG12	2.17	0.45
1:B:218:LEU:HA	1:B:235:LYS:HA	1.98	0.45
1:A:72:PHE:HD2	1:A:73:PHE:CD2	2.34	0.45
1:B:204:ILE:HG23	1:B:208:LEU:C	2.36	0.45
1:B:51:ILE:O	1:B:51:ILE:HD12	2.17	0.45
1:B:264:ILE:HG13	1:B:265:PHE:CD2	2.51	0.45
1:A:779:GLN:NE2	1:B:779:GLN:OE1	2.48	0.45
2:C:1633:U:N3	2:C:1636:C:N4	2.62	0.45
1:A:249:ARG:NH1	3:A:1001:A5A:H2'	2.32	0.45
1:A:281:ASN:O	1:A:287:VAL:HG21	2.17	0.45
1:B:538:PRO:O	1:B:539:GLU:HG3	2.17	0.45
1:B:272:ILE:HB	1:B:337:VAL:HG23	1.99	0.45
1:B:714:ILE:HD12	1:B:715:GLY:O	2.15	0.45
1:A:105:GLN:HA	1:A:106:PRO:HA	1.74	0.45
1:A:197:ALA:HB3	1:A:218:LEU:HD11	1.98	0.45
1:A:24:PRO:HG2	1:A:41:GLY:HA2	1.98	0.45
1:B:252:TRP:CH2	1:B:259:THR:N	2.85	0.45
1:B:855:LYS:HA	1:B:855:LYS:HD2	1.64	0.45
1:A:868:VAL:HG23	1:A:888:LEU:HD11	1.98	0.45
1:B:284:ASP:O	1:B:288:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:TYR:CE1	1:A:199:PRO:HB2	2.52	0.45
1:B:34:ASP:HB2	1:B:182:GLU:HB3	1.99	0.45
1:B:577:LYS:HA	1:B:578:PRO:HD3	1.82	0.45
1:B:58:LYS:O	1:B:254:SER:OG	2.34	0.45
1:B:602:ALA:O	1:B:605:VAL:HG12	2.17	0.45
1:B:669:ARG:NH1	1:B:673:GLU:OE2	2.49	0.45
1:B:827:GLU:HG3	1:B:828:ARG:N	2.31	0.45
1:A:13:LEU:HA	1:A:18:PHE:HB2	1.99	0.45
1:A:146:GLU:N	1:A:248:GLU:OE1	2.41	0.45
1:A:42:ASP:HA	1:A:43:PRO:HD2	1.80	0.45
1:B:119:PRO:HB3	1:B:160:ILE:HG21	1.98	0.45
1:B:268:VAL:O	1:B:272:ILE:HG13	2.17	0.45
1:B:67:GLU:HA	1:B:70:LEU:HD12	1.98	0.45
1:A:656:ILE:HG12	1:A:714:ILE:HD11	1.99	0.44
1:B:652:ALA:HB1	1:B:717:LEU:HD21	1.99	0.44
1:A:237:ASP:N	1:A:237:ASP:OD1	2.50	0.44
1:A:367:ARG:NH1	1:A:415:GLU:OE2	2.50	0.44
1:A:397:LEU:HB3	1:A:399:PHE:CD1	2.50	0.44
1:A:511:ASP:OD1	1:A:514:LEU:HG	2.17	0.44
1:A:305:ARG:HA	1:A:309:LEU:HB2	1.99	0.44
1:A:561:ASP:OD1	1:A:562:VAL:N	2.49	0.44
1:A:607:LEU:O	1:A:611:GLN:HG2	2.16	0.44
1:A:772:PHE:O	1:A:776:TRP:N	2.39	0.44
1:B:12:PHE:CZ	1:B:168:ALA:HA	2.53	0.44
1:B:259:THR:HG1	1:B:338:TYR:HH	1.58	0.44
1:B:456:VAL:O	1:B:460:VAL:HG23	2.17	0.44
1:A:154:ASN:HB3	1:A:159:GLU:HB3	1.98	0.44
1:A:249:ARG:HD2	3:A:1001:A5A:O2'	2.16	0.44
1:A:489:LYS:HD3	1:A:489:LYS:HA	1.70	0.44
1:A:558:GLU:O	1:A:573:VAL:HG13	2.17	0.44
1:A:601:SER:O	1:A:605:VAL:HG23	2.17	0.44
1:B:740:ALA:O	1:B:744:VAL:HG23	2.18	0.44
1:B:869:ALA:HB3	1:B:884:VAL:HG21	1.99	0.44
1:B:888:LEU:HG	1:B:892:GLU:HB3	1.98	0.44
1:A:767:LYS:HA	1:A:767:LYS:HD3	1.59	0.44
1:A:833:GLY:HA2	1:A:853:GLY:HA3	1.99	0.44
1:B:252:TRP:CZ3	1:B:257:THR:HB	2.52	0.44
1:A:69:TYR:CE2	1:A:245:TYR:HD2	2.36	0.44
1:B:330:ILE:O	1:B:333:PRO:HD2	2.18	0.44
1:B:9:ASP:CG	1:B:10:ILE:HG23	2.37	0.44
1:A:197:ALA:HB3	1:A:218:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLN:O	1:A:545:ASN:N	2.51	0.44
1:A:890:ARG:HE	1:A:894:LEU:HD11	1.82	0.44
1:B:259:THR:O	1:B:261:TYR:N	2.51	0.44
1:B:405:LEU:O	1:B:408:VAL:HG12	2.18	0.44
1:B:537:TYR:HD1	1:B:538:PRO:HD2	1.82	0.44
1:B:819:MET:O	1:B:822:LEU:N	2.51	0.44
2:C:1643:G:H2'	2:C:1644:A:C8	2.52	0.44
1:A:122:ILE:O	1:A:148:MET:HA	2.18	0.44
1:A:69:TYR:HE2	1:A:245:TYR:CD2	2.35	0.44
1:B:13:LEU:HA	1:B:13:LEU:HD23	1.67	0.44
1:B:865:ILE:O	1:B:868:VAL:HG22	2.18	0.44
1:A:501:TYR:HE2	1:A:523:GLY:HA3	1.81	0.43
1:A:530:ILE:HD13	1:A:569:VAL:H	1.82	0.43
1:A:626:GLU:OE2	1:A:629:LYS:HD2	2.18	0.43
1:A:73:PHE:HE2	1:A:173:LEU:HD22	1.83	0.43
1:B:600:HIS:HB3	1:B:707:HIS:CE1	2.53	0.43
1:B:662:ILE:HA	1:B:695:GLN:O	2.17	0.43
2:C:1634:U:O2	2:C:1636:C:OP2	2.36	0.43
1:A:656:ILE:O	1:A:711:THR:OG1	2.37	0.43
1:A:78:HIS:HB3	1:A:119:PRO:HG2	2.00	0.43
1:A:442:LYS:HA	1:A:445:LEU:HB2	2.00	0.43
1:B:72:PHE:O	1:B:76:ARG:HD3	2.18	0.43
1:A:150:HIS:N	1:A:243:THR:OG1	2.45	0.43
1:A:537:TYR:HA	1:A:538:PRO:HD3	1.87	0.43
1:A:543:GLN:HE21	1:A:596:HIS:CE1	2.36	0.43
1:A:750:LEU:HD13	1:B:763:ALA:HA	2.01	0.43
1:B:351:LEU:HD23	1:B:408:VAL:HG23	2.00	0.43
1:B:779:GLN:O	1:B:783:ILE:HG13	2.19	0.43
1:B:234:ARG:HG2	1:B:235:LYS:N	2.33	0.43
1:A:281:ASN:HD21	1:A:283:GLU:HB2	1.84	0.43
1:A:537:TYR:HB3	1:A:546:ASP:OD2	2.19	0.43
1:B:252:TRP:HE3	1:B:263:ALA:HB3	1.83	0.43
1:B:285:GLU:O	1:B:289:ARG:HG2	2.19	0.43
1:A:738:GLU:O	1:A:741:ILE:HG13	2.18	0.43
1:A:891:GLU:HG3	1:A:892:GLU:N	2.34	0.43
1:A:31:TRP:NE1	1:A:188:GLU:OE1	2.51	0.43
1:A:660:LYS:NZ	1:A:696:VAL:O	2.47	0.43
1:B:198:GLY:HA3	1:B:216:MET:HA	2.00	0.43
1:B:428:ARG:HE	1:B:432:ARG:HH22	1.67	0.43
1:B:78:HIS:HE2	1:B:161:TYR:HE2	1.67	0.43
2:C:1648:C:C2	2:C:1659:A:H1'	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:TYR:HB3	1:B:362:ALA:HB2	2.01	0.43
1:B:456:VAL:HG21	1:B:476:ILE:HD11	2.01	0.43
1:A:70:LEU:HD13	1:A:80:ARG:NH1	2.34	0.42
1:B:476:ILE:HG13	1:B:477:TYR:N	2.34	0.42
1:A:122:ILE:HD12	1:A:123:SER:N	2.34	0.42
1:A:328:GLU:OE1	1:A:328:GLU:N	2.52	0.42
1:A:549:TYR:HE1	1:A:558:GLU:HG3	1.84	0.42
1:A:69:TYR:CE2	1:A:245:TYR:CD2	3.07	0.42
1:B:270:ASP:OD2	1:B:282:ARG:NH1	2.52	0.42
1:B:499:ASN:ND2	1:B:499:ASN:O	2.52	0.42
1:B:681:TYR:CE2	1:B:686:PRO:HD2	2.53	0.42
1:A:281:ASN:OD1	1:A:282:ARG:N	2.52	0.42
1:B:150:HIS:CE1	1:B:243:THR:HG21	2.55	0.42
1:A:512:PRO:HB2	1:A:597:MET:CE	2.49	0.42
1:B:25:LYS:HE2	1:B:25:LYS:HB3	1.77	0.42
1:B:462:ILE:HA	1:B:465:GLU:HB3	2.01	0.42
1:A:156:PRO:HG3	1:A:237:ASP:O	2.19	0.42
1:A:510:ASP:N	1:A:510:ASP:OD1	2.52	0.42
1:B:419:TYR:O	1:B:423:VAL:HG13	2.19	0.42
1:B:50:PHE:CE1	1:B:51:ILE:HG23	2.54	0.42
1:B:813:GLU:HB2	1:B:838:LEU:CD2	2.49	0.42
1:A:138:THR:HG23	1:A:140:ARG:H	1.85	0.42
1:A:268:VAL:HG11	1:A:393:HIS:NE2	2.34	0.42
1:B:218:LEU:HD23	1:B:235:LYS:N	2.34	0.42
1:B:51:ILE:HG13	1:B:51:ILE:H	1.59	0.42
1:B:656:ILE:CD1	1:B:714:ILE:HD11	2.48	0.42
1:B:670:ILE:HG13	1:B:671:GLU:N	2.34	0.42
1:B:730:ILE:HG23	1:B:732:PHE:HE1	1.85	0.42
1:A:201:LEU:HB2	1:A:213:LEU:CD1	2.49	0.42
1:A:679:ARG:O	1:A:682:GLN:HG3	2.20	0.42
2:C:1635:G:HO2'	2:C:1637:G:N2	2.18	0.42
1:A:519:ALA:HB1	1:A:532:ASN:HD21	1.85	0.42
2:C:1630:C:H2'	2:C:1631:C:C6	2.54	0.42
2:C:1633:U:H2'	2:C:1634:U:H5"	2.02	0.42
1:A:171:THR:HA	1:A:174:LEU:HD21	2.02	0.42
1:A:805:PHE:N	1:A:808:MET:O	2.47	0.42
1:A:545:ASN:O	1:A:592:VAL:HG21	2.20	0.41
1:B:71:ASN:OD1	1:B:72:PHE:N	2.53	0.41
1:B:723:GLU:HG3	1:B:731:ARG:HB3	2.01	0.41
1:B:893:MET:O	1:B:897:ILE:HG12	2.20	0.41
1:A:47:SER:OG	1:A:296:LYS:O	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:TYR:CE1	1:A:409:GLN:HB2	2.54	0.41
1:A:434:VAL:HG11	1:A:466:LYS:CD	2.49	0.41
1:A:448:LEU:HA	1:A:448:LEU:HD23	1.85	0.41
2:C:1632:U:H2'	2:C:1633:U:O4'	2.19	0.41
1:A:78:HIS:HB3	1:A:119:PRO:CG	2.50	0.41
1:A:219:GLU:HG3	1:A:236:MET:HG2	2.02	0.41
1:B:186:TYR:HB3	1:B:201:LEU:HG	2.02	0.41
1:B:720:LEU:N	1:B:733:GLU:O	2.53	0.41
1:A:105:GLN:NE2	1:A:196:ASN:HD22	2.18	0.41
1:A:686:PRO:HA	1:A:687:PRO:HD3	1.94	0.41
1:B:175:ASN:C	1:B:175:ASN:HD22	2.24	0.41
1:A:653:ASN:HA	1:A:656:ILE:HD12	2.01	0.41
1:B:218:LEU:HA	1:B:236:MET:N	2.35	0.41
1:B:605:VAL:O	1:B:609:SER:OG	2.32	0.41
1:B:718:LYS:HD2	1:B:718:LYS:HA	1.42	0.41
1:B:767:LYS:H	1:B:767:LYS:HD2	1.85	0.41
1:A:720:LEU:N	1:A:733:GLU:O	2.47	0.41
1:A:765:LEU:HB3	1:A:766:PRO:HD3	2.02	0.41
1:B:174:LEU:O	1:B:179:VAL:HG22	2.20	0.41
1:A:511:ASP:OD1	1:A:513:THR:HG22	2.21	0.41
1:B:123:SER:O	1:B:125:PRO:HD3	2.20	0.41
1:B:56:PHE:HD2	1:B:254:SER:HA	1.85	0.41
1:B:407:THR:O	1:B:411:ILE:HG13	2.21	0.41
1:B:515:LEU:HD21	1:B:590:SER:CA	2.51	0.41
1:B:755:SER:HB3	1:B:760:VAL:O	2.21	0.41
1:B:856:TYR:HB3	1:B:900:PHE:HE2	1.84	0.41
1:A:463:ALA:HB1	1:A:468:ALA:HB3	2.03	0.41
1:A:624:ARG:HD2	1:A:631:ARG:NH2	2.29	0.41
1:A:695:GLN:HG3	1:A:700:VAL:HG22	2.03	0.41
1:A:716:MET:H	1:A:716:MET:HE3	1.86	0.41
1:B:152:ALA:O	1:B:240:ILE:HD12	2.20	0.41
1:B:442:LYS:HD3	1:B:473:PRO:HG3	2.02	0.41
1:B:509:TYR:HD1	1:B:692:ARG:HD2	1.86	0.41
1:B:676:PHE:CD2	1:B:700:VAL:HG11	2.56	0.41
1:A:144:LEU:HD21	1:A:349:PHE:CD1	2.56	0.41
1:B:305:ARG:HG3	1:B:309:LEU:HD23	2.03	0.41
1:A:436:ARG:NH1	2:C:1615:G:OP1	2.53	0.41
2:C:1634:U:C5	2:C:1636:C:N4	2.89	0.41
1:A:186:TYR:HE1	1:A:203:ALA:HB2	1.86	0.41
1:A:2:THR:OG1	1:A:3:LEU:N	2.52	0.41
1:A:71:ASN:O	1:A:75:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:PRO:O	1:B:407:THR:OG1	2.38	0.41
1:A:520:GLU:H	1:A:532:ASN:ND2	2.18	0.40
1:A:803:GLU:O	1:A:810:VAL:HG22	2.22	0.40
1:B:476:ILE:O	1:B:479:GLU:HB2	2.21	0.40
1:B:530:ILE:C	1:B:531:LEU:HD12	2.42	0.40
1:A:242:ASP:OD1	3:A:1001:A5A:HB3	2.22	0.40
1:A:184:ILE:HD11	1:A:186:TYR:CE1	2.57	0.40
1:B:6:GLU:O	1:B:13:LEU:HD12	2.22	0.40
1:B:39:ILE:CG2	1:B:185:VAL:HG11	2.51	0.40
1:A:213:LEU:O	1:A:213:LEU:HD12	2.22	0.40
1:A:252:TRP:CZ2	1:A:259:THR:HA	2.57	0.40
1:A:7:TYR:CE2	1:A:188:GLU:HB3	2.56	0.40
1:B:26:CYS:SG	1:B:28:LYS:HB2	2.62	0.40
1:B:30:PHE:HD1	1:B:32:THR:HG23	1.85	0.40
1:B:889:ASP:O	1:B:893:MET:HG3	2.20	0.40
1:A:281:ASN:ND2	1:A:283:GLU:HB2	2.36	0.40
1:A:47:SER:HB3	1:A:300:ILE:CG1	2.50	0.40
1:A:643:GLU:OE1	1:A:643:GLU:N	2.31	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%)	864 (96%)	35 (4%)	4 (0%)	34	66
1	B	903/906 (100%)	855 (95%)	44 (5%)	4 (0%)	34	66
All	All	1806/1812 (100%)	1719 (95%)	79 (4%)	8 (0%)	34	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PRO
1	A	544	ASP
1	B	502	PRO
1	B	870	LYS
1	B	260	VAL
1	A	17	GLY
1	A	512	PRO
1	B	258	PRO

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	766/767 (100%)	716 (94%)	50 (6%)	17	46
1	B	767/767 (100%)	707 (92%)	60 (8%)	12	38
All	All	1533/1534 (100%)	1423 (93%)	110 (7%)	14	41

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	12	PHE
1	A	14	THR
1	A	28	LYS
1	A	45	CYS
1	A	46	GLU
1	A	78	HIS
1	A	104	PHE
1	A	107	PHE
1	A	128	ARG
1	A	148	MET
1	A	158	LYS
1	A	162	TRP
1	A	179	VAL
1	A	184	ILE
1	A	204	ILE

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Mol	Chain	Res	Type
1	A	205	VAL
1	A	210	VAL
1	A	213	LEU
1	A	218	LEU
1	A	248	GLU
1	A	250	PHE
1	A	254	SER
1	A	273	ILE
1	A	397	LEU
1	A	412	LEU
1	A	477	TYR
1	A	482	LYS
1	A	490	VAL
1	A	514	LEU
1	A	525	GLU
1	A	528	PHE
1	A	530	ILE
1	A	531	LEU
1	A	543	GLN
1	A	544	ASP
1	A	559	VAL
1	A	572	VAL
1	A	592	VAL
1	A	607	LEU
1	A	611	GLN
1	A	625	LYS
1	A	679	ARG
1	A	710	SER
1	A	711	THR
1	A	794	TRP
1	A	823	GLN
1	A	837	CYS
1	A	838	LEU
1	A	862	LEU
1	B	6	GLU
1	B	42	ASP
1	B	48	TYR
1	B	87	VAL
1	B	92	THR
1	B	93	ASP
1	B	97	THR
1	B	121	THR

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Mol	Chain	Res	Type
1	B	131	ASP
1	B	158	LYS
1	B	161	TYR
1	B	162	TRP
1	B	163	LYS
1	B	164	ASN
1	B	171	THR
1	B	175	ASN
1	B	237	ASP
1	B	240	ILE
1	B	241	VAL
1	B	242	ASP
1	B	257	THR
1	B	259	THR
1	B	261	TYR
1	B	290	ILE
1	B	309	LEU
1	B	311	GLN
1	B	316	VAL
1	B	320	VAL
1	B	322	VAL
1	B	328	GLU
1	B	332	VAL
1	B	342	ASP
1	B	440	LEU
1	B	441	GLU
1	B	448	LEU
1	B	497	LEU
1	B	504	THR
1	B	513	THR
1	B	522	ILE
1	B	530	ILE
1	B	537	TYR
1	B	562	VAL
1	B	563	LEU
1	B	574	LYS
1	B	587	VAL
1	B	609	SER
1	B	653	ASN
1	B	659	ASN
1	B	669	ARG
1	B	706	THR

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Mol	Chain	Res	Type
1	B	717	LEU
1	B	722	VAL
1	B	772	PHE
1	B	797	ILE
1	B	798	LEU
1	B	807	SER
1	B	815	VAL
1	B	825	LEU
1	B	868	VAL
1	B	884	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	151	HIS
1	A	196	ASN
1	A	532	ASN
1	A	596	HIS
1	B	16	ASN
1	B	29	HIS
1	B	105	GLN
1	B	164	ASN
1	B	499	ASN
1	B	545	ASN
1	B	571	HIS
1	B	596	HIS
1	B	823	GLN
1	B	854	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	74/75 (98%)	20 (27%)	2 (2%)

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	1603	G
2	C	1609	A

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Mol	Chain	Res	Type
2	C	1613	C
2	C	1616	C
2	C	1619	G
2	C	1620	G
2	C	1621	A
2	C	1622	G
2	C	1635	G
2	C	1636	C
2	C	1637	G
2	C	1638	A
2	C	1648	C
2	C	1649	G
2	C	1652	G
2	C	1653	G
2	C	1660	U
2	C	1674	C
2	C	1675	C
2	C	1676	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	1634	U
2	C	1636	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 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	A	1001	-	26,30,30	2.54	10 (38%)	30,45,45	2.41	8 (26%)
3	A5A	B	1001	-	26,30,30	2.60	10 (38%)	30,45,45	2.25	9 (30%)

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	A	1001	-	-	2/14/35/35	0/3/3/3
3	A5A	B	1001	-	-	3/14/35/35	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	A5A	O5'-S	-6.17	1.46	1.59
3	A	1001	A5A	O5'-S	-5.59	1.48	1.59
3	A	1001	A5A	O1S-S	5.56	1.47	1.42
3	B	1001	A5A	O1S-S	5.12	1.46	1.42
3	B	1001	A5A	C-N3S	4.66	1.46	1.37
3	B	1001	A5A	C2'-C1'	-4.64	1.46	1.53
3	A	1001	A5A	C-N3S	4.35	1.45	1.37
3	A	1001	A5A	C2'-C1'	-4.26	1.47	1.53
3	B	1001	A5A	C3'-C4'	-3.44	1.44	1.53
3	B	1001	A5A	C2'-C3'	-3.31	1.44	1.53
3	A	1001	A5A	C3'-C4'	-3.28	1.44	1.53
3	A	1001	A5A	C2'-C3'	-3.11	1.44	1.53
3	A	1001	A5A	S-N3S	3.05	1.65	1.59
3	A	1001	A5A	C6-N6	2.91	1.44	1.34
3	B	1001	A5A	S-N3S	2.82	1.64	1.59
3	B	1001	A5A	C6-N6	2.75	1.44	1.34
3	A	1001	A5A	C4-N3	2.59	1.39	1.35
3	A	1001	A5A	C2-N3	2.52	1.36	1.32
3	B	1001	A5A	C4-N3	2.45	1.39	1.35
3	B	1001	A5A	C2-N3	2.43	1.36	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	-7.98	108.33	120.76
3	B	1001	A5A	O2S-S-O1S	-6.62	110.44	120.76
3	B	1001	A5A	N3-C2-N1	-5.65	119.85	128.68
3	A	1001	A5A	N3-C2-N1	-5.10	120.70	128.68
3	A	1001	A5A	O5'-C5'-C4'	4.37	115.77	107.62
3	B	1001	A5A	O5'-C5'-C4'	3.86	114.82	107.62
3	B	1001	A5A	C-N3S-S	-3.84	118.39	124.61
3	A	1001	A5A	C-N3S-S	-3.43	119.05	124.61
3	A	1001	A5A	CB-CA-C	-3.25	103.97	110.14
3	B	1001	A5A	CA-C-N3S	2.92	120.51	114.34
3	A	1001	A5A	CA-C-N3S	2.75	120.16	114.34
3	A	1001	A5A	C4-C5-N7	-2.46	106.83	109.40
3	B	1001	A5A	C2-N1-C6	2.38	122.83	118.75
3	B	1001	A5A	C4-C5-N7	-2.26	107.04	109.40
3	B	1001	A5A	C3'-C2'-C1'	2.26	104.39	100.98
3	A	1001	A5A	C5'-O5'-S	2.18	121.87	117.37
3	B	1001	A5A	C5'-C4'-C3'	-2.16	107.08	115.18

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1001	A5A	C5'-O5'-S-N3S
3	A	1001	A5A	O4'-C4'-C5'-O5'
3	A	1001	A5A	C3'-C4'-C5'-O5'
3	B	1001	A5A	O4'-C4'-C5'-O5'
3	B	1001	A5A	C5'-O5'-S-O2S

There are no ring outliers.

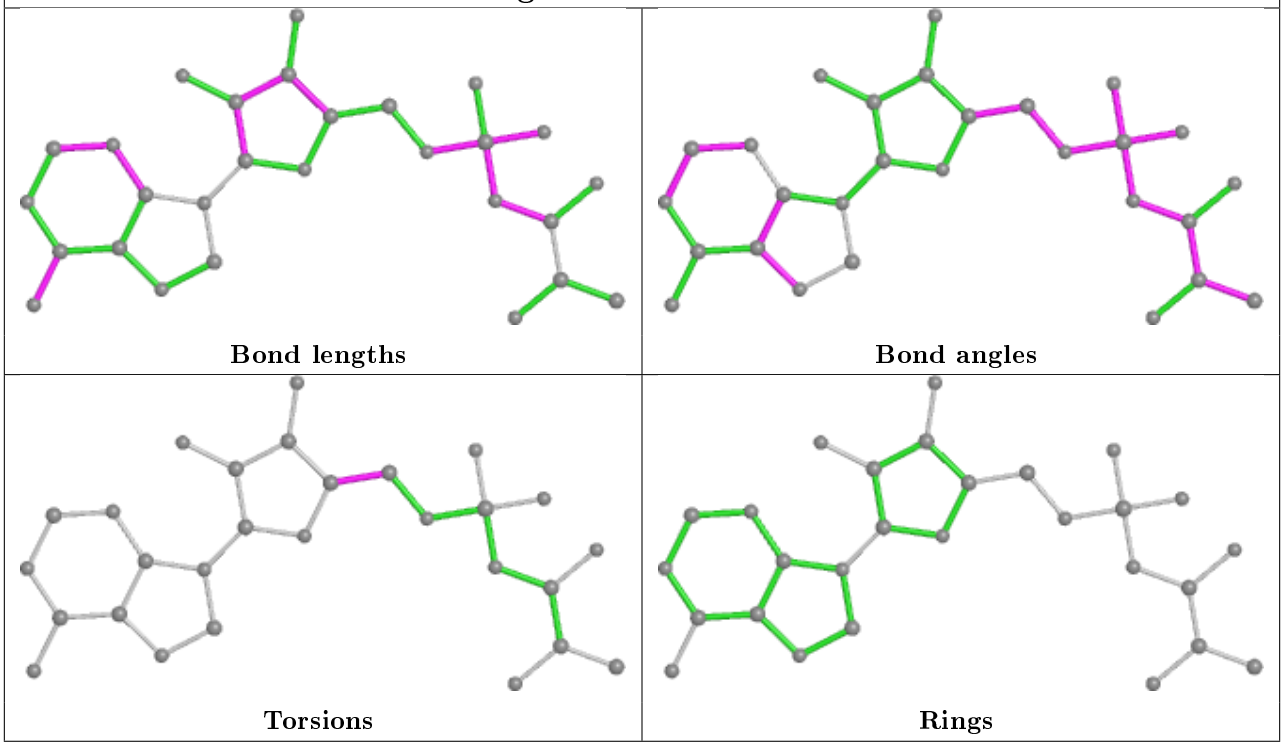
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	A5A	5	0

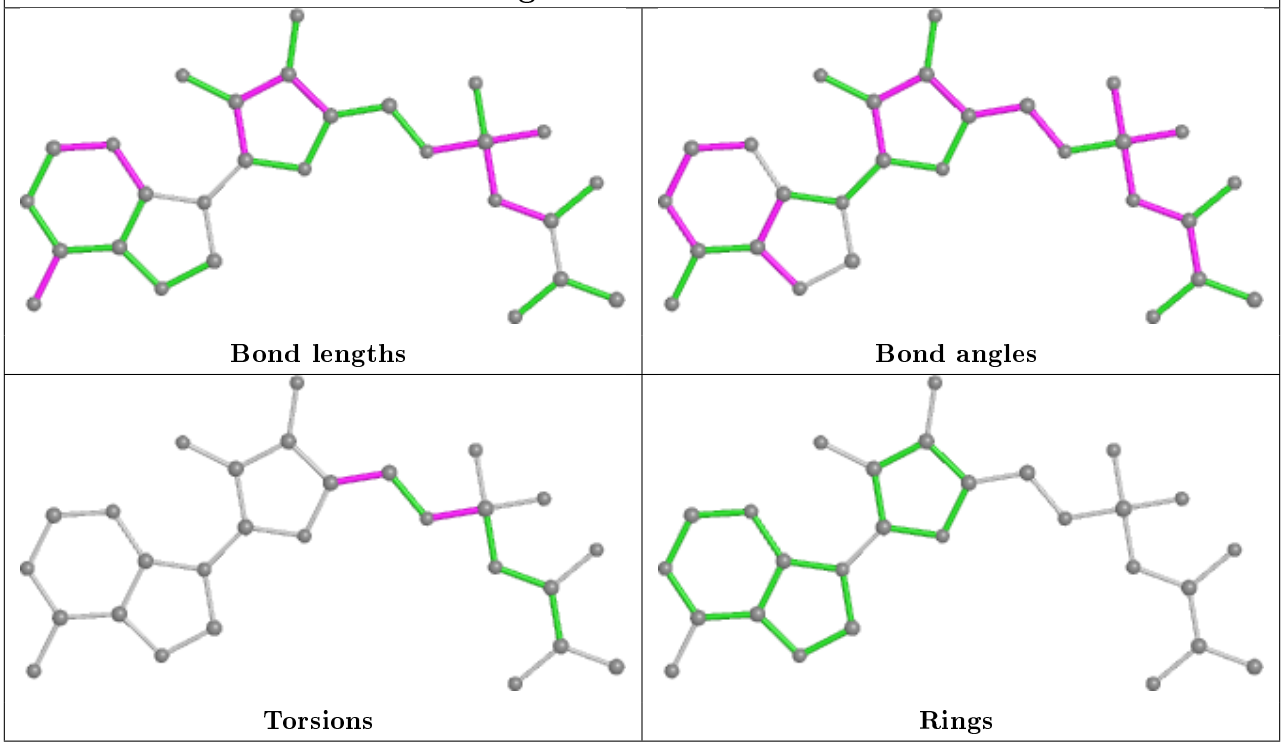
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A5A A 1001



Ligand A5A B 1001



5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.13	49 (5%)	25	24	22, 93, 184, 291	0
1	B	905/906 (99%)	0.20	40 (4%)	34	33	18, 99, 170, 282	0
2	C	75/75 (100%)	-0.48	1 (1%)	77	77	27, 51, 129, 240	0
All	All	1885/1887 (99%)	0.14	90 (4%)	30	28	18, 95, 179, 291	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	628	SER	8.6
1	B	42	ASP	7.9
1	B	503	ALA	7.9
1	A	487	ALA	6.6
1	A	488	GLU	6.6
1	A	502	PRO	6.2
1	A	45	CYS	6.2
1	A	46	GLU	5.7
1	A	503	ALA	5.6
1	B	43	PRO	5.6
1	A	490	VAL	5.6
1	B	41	GLY	5.5
1	B	40	CYS	5.4
1	A	524	VAL	5.2
1	A	491	GLN	5.0
1	B	570	LEU	4.7
1	A	492	GLU	4.7
1	A	526	GLY	4.5
1	B	629	LYS	4.5
1	B	426	GLY	4.3
1	A	499	ASN	4.3
1	A	497	LEU	4.3
1	A	484	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	547	VAL	4.2
1	A	489	LYS	4.1
1	B	26	CYS	4.1
1	A	485	SER	4.0
1	A	486	LYS	4.0
1	B	197	ALA	4.0
1	A	304	LEU	3.9
1	A	494	LYS	3.8
1	B	517	PHE	3.8
1	B	502	PRO	3.4
1	A	496	THR	3.4
1	B	550	LEU	3.3
1	A	552	ALA	3.3
1	B	7	TYR	3.3
1	B	9	ASP	3.2
1	A	523	GLY	3.2
1	A	566	ASP	3.1
1	A	498	GLN	3.0
1	A	483	ARG	3.0
1	B	626	GLU	3.0
1	B	186	TYR	3.0
1	A	47	SER	3.0
1	B	25	LYS	3.0
1	A	26	CYS	2.9
1	A	548	GLY	2.9
1	A	906	GLY	2.9
1	A	628	SER	2.8
1	B	160	ILE	2.8
1	B	44	PRO	2.8
1	B	560	VAL	2.8
1	B	470	VAL	2.7
1	B	463	ALA	2.6
1	B	313	ARG	2.6
1	B	547	VAL	2.6
1	A	627	PHE	2.6
1	A	522	ILE	2.5
1	A	567	GLY	2.5
1	B	164	ASN	2.5
1	B	572	VAL	2.5
1	B	328	GLU	2.5
1	B	627	PHE	2.4
1	A	472	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	511	ASP	2.4
1	A	556	LYS	2.4
2	C	1676	A	2.4
1	B	561	ASP	2.3
1	A	2	THR	2.3
1	A	517	PHE	2.3
1	A	501	TYR	2.3
1	A	40	CYS	2.3
1	A	521	VAL	2.3
1	B	431	GLU	2.3
1	A	495	ILE	2.2
1	A	493	LYS	2.2
1	B	526	GLY	2.2
1	B	4	ASP	2.2
1	A	504	THR	2.2
1	A	531	LEU	2.2
1	A	528	PHE	2.1
1	B	30	PHE	2.1
1	B	301	MET	2.1
1	B	161	TYR	2.1
1	B	8	LEU	2.1
1	A	506	LYS	2.1
1	A	44	PRO	2.0
1	B	564	GLU	2.0
1	B	575	GLY	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 carbohydrates in this entry.

6.4 Ligands (i)

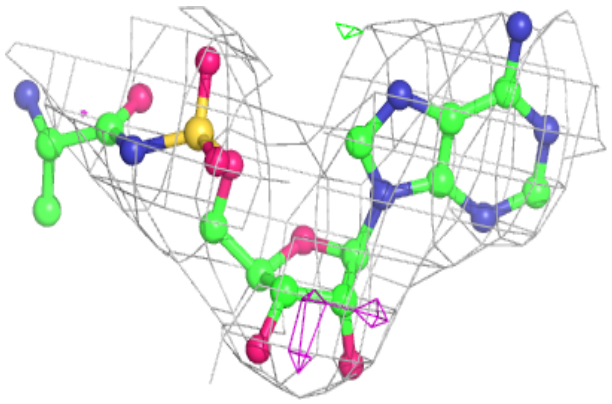
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

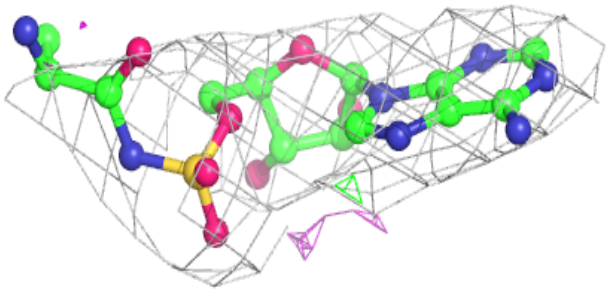
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	C	1701	1/1	0.61	0.61	52,52,52,52	0
4	MG	C	1703	1/1	0.90	0.14	63,63,63,63	0
3	A5A	B	1001	28/28	0.93	0.28	46,70,102,105	0
3	A5A	A	1001	28/28	0.95	0.27	51,66,91,96	0
4	MG	C	1702	1/1	0.97	0.13	13,13,13,13	0

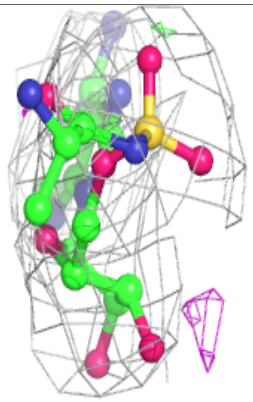
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

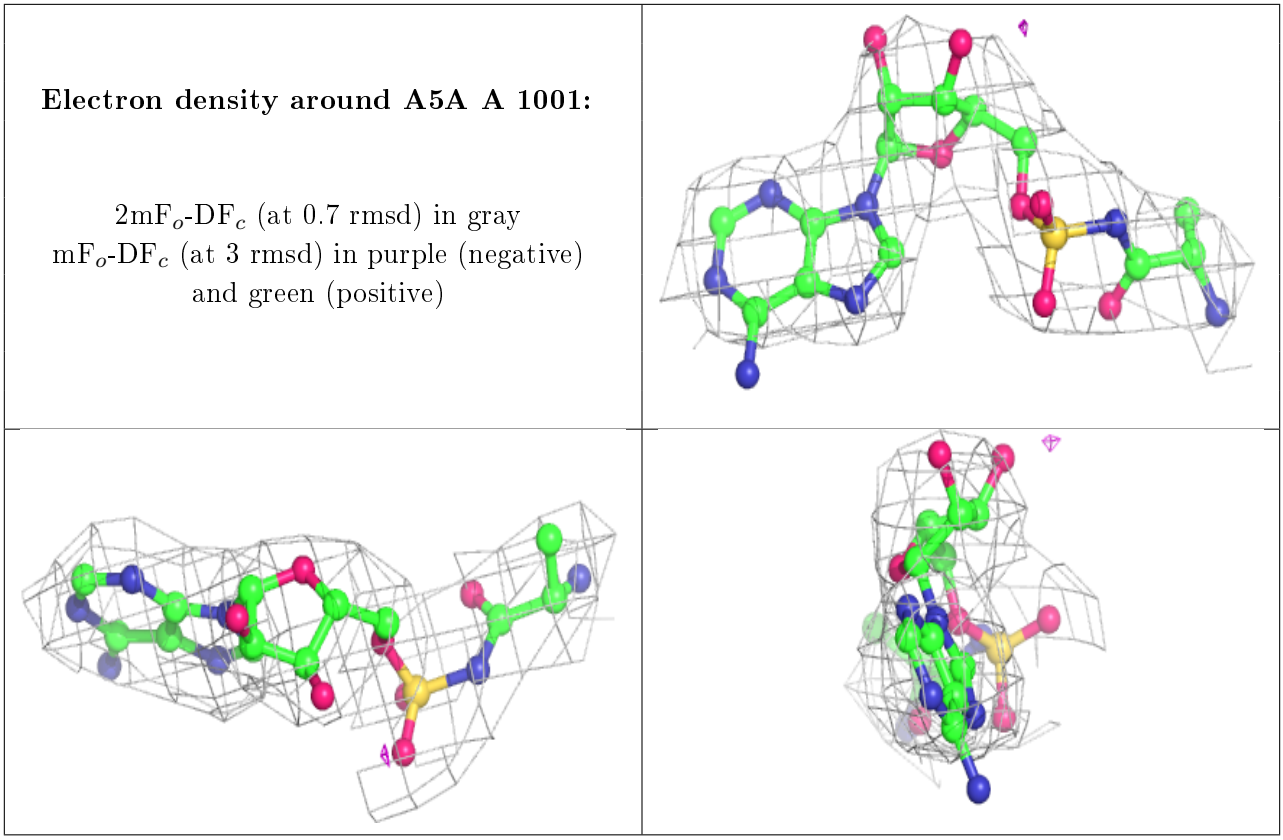






Electron density around A5A A 1001:

$2mF_o$-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.