Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 12:17 PM EDT

PDB ID	:	3AKZ
Title	:	Crystal structure of Thermotoga maritima nondiscriminating glutamyl-tRNA synthetase in complex with tRNAGln and a glutamyl-AMP analog
Authors	:	Ito, T.; Yokoyama, S.
Deposited on	:	2010-07-19
Resolution	:	2.90 Å(reported)

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

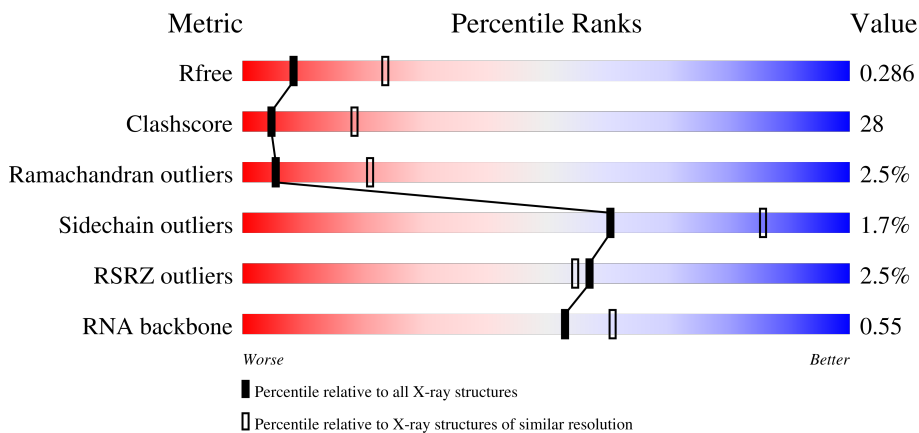|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.
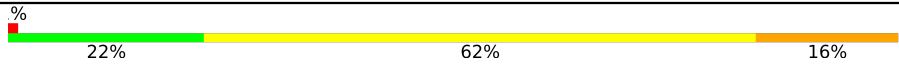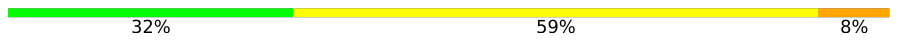
Metric	Percentile Ranks	Value
Rfree		0.286
Clashscore		28
Ramachandran outliers		2.5%
Sidechain outliers		1.7%
RSRZ outliers		2.5%
RNA backbone		0.55

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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	487	% 40% 51% · 5%
1	B	487	% 45% 47% · 5%
1	C	487	5% 46% 47% · 5%
1	D	487	3% 39% 54% · 5%

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Mol	Chain	Length	Quality of chain
2	E	74	22% · 62% · 16%
2	F	74	32% · 59% · 8%
2	G	74	27% · 66% · 7%
2	H	74	30% · 59% · 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21872 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 Glutamyl-tRNA synthetase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	463	Total	C	N	O	S	0	0	0
			3855	2475	652	715	13			
1	D	463	Total	C	N	O	S	0	0	0
			3855	2475	652	715	13			
1	C	463	Total	C	N	O	S	0	0	0
			3855	2475	652	715	13			
1	A	463	Total	C	N	O	S	0	0	0
			3855	2475	652	715	13			

- Molecule 2 is a RNA chain called tRNAGln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	74	Total	C	N	O	P	0	0	0
			1581	703	281	523	74			
2	H	74	Total	C	N	O	P	0	0	0
			1581	703	281	523	74			
2	G	74	Total	C	N	O	P	0	0	0
			1581	703	281	523	74			
2	E	74	Total	C	N	O	P	0	0	0
			1581	703	281	523	74			

- Molecule 3 is O5'-(L-GLUTAMYL-SULFAMOYL)-ADENOSINE (three-letter code: GSU) (formula: $C_{15}H_{21}N_7O_9S$).

GSU

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

3 Residue-property plots ⓘ

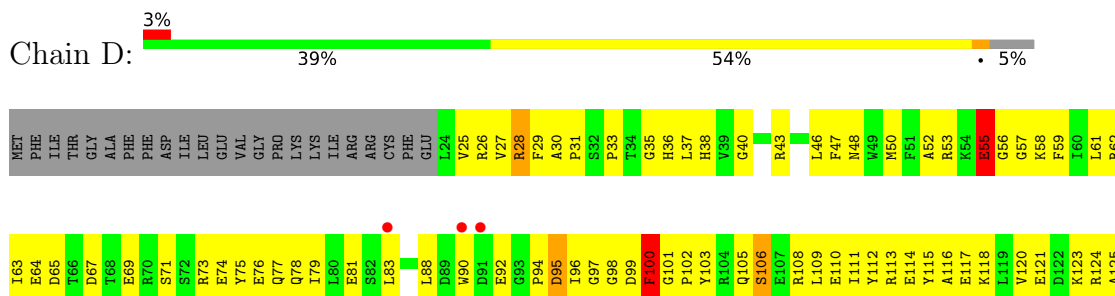These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Glutamyl-tRNA synthetase 2
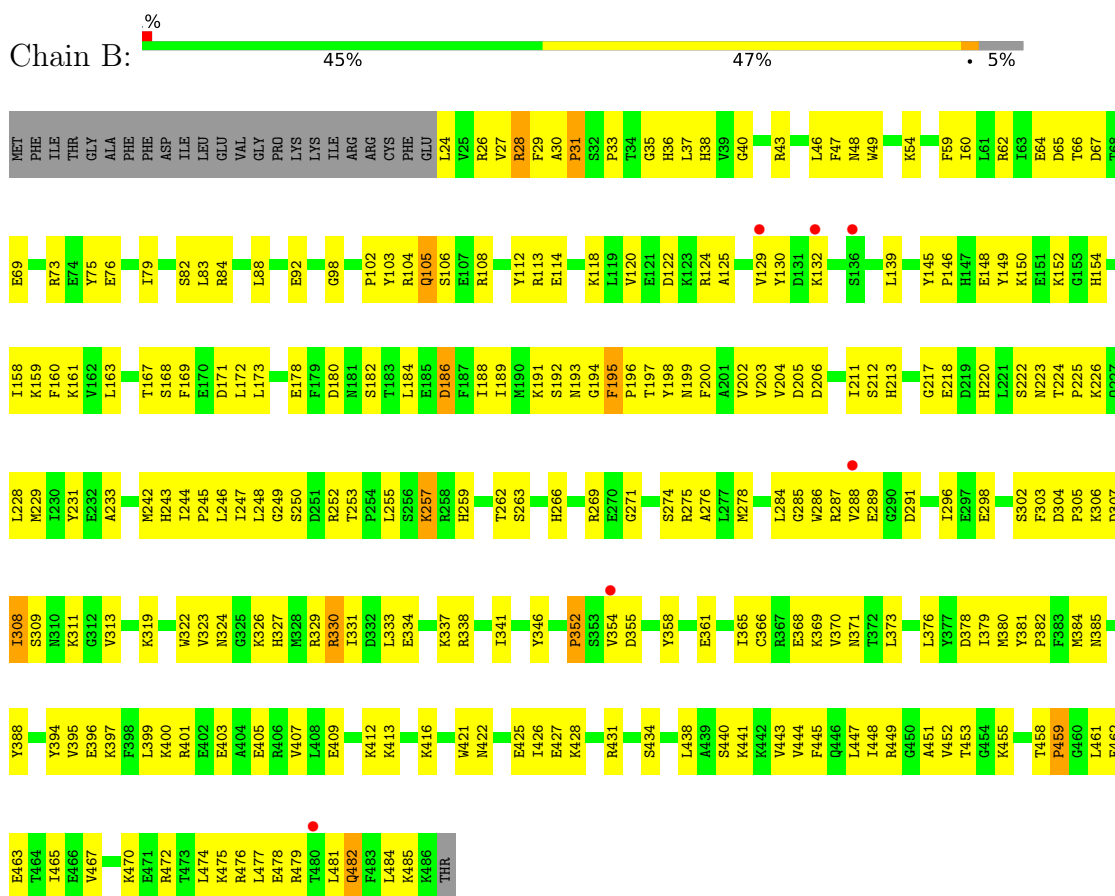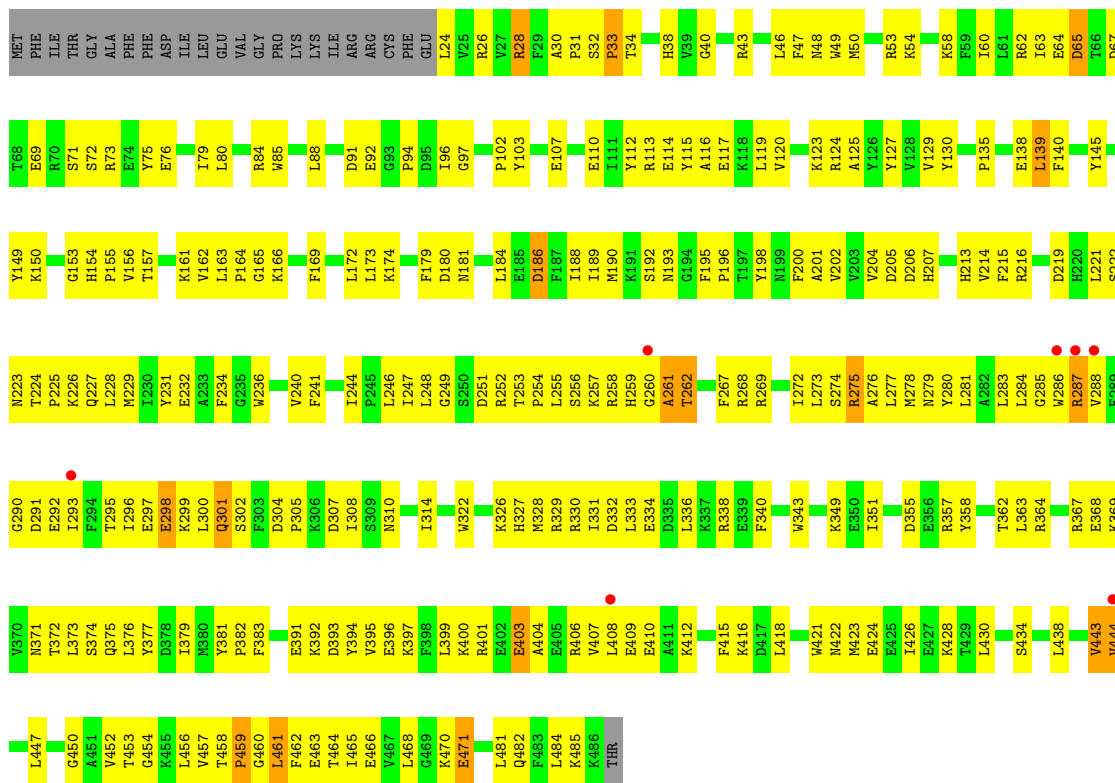
• Molecule 1: Glutamyl-tRNA synthetase 2

• Molecule 1: Glutamyl-tRNA synthetase 2

Chain C:

• Molecule 1: Glutamyl-tRNA synthetase 2

Chain A:

• Molecule 2: tRNAGln

Chain F:

• Molecule 2: tRNAGln

Chain H:

• Molecule 2: tRNAGln

Chain G:

U68 C69 C70 C71 A72 C75 A76

• Molecule 2: tRNAGln

Chain E:

%

22%　　　　　　　　　62%　　　　　　　16%

U1 G2 G3 G4 A5 G6 G7 U8 C9 G10 U11 C12 U13 A14 A15 C16 G18 G19 U20 A21 A24 C25 G26 G27 C28 G29 U33 C34 U35 G36 G37 A38 U44 G45 G46 U48 G49 G50 A51 G52 G53 U54 U55 C56 G57 A58 G59 U60 C61 C62 U63 C64 C65 C66 C67 U68 C69

C70 C71 A72 G73 C74 C75 A76
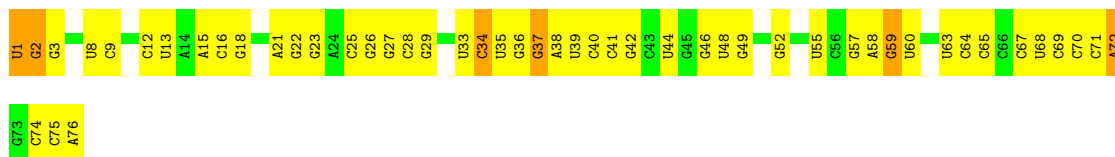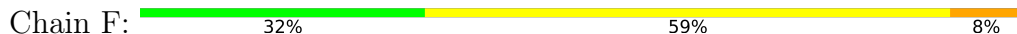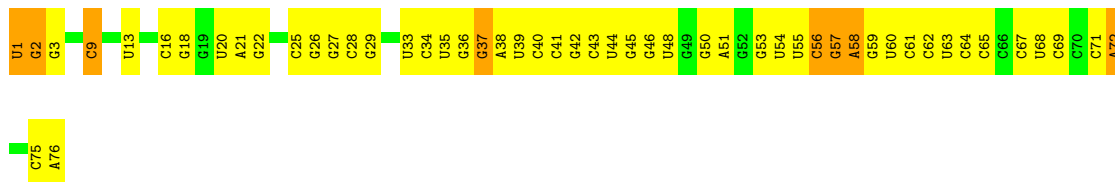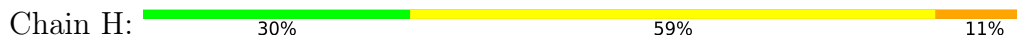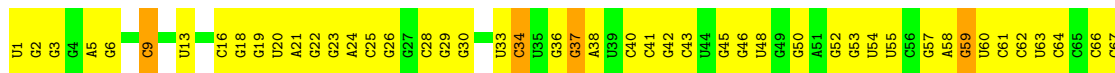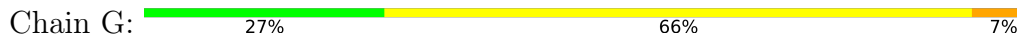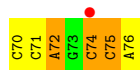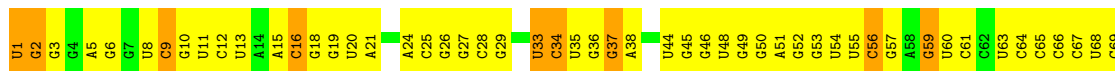
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.20Å 159.90Å 156.17Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 49.10 – 2.89	Depositor EDS
% Data completeness (in resolution range)	81.6 (50.00-2.90) 87.3 (49.10-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.200 , 0.282 0.211 , 0.286	Depositor DCC
R_{free} test set	2692 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å^2)	48.3	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.7	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.054 for -h,-l,-k 0.047 for -h,l,k 0.430 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	0 of 60407 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	21872	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: GSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z|>5$	RMSZ	$\#|Z|>5$
1	A	0.26	0/3947	0.42	0/5313
1	B	0.26	0/3947	0.41	0/5313
1	C	0.26	0/3947	0.41	0/5313
1	D	0.26	0/3947	0.41	0/5313
2	E	0.27	1/1765 (0.1%)	0.65	0/2749
2	F	0.27	1/1765 (0.1%)	0.65	0/2749
2	G	0.27	1/1765 (0.1%)	0.65	0/2749
2	H	0.26	1/1765 (0.1%)	0.65	0/2749
All	All	0.26	4/22848 (0.0%)	0.51	0/32248

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	U	OP3-P	-7.25	1.52	1.61
2	H	1	U	OP3-P	-7.23	1.52	1.61
2	G	1	U	OP3-P	-7.20	1.52	1.61
2	F	1	U	OP3-P	-7.20	1.52	1.61

There are no bond angle outliers.

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.

WORLDWIDE PDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3805	271	0
1	B	3855	0	3805	244	0
1	C	3855	0	3805	227	0
1	D	3855	0	3805	259	0
2	E	1581	0	800	59	0
2	F	1581	0	800	49	0
2	G	1581	0	800	55	0
2	H	1581	0	800	46	0
3	A	32	0	20	0	0
3	B	32	0	20	2	0
3	C	32	0	20	2	0
3	D	32	0	20	1	0
All	All	21872	0	18500	1126	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 28.

All (1126) 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:F:71:C:H2'	2:F:72:A:H5"	1.41	1.03
1:D:40:GLY:HA2	1:D:247:ILE:HD12	1.45	0.98
1:D:351:ILE:HG13	1:D:385:ASN:HD21	1.26	0.98
1:D:102:PRO:HD3	1:A:165:GLY:HA2	1.44	0.97
1:A:43:ARG:HD3	1:A:247:ILE:HD11	1.46	0.97
1:A:421:TRP:HE1	1:A:466:GLU:HA	1.29	0.96
1:B:304:ASP:HB3	1:B:307:ASP:HB2	1.49	0.93
1:C:460:GLY:HA2	2:G:34:C:H42	1.35	0.92
1:C:28:ARG:HG3	1:C:62:ARG:HH12	1.35	0.91
1:B:250:SER:HB3	1:D:251:ASP:HB3	1.53	0.90
1:A:40:GLY:HA2	1:A:247:ILE:HD12	1.55	0.89
1:A:219:ASP:HB3	1:A:246:LEU:HD11	1.56	0.87
1:A:369:LYS:HD2	2:E:36:G:H1	1.39	0.87
2:H:21:A:H61	2:H:46:G:H2'	1.40	0.85
2:G:71:C:H2'	2:G:72:A:H5"	1.60	0.84
1:B:64:GLU:HA	1:B:105:GLN:HG3	1.57	0.82
1:B:129:VAL:HG12	1:B:139:LEU:HD12	1.61	0.82
1:D:199:ASN:HD21	1:D:223:ASN:HD22	1.27	0.82
2:E:21:A:H61	2:E:46:G:H2'	1.42	0.82
1:D:406:ARG:HD3	1:D:438:LEU:HD22	1.60	0.82
2:G:21:A:H61	2:G:46:G:H2'	1.42	0.81
1:B:40:GLY:HA2	1:B:247:ILE:HD12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:VAL:HB	1:D:57:GLY:HA3	1.62	0.80
1:B:395:VAL:HA	1:B:399:LEU:HB3	1.64	0.80
1:B:329:ARG:NH2	2:F:38:A:H4'	1.98	0.78
1:B:37:LEU:HD23	1:B:37:LEU:H	1.49	0.78
1:B:472:ARG:HA	1:B:475:LYS:HE2	1.64	0.78
1:C:426:ILE:HD13	1:C:465:ILE:HB	1.63	0.78
1:D:36:HIS:HB3	1:D:264:VAL:HG23	1.67	0.77
1:D:279:ASN:HD21	1:D:294:PHE:H	1.30	0.77
1:A:301:GLN:H	1:A:301:GLN:NE2	1.82	0.77
1:B:434:SER:HB2	1:B:441:LYS:HA	1.65	0.76
1:D:64:GLU:HB3	1:D:105:GLN:NE2	2.00	0.76
1:C:329:ARG:HH21	2:G:38:A:H4'	1.50	0.76
1:C:334:GLU:HB3	1:C:338:ARG:HH12	1.49	0.76
1:A:46:LEU:HD22	1:A:278:MET:HE3	1.64	0.76
1:C:245:PRO:HG3	1:C:310:ASN:HA	1.66	0.76
1:B:33:PRO:HB3	1:B:76:GLU:HB2	1.65	0.76
1:A:369:LYS:HD2	2:E:36:G:H22	1.49	0.76
1:B:371:ASN:HD21	2:F:38:A:H5'	1.49	0.75
1:C:120:VAL:HG13	1:C:126:TYR:HA	1.67	0.75
1:D:295:THR:HB	1:D:298:GLU:HG2	1.67	0.75
1:B:29:PHE:O	1:B:31:PRO:HD3	1.86	0.75
1:C:64:GLU:HG3	3:C:1001:GSU:H	1.51	0.75
1:A:287:ARG:HB3	2:E:13:U:O2'	1.87	0.74
1:A:288:VAL:HG22	1:A:290:GLY:H	1.52	0.74
2:G:70:C:H2'	2:G:71:C:C6	2.23	0.74
1:A:254:PRO:HD3	2:E:69:C:H4'	1.69	0.73
1:B:172:LEU:HB3	1:B:242:MET:HB2	1.70	0.73
1:C:64:GLU:HG3	3:C:1001:GSU:N	2.04	0.73
1:C:40:GLY:HA2	1:C:247:ILE:HD12	1.70	0.73
1:D:94:PRO:HD3	1:D:103:TYR:H	1.52	0.73
1:A:421:TRP:NE1	1:A:466:GLU:HA	2.03	0.72
1:B:113:ARG:HH22	1:B:194:GLY:HA3	1.53	0.72
1:D:369:LYS:HD2	2:H:36:G:H22	1.51	0.72
1:D:25:VAL:HG11	1:D:52:ALA:HA	1.72	0.72
1:C:172:LEU:HB3	1:C:242:MET:HB2	1.71	0.72
1:C:218:GLU:HA	1:C:243:HIS:HB3	1.71	0.72
1:A:415:PHE:HA	1:A:418:LEU:HG	1.70	0.72
1:C:424:GLU:HA	1:C:427:GLU:HB3	1.71	0.72
1:A:157:THR:HG22	1:A:192:SER:N	2.05	0.71
1:D:369:LYS:HD2	2:H:36:G:H1	1.55	0.71
2:E:36:G:O2'	2:E:37:G:H5"	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:LYS:HG3	1:B:474:LEU:HD22	1.71	0.71
1:B:43:ARG:HH21	1:B:285:GLY:HA3	1.54	0.70
1:C:478:GLU:HA	1:C:481:LEU:HD12	1.73	0.70
1:C:203:VAL:HG21	1:C:230:ILE:HB	1.72	0.70
1:B:478:GLU:HB3	1:B:482:GLN:HE22	1.57	0.70
1:B:369:LYS:HE3	1:B:459:PRO:HA	1.72	0.70
1:D:458:THR:HB	1:D:459:PRO:HD2	1.73	0.69
1:D:28:ARG:C	1:D:28:ARG:HD2	2.13	0.69
1:B:354:VAL:HG12	1:B:355:ASP:H	1.57	0.69
1:D:264:VAL:HA	1:D:267:PHE:CZ	2.28	0.69
1:C:396:GLU:HB3	1:A:73:ARG:HH11	1.56	0.69
2:H:21:A:N6	2:H:46:G:H2'	2.08	0.69
1:D:282:ALA:O	1:D:286:TRP:HB3	1.93	0.69
1:C:173:LEU:HB2	1:C:242:MET:HG3	1.75	0.69
1:A:369:LYS:HD2	2:E:36:G:N1	2.08	0.69
1:A:407:VAL:HG11	1:A:447:LEU:HD13	1.75	0.69
1:D:38:HIS:CE1	1:D:255:LEU:HB2	2.26	0.68
1:B:440:SER:HB3	1:B:443:VAL:HG23	1.74	0.68
1:A:76:GLU:O	1:A:80:LEU:HD13	1.94	0.68
1:A:257:LYS:HG3	1:A:261:ALA:HA	1.75	0.68
1:B:485:LYS:H	1:B:485:LYS:HD2	1.58	0.68
1:C:369:LYS:HD2	2:G:36:G:N2	2.09	0.68
1:D:295:THR:HG22	1:D:297:GLU:H	1.56	0.68
1:A:269:ARG:HD2	1:A:269:ARG:O	1.94	0.68
1:A:452:VAL:HG23	1:A:453:THR:HG23	1.76	0.67
1:C:349:LYS:H	1:C:349:LYS:HD3	1.60	0.67
1:D:130:TYR:HE1	1:D:138:GLU:HG2	1.60	0.67
1:C:84:ARG:NE	1:C:89:ASP:HB3	2.10	0.67
1:B:66:THR:HG23	1:B:105:GLN:HB3	1.76	0.67
1:A:130:TYR:HD2	1:A:155:PRO:HB2	1.59	0.67
1:B:287:ARG:CZ	2:F:13:U:H4'	2.25	0.67
1:B:354:VAL:HG12	1:B:355:ASP:N	2.09	0.67
2:E:25:C:H2'	2:E:26:G:O4'	1.94	0.67
1:C:26:ARG:HH22	1:C:100:PHE:HE2	1.40	0.66
1:B:30:ALA:HB1	1:B:64:GLU:HG3	1.77	0.66
1:B:64:GLU:HA	1:B:105:GLN:CG	2.25	0.66
1:C:158:ILE:HB	1:C:190:MET:HB2	1.75	0.66
1:C:370:VAL:HG21	1:C:376:LEU:HB2	1.77	0.66
1:B:276:ALA:HB1	1:B:324:ASN:HA	1.77	0.66
2:F:15:A:H2'	2:F:59:G:O6	1.94	0.66
1:D:279:ASN:ND2	1:D:294:PHE:H	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:VAL:HG12	1:A:447:LEU:HD12	1.78	0.66
1:D:112:TYR:CD2	1:D:196:PRO:HG3	2.30	0.66
1:D:468:LEU:HA	1:D:472:ARG:HD2	1.78	0.66
1:C:322:TRP:O	1:C:326:LYS:HG2	1.96	0.65
1:A:198:TYR:CE2	1:A:202:VAL:HG21	2.31	0.65
1:C:73:ARG:HB3	1:C:73:ARG:NH1	2.10	0.65
1:B:60:ILE:N	1:B:60:ILE:HD12	2.11	0.65
1:D:173:LEU:HB2	1:D:242:MET:SD	2.36	0.65
1:C:452:VAL:HG23	1:C:453:THR:HG23	1.78	0.65
1:B:184:LEU:HD21	1:B:226:LYS:HG2	1.78	0.65
1:C:27:VAL:HG12	1:C:213:HIS:HB2	1.79	0.65
1:B:485:LYS:HD2	1:B:485:LYS:N	2.10	0.65
1:B:218:GLU:HA	1:B:243:HIS:HB3	1.79	0.65
1:C:397:LYS:NZ	1:A:72:SER:HA	2.12	0.65
2:F:71:C:C2'	2:F:72:A:H5"	2.24	0.65
1:C:190:MET:SD	1:C:196:PRO:HB3	2.37	0.64
1:B:37:LEU:HD22	1:B:79:ILE:HA	1.80	0.64
1:D:332:ASP:HB3	1:D:335:ASP:HB2	1.79	0.64
1:D:286:TRP:NE1	1:D:307:ASP:HB2	2.12	0.64
1:A:383:PHE:HZ	1:A:464:THR:HG23	1.62	0.64
1:A:63:ILE:HG12	1:A:94:PRO:HG3	1.80	0.64
2:E:71:C:H3'	2:E:72:A:H5"	1.80	0.64
1:D:118:LYS:NZ	1:D:118:LYS:HB3	2.12	0.64
1:A:401:ARG:HB2	1:A:404:ALA:HB2	1.80	0.64
1:D:223:ASN:HA	1:D:226:LYS:HE2	1.78	0.64
1:D:108:ARG:HB2	1:D:111:ILE:HD12	1.78	0.64
1:A:392:LYS:HE3	1:A:396:GLU:HG3	1.80	0.64
2:H:38:A:H2'	2:H:39:U:C6	2.32	0.64
1:D:447:LEU:O	1:D:451:ALA:HB2	1.97	0.64
2:F:21:A:H61	2:F:46:G:H2'	1.63	0.64
1:D:163:LEU:HD23	1:D:163:LEU:H	1.63	0.63
1:A:226:LYS:HA	1:A:229:MET:HE2	1.80	0.63
1:B:255:LEU:HD11	1:B:262:THR:HG21	1.79	0.63
1:C:288:VAL:HG22	1:C:290:GLY:H	1.63	0.63
1:A:161:LYS:HA	1:A:186:ASP:OD2	1.99	0.63
1:D:452:VAL:HG23	1:D:453:THR:HG23	1.81	0.63
1:C:114:GLU:HB3	1:C:118:LYS:NZ	2.13	0.62
1:A:369:LYS:HD2	2:E:36:G:N2	2.14	0.62
1:A:248:LEU:HD13	1:A:252:ARG:HA	1.80	0.62
1:A:85:TRP:CZ2	1:A:268:ARG:HG3	2.34	0.62
1:B:43:ARG:HD3	1:B:247:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ILE:HG22	1:B:459:PRO:HB3	1.82	0.62
2:G:21:A:N6	2:G:46:G:H2'	2.14	0.62
1:A:139:LEU:HD12	1:A:140:PHE:CD1	2.34	0.62
2:G:75:C:H2'	2:G:76:A:O4'	2.00	0.62
1:A:286:TRP:CD1	1:A:307:ASP:HB3	2.35	0.62
1:B:28:ARG:H	1:B:28:ARG:HD3	1.65	0.62
1:C:404:ALA:HA	1:C:447:LEU:HD11	1.82	0.62
2:F:1:U:H2'	2:F:2:G:H5'	1.82	0.62
1:B:286:TRP:HD1	1:B:308:ILE:HG12	1.65	0.62
1:B:394:TYR:HE1	1:B:447:LEU:HA	1.65	0.62
1:A:329:ARG:HH21	2:E:38:A:H4'	1.64	0.62
1:C:134:ASP:HB3	1:C:137:LYS:HB2	1.82	0.61
1:A:457:VAL:HG11	2:E:37:G:N7	2.15	0.61
1:D:395:VAL:HA	1:D:399:LEU:HB3	1.81	0.61
1:C:183:THR:HG21	2:G:3:G:H4'	1.81	0.61
1:C:477:LEU:O	1:C:481:LEU:HG	2.00	0.61
1:B:440:SER:HB3	1:B:443:VAL:CG2	2.30	0.61
1:D:108:ARG:HA	1:A:164:PRO:HG3	1.82	0.61
1:A:283:LEU:HG	1:A:287:ARG:NH2	2.15	0.61
2:F:71:C:H2'	2:F:72:A:C5'	2.26	0.61
1:C:403:GLU:HA	1:C:406:ARG:NH1	2.16	0.61
1:A:38:HIS:HE1	1:A:255:LEU:HG	1.64	0.61
1:A:54:LYS:O	1:A:54:LYS:HD3	2.00	0.61
1:D:248:LEU:O	1:D:314:ILE:HA	2.00	0.61
1:A:415:PHE:O	1:A:470:LYS:HE3	2.00	0.61
1:D:65:ASP:OD1	1:D:106:SER:HB3	2.00	0.61
2:G:37:G:O2'	2:G:38:A:H5'	2.01	0.61
1:A:277:LEU:O	1:A:281:LEU:HG	2.01	0.61
1:A:369:LYS:HB3	2:E:36:G:H22	1.66	0.61
1:A:169:PHE:CD2	1:A:228:LEU:HD11	2.36	0.61
1:B:381:TYR:N	1:B:382:PRO:HD2	2.16	0.60
1:C:129:VAL:HG12	1:C:139:LEU:HD12	1.83	0.60
1:A:434:SER:HB3	1:A:444:VAL:HG11	1.83	0.60
1:C:399:LEU:HG	1:C:484:LEU:HD13	1.82	0.60
1:B:484:LEU:HD13	1:B:484:LEU:O	2.02	0.60
1:D:224:THR:HB	1:D:225:PRO:HD3	1.84	0.60
2:H:71:C:H2'	2:H:72:A:H5"	1.82	0.60
1:D:315:PHE:HZ	1:D:320:LEU:HD22	1.64	0.60
1:A:304:ASP:HB3	1:A:307:ASP:OD2	2.02	0.60
2:H:59:G:H2'	2:H:60:U:H5'	1.82	0.60
1:B:73:ARG:HB3	1:B:73:ARG:NH1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ILE:HD13	1:C:326:LYS:HG3	1.83	0.60
1:D:77:GLN:O	1:D:81:GLU:HG3	2.01	0.60
1:D:432:ASP:O	1:D:436:LYS:HG3	2.02	0.60
1:A:139:LEU:HD12	1:A:140:PHE:HD1	1.67	0.60
1:A:110:GLU:O	1:A:114:GLU:HG2	2.01	0.59
2:G:71:C:H2'	2:G:72:A:C5'	2.30	0.59
1:B:102:PRO:HG2	1:B:108:ARG:HG2	1.83	0.59
1:A:461:LEU:O	1:A:465:ILE:HG13	2.02	0.59
1:D:131:ASP:OD1	1:D:139:LEU:HD11	2.03	0.59
1:A:369:LYS:HB3	2:E:36:G:N2	2.18	0.59
1:A:403:GLU:O	1:A:407:VAL:HG23	2.03	0.59
2:H:59:G:C2'	2:H:60:U:H5'	2.33	0.59
1:B:249:GLY:HA3	1:B:259:HIS:HD2	1.67	0.59
1:A:161:LYS:HE2	1:A:163:LEU:HD21	1.83	0.59
2:E:28:C:O2'	2:E:29:G:H5'	2.03	0.59
2:F:37:G:O2'	2:F:38:A:H5'	2.03	0.58
1:B:226:LYS:HA	1:B:229:MET:HE2	1.83	0.58
1:C:28:ARG:CZ	1:C:62:ARG:HH22	2.16	0.58
1:C:198:TYR:O	1:C:202:VAL:HG23	2.03	0.58
1:B:33:PRO:HB3	1:B:76:GLU:CB	2.32	0.58
1:D:338:ARG:O	1:D:342:GLU:HG3	2.03	0.58
1:C:223:ASN:HD21	2:G:76:A:N6	2.01	0.58
1:B:65:ASP:H	1:B:105:GLN:HB2	1.68	0.58
1:D:33:PRO:HB3	1:D:76:GLU:HB2	1.85	0.58
1:D:35:GLY:HA3	1:D:257:LYS:HE3	1.85	0.58
2:F:8:U:H5'	2:F:49:G:OP2	2.04	0.58
1:B:395:VAL:HG12	1:B:400:LYS:HG3	1.86	0.58
1:D:304:ASP:HB2	1:D:307:ASP:OD2	2.04	0.58
1:C:381:TYR:N	1:C:382:PRO:HD2	2.19	0.58
1:C:396:GLU:HB3	1:A:73:ARG:NH1	2.17	0.58
1:A:48:ASN:OD1	1:A:215:PHE:HB2	2.03	0.58
1:A:457:VAL:HA	2:E:35:U:O2	2.04	0.58
2:F:12:C:H2'	2:F:13:U:O4'	2.04	0.58
2:F:59:G:H2'	2:F:60:U:H5'	1.84	0.58
2:E:15:A:H2'	2:E:59:G:O6	2.04	0.58
1:C:271:GLY:HA3	1:C:373:LEU:HB2	1.86	0.58
1:A:372:THR:OG1	1:A:375:GLN:HG3	2.03	0.58
1:D:256:SER:OG	1:D:258:ARG:HG2	2.03	0.58
1:A:30:ALA:HA	1:A:62:ARG:O	2.04	0.58
1:D:36:HIS:CG	1:D:262:THR:HA	2.39	0.58
1:D:199:ASN:HD21	1:D:223:ASN:ND2	1.97	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:HIS:HA	1:A:259:HIS:HB3	1.84	0.58
1:A:287:ARG:NH1	2:E:12:C:H1'	2.18	0.58
2:E:16:C:H3'	2:E:19:G:OP1	2.03	0.58
1:D:75:TYR:O	1:D:79:ILE:HG13	2.04	0.58
1:B:43:ARG:NH2	1:B:285:GLY:HA3	2.19	0.57
1:B:114:GLU:O	1:B:118:LYS:HG3	2.04	0.57
1:D:318:GLN:HG2	2:H:26:G:H4'	1.86	0.57
1:A:280:TYR:CZ	1:A:284:LEU:HD21	2.39	0.57
1:A:174:LYS:HE2	1:A:221:LEU:HD22	1.86	0.57
1:B:73:ARG:HA	1:B:76:GLU:HB3	1.85	0.57
1:C:351:ILE:HG23	1:C:384:MET:HB3	1.86	0.57
1:A:395:VAL:HG13	1:A:399:LEU:HD23	1.86	0.57
1:A:422:ASN:HD21	1:A:424:GLU:HB3	1.69	0.57
1:B:337:LYS:O	1:B:341:ILE:HG13	2.04	0.57
1:D:67:ASP:OD2	1:D:69:GLU:HB2	2.04	0.57
1:A:92:GLU:HB3	1:A:103:TYR:OH	2.04	0.57
1:A:293:ILE:HG22	1:A:330:ARG:NH1	2.20	0.57
1:B:148:GLU:HA	1:B:152:LYS:NZ	2.20	0.57
1:A:84:ARG:HD3	1:A:84:ARG:O	2.05	0.57
1:A:172:LEU:HD11	1:A:240:VAL:HG13	1.87	0.57
1:B:27:VAL:HB	1:B:48:ASN:HD22	1.69	0.57
1:B:112:TYR:CD2	1:B:196:PRO:HG3	2.40	0.57
1:D:271:GLY:HA3	1:D:373:LEU:HB2	1.86	0.57
1:A:395:VAL:HA	1:A:399:LEU:HB3	1.86	0.57
2:H:55:U:C3'	2:H:56:C:H5''	2.35	0.57
2:G:71:C:C2'	2:G:72:A:H5''	2.33	0.57
1:B:46:LEU:HD13	1:B:278:MET:HE3	1.87	0.57
1:C:28:ARG:H	1:C:28:ARG:HD3	1.69	0.56
1:C:33:PRO:HD3	1:C:63:ILE:HG23	1.86	0.56
2:E:59:G:O2'	2:E:60:U:H5'	2.04	0.56
1:D:130:TYR:HD2	1:D:155:PRO:HB2	1.70	0.56
1:C:294:PHE:HA	1:C:330:ARG:HH12	1.70	0.56
1:C:349:LYS:HD3	1:C:349:LYS:N	2.20	0.56
1:C:460:GLY:CA	2:G:34:C:H42	2.13	0.56
1:A:224:THR:O	1:A:228:LEU:HG	2.06	0.56
1:A:278:MET:O	1:A:296:ILE:HD11	2.04	0.56
1:A:369:LYS:CD	2:E:36:G:H22	2.18	0.56
1:A:410:GLU:OE1	1:A:438:LEU:HD11	2.05	0.56
1:B:160:PHE:O	1:B:186:ASP:HA	2.06	0.56
1:D:109:LEU:HD12	1:D:110:GLU:N	2.20	0.56
1:C:157:THR:HG22	1:C:192:SER:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:LYS:O	1:C:446:GLN:HG2	2.05	0.56
1:B:193:ASN:OD1	1:B:195:PHE:HB2	2.05	0.56
1:B:405:GLU:O	1:B:409:GLU:HG2	2.05	0.56
1:A:234:PHE:HB3	1:A:236:TRP:CE2	2.41	0.56
1:C:148:GLU:O	1:C:152:LYS:HG3	2.06	0.56
1:C:131:ASP:CG	1:C:132:LYS:H	2.09	0.56
1:C:163:LEU:HB3	1:C:164:PRO:HD2	1.88	0.56
1:C:298:GLU:HG3	1:C:299:LYS:H	1.70	0.56
1:A:275:ARG:H	1:A:275:ARG:HD3	1.70	0.56
1:C:109:LEU:HD21	1:C:195:PHE:CE1	2.40	0.56
2:G:42:G:O2'	2:G:43:C:H5'	2.06	0.56
1:B:303:PHE:O	1:B:305:PRO:HD3	2.06	0.56
1:D:95:ASP:CG	1:D:96:ILE:H	2.09	0.56
1:A:166:LYS:NZ	1:A:180:ASP:HB2	2.21	0.56
1:A:343:TRP:CH2	1:A:374:SER:HA	2.41	0.56
1:B:319:LYS:O	1:B:323:VAL:HG23	2.06	0.56
1:A:301:GLN:H	1:A:301:GLN:HE21	1.54	0.56
1:D:100:PHE:HB3	1:D:103:TYR:OH	2.04	0.56
1:D:369:LYS:HD2	2:H:36:G:N2	2.19	0.56
1:A:47:PHE:CD2	1:A:244:ILE:HD11	2.40	0.56
1:A:422:ASN:ND2	1:A:424:GLU:HB3	2.21	0.56
1:A:430:LEU:HD12	1:A:462:PHE:HE1	1.71	0.56
1:D:169:PHE:HE1	1:D:171:ASP:HB2	1.70	0.55
1:C:270:GLU:O	1:C:374:SER:HB2	2.05	0.55
1:B:26:ARG:O	1:B:211:ILE:HG23	2.06	0.55
1:A:393:ASP:O	1:A:456:LEU:HD11	2.06	0.55
1:A:447:LEU:HD23	1:A:447:LEU:O	2.06	0.55
1:D:117:GLU:OE2	1:A:123:LYS:HE2	2.05	0.55
1:D:315:PHE:CZ	1:D:320:LEU:HD22	2.41	0.55
1:C:162:VAL:HG23	1:C:186:ASP:HA	1.88	0.55
1:A:161:LYS:NZ	1:A:161:LYS:HB3	2.21	0.55
1:A:381:TYR:N	1:A:382:PRO:HD2	2.22	0.55
1:A:401:ARG:HD3	1:A:443:VAL:HG11	1.88	0.55
1:B:286:TRP:CD1	1:B:308:ILE:HG12	2.42	0.55
1:C:251:ASP:O	1:C:253:THR:HG23	2.07	0.55
1:A:75:TYR:O	1:A:79:ILE:HG13	2.06	0.55
2:G:24:A:N6	2:G:45:G:H22	2.03	0.55
1:A:222:SER:O	1:A:225:PRO:HD2	2.07	0.55
2:E:53:G:O2'	2:E:54:U:H5'	2.07	0.55
1:D:114:GLU:O	1:D:118:LYS:HG3	2.05	0.55
1:C:279:ASN:HD22	1:C:323:VAL:HG11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TYR:CD2	1:A:155:PRO:HB2	2.42	0.55
2:E:19:G:O2'	2:E:20:U:H5'	2.07	0.55
1:B:167:THR:HG22	1:B:228:LEU:HD12	1.89	0.54
1:B:428:LYS:HA	1:B:431:ARG:HE	1.73	0.54
1:D:268:ARG:HG3	1:D:268:ARG:HH11	1.72	0.54
1:C:279:ASN:HD21	1:C:293:ILE:HA	1.72	0.54
1:C:369:LYS:HD2	2:G:36:G:H22	1.71	0.54
2:G:24:A:H62	2:G:45:G:H22	1.54	0.54
1:C:60:ILE:HG23	1:C:92:GLU:HB2	1.88	0.54
1:C:363:LEU:HD13	1:C:380:MET:HE1	1.89	0.54
1:A:149:TYR:O	1:A:154:HIS:HB2	2.07	0.54
1:B:104:ARG:C	1:B:106:SER:H	2.10	0.54
1:B:180:ASP:OD2	1:B:182:SER:HB2	2.06	0.54
1:D:425:GLU:O	1:D:428:LYS:HG2	2.08	0.54
1:B:30:ALA:HA	1:B:62:ARG:O	2.07	0.54
1:B:396:GLU:HB3	1:D:73:ARG:HD3	1.89	0.54
1:D:115:TYR:OH	1:D:208:LEU:HD21	2.08	0.54
1:D:264:VAL:O	1:D:268:ARG:HG2	2.07	0.54
1:D:326:LYS:NZ	1:D:329:ARG:HH12	2.04	0.54
2:H:26:G:H2'	2:H:27:G:O4'	2.07	0.54
1:B:361:GLU:O	1:B:365:ILE:HG13	2.07	0.54
1:B:413:LYS:HA	1:B:416:LYS:HZ2	1.72	0.54
1:D:216:ARG:HH22	1:D:227:GLN:HE22	1.56	0.54
1:A:49:TRP:O	1:A:53:ARG:HG2	2.08	0.54
1:A:422:ASN:O	1:A:426:ILE:HG13	2.08	0.54
1:D:129:VAL:HG22	1:D:146:PRO:HG3	1.90	0.54
1:A:371:ASN:HB2	1:A:375:GLN:HE22	1.72	0.54
2:E:9:C:O2	2:E:45:G:H2'	2.08	0.54
1:B:286:TRP:HZ2	1:B:304:ASP:H	1.54	0.54
2:F:68:U:H2'	2:F:69:C:C6	2.43	0.54
1:D:38:HIS:ND1	1:D:40:GLY:N	2.55	0.54
1:D:215:PHE:HD1	1:D:242:MET:HB3	1.73	0.54
2:G:22:G:O2'	2:G:23:G:H5'	2.08	0.54
1:B:36:HIS:CE1	1:B:257:LYS:HD3	2.43	0.54
1:A:190:MET:SD	1:A:196:PRO:HB3	2.47	0.54
1:B:434:SER:HA	1:B:444:VAL:HG21	1.90	0.53
1:D:36:HIS:HB3	1:D:264:VAL:CG2	2.37	0.53
1:A:64:GLU:OE2	1:A:202:VAL:HG22	2.08	0.53
1:A:113:ARG:HA	1:A:190:MET:HE2	1.89	0.53
1:A:288:VAL:HG21	1:A:291:ASP:O	2.08	0.53
2:F:75:C:H2'	2:F:76:A:O4'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:69:C:H2'	2:E:70:C:H6	1.72	0.53
1:D:265:GLU:OE2	1:D:268:ARG:HD3	2.09	0.53
1:D:283:LEU:HD11	1:D:292:GLU:OE1	2.07	0.53
1:D:468:LEU:HB3	1:D:472:ARG:HB2	1.90	0.53
2:G:9:C:O2	2:G:45:G:H2'	2.08	0.53
1:D:33:PRO:HA	1:D:79:ILE:HD12	1.90	0.53
1:D:128:VAL:HB	1:D:157:THR:CG2	2.39	0.53
1:D:218:GLU:OE1	1:D:245:PRO:HA	2.09	0.53
1:A:24:LEU:N	1:A:24:LEU:HD23	2.23	0.53
1:A:198:TYR:CD2	1:A:202:VAL:HG21	2.44	0.53
1:A:278:MET:SD	1:A:281:LEU:HD12	2.48	0.53
1:A:368:GLU:O	1:A:369:LYS:HD3	2.09	0.53
1:A:383:PHE:CZ	1:A:464:THR:HG23	2.44	0.53
1:C:314:ILE:HG22	1:C:315:PHE:N	2.23	0.53
1:A:363:LEU:O	1:A:367:ARG:HG2	2.08	0.53
1:B:452:VAL:HG23	1:B:453:THR:HG23	1.90	0.53
1:B:472:ARG:O	1:B:476:ARG:HG3	2.07	0.53
1:D:223:ASN:HA	1:D:226:LYS:CE	2.39	0.53
1:C:293:ILE:CD1	1:C:326:LYS:HG3	2.38	0.53
1:A:117:GLU:C	1:A:119:LEU:H	2.11	0.53
1:A:223:ASN:HD21	2:E:76:A:N6	2.07	0.53
1:A:255:LEU:HD11	1:A:262:THR:HG21	1.89	0.53
1:A:430:LEU:HD12	1:A:462:PHE:CE1	2.44	0.53
1:A:471:GLU:CD	1:A:471:GLU:H	2.12	0.53
1:B:199:ASN:HD22	1:B:226:LYS:HB2	1.72	0.53
1:D:88:LEU:HB2	1:D:90:TRP:NE1	2.23	0.53
1:C:421:TRP:CZ3	1:C:470:LYS:HA	2.44	0.53
1:C:430:LEU:N	1:C:430:LEU:HD12	2.23	0.53
1:A:189:ILE:HB	1:A:200:PHE:CG	2.43	0.53
1:A:226:LYS:HA	1:A:229:MET:CE	2.39	0.53
1:B:54:LYS:HD2	1:B:303:PHE:HB3	1.90	0.53
1:B:412:LYS:HE2	1:B:478:GLU:OE1	2.08	0.53
1:D:273:LEU:HD13	1:D:324:ASN:OD1	2.09	0.53
1:C:95:ASP:OD2	1:C:96:ILE:HG13	2.09	0.53
2:G:25:C:H2'	2:G:26:G:O4'	2.08	0.53
1:D:278:MET:HB3	1:D:296:ILE:HG13	1.90	0.53
1:A:28:ARG:HD3	1:A:28:ARG:N	2.24	0.53
1:A:286:TRP:CG	1:A:307:ASP:HB3	2.43	0.53
2:E:55:U:H2'	2:E:56:C:H5"	1.91	0.53
1:D:130:TYR:CD2	1:D:155:PRO:HB2	2.44	0.53
1:C:24:LEU:N	1:C:24:LEU:HD23	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:71:C:H2'	2:E:72:A:H4'	1.89	0.53
1:B:98:GLY:HA3	1:B:103:TYR:HE2	1.73	0.52
1:B:169:PHE:CD2	1:B:228:LEU:HD11	2.44	0.52
1:D:337:LYS:O	1:D:341:ILE:HG13	2.09	0.52
1:C:215:PHE:CD1	1:C:242:MET:HB3	2.44	0.52
1:A:145:TYR:OH	1:A:150:LYS:HG3	2.09	0.52
1:A:481:LEU:O	1:A:485:LYS:HG3	2.10	0.52
1:B:329:ARG:HH21	2:F:38:A:H4'	1.72	0.52
1:B:413:LYS:O	1:B:416:LYS:HB3	2.10	0.52
1:D:99:ASP:C	1:D:101:GLY:H	2.11	0.52
1:D:219:ASP:HB3	1:D:246:LEU:HD11	1.90	0.52
1:A:161:LYS:HB3	1:A:161:LYS:HZ3	1.73	0.52
1:A:297:GLU:C	1:A:299:LYS:H	2.12	0.52
1:A:450:GLY:O	1:A:454:GLY:HA2	2.09	0.52
1:C:61:LEU:HD22	1:C:90:TRP:CE3	2.44	0.52
1:C:440:SER:OG	1:C:443:VAL:HG23	2.08	0.52
1:C:250:SER:H	1:C:259:HIS:CE1	2.27	0.52
2:E:59:G:C2'	2:E:60:U:H5'	2.40	0.52
1:B:304:ASP:CB	1:B:307:ASP:HB2	2.30	0.52
1:D:30:ALA:HB1	1:D:64:GLU:OE1	2.10	0.52
1:D:228:LEU:HA	1:D:231:TYR:HD2	1.73	0.52
1:D:369:LYS:HB3	2:H:36:G:N2	2.24	0.52
1:C:304:ASP:HB3	1:C:307:ASP:OD1	2.10	0.52
2:G:68:U:H2'	2:G:69:C:C6	2.44	0.52
1:B:30:ALA:HB1	1:B:64:GLU:CG	2.37	0.52
1:D:299:LYS:HA	1:D:302:SER:OG	2.10	0.52
1:B:31:PRO:O	1:B:64:GLU:HB2	2.10	0.52
1:D:88:LEU:HB2	1:D:90:TRP:HE1	1.75	0.52
1:D:430:LEU:HD12	1:D:430:LEU:N	2.24	0.52
2:G:41:C:O2'	2:G:42:G:H5'	2.10	0.52
2:G:62:C:H2'	2:G:63:U:C6	2.44	0.52
1:B:369:LYS:NZ	2:F:36:G:N2	2.58	0.52
1:C:95:ASP:CG	1:C:96:ILE:H	2.14	0.52
1:A:322:TRP:O	1:A:326:LYS:HG3	2.09	0.52
1:B:169:PHE:HD2	1:B:228:LEU:HD11	1.75	0.52
1:C:37:LEU:HG	1:C:264:VAL:HG21	1.91	0.52
1:C:278:MET:HB3	1:C:296:ILE:HG13	1.91	0.52
1:A:275:ARG:O	1:A:279:ASN:HB2	2.10	0.52
1:A:326:LYS:O	1:A:330:ARG:HB2	2.10	0.52
1:A:223:ASN:HD21	2:E:76:A:H61	1.57	0.52
2:G:59:G:O2'	2:G:60:U:H5'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:HIS:CE1	1:D:262:THR:HG22	2.45	0.51
1:D:357:ARG:O	1:D:361:GLU:HG2	2.10	0.51
1:C:298:GLU:HG3	1:C:299:LYS:N	2.25	0.51
1:B:83:LEU:HD22	1:B:88:LEU:HD12	1.91	0.51
1:D:48:ASN:OD1	1:D:215:PHE:HB2	2.09	0.51
1:D:64:GLU:HA	1:D:105:GLN:HB2	1.91	0.51
1:D:73:ARG:HA	1:D:76:GLU:HB3	1.91	0.51
1:D:223:ASN:HD21	2:H:76:A:N6	2.09	0.51
1:C:333:LEU:HD11	1:C:364:ARG:HG3	1.91	0.51
2:F:41:C:O2'	2:F:42:G:H5'	2.10	0.51
1:D:304:ASP:C	1:D:306:LYS:H	2.14	0.51
1:C:104:ARG:HB2	1:C:107:GLU:HB2	1.93	0.51
1:B:125:ALA:HA	1:B:159:LYS:O	2.11	0.51
1:D:62:ARG:HD3	1:D:209:MET:SD	2.51	0.51
1:D:376:LEU:O	1:D:379:ILE:HG22	2.10	0.51
1:C:73:ARG:HA	1:C:73:ARG:HH11	1.76	0.51
1:A:369:LYS:CD	2:E:36:G:H1	2.18	0.51
1:A:426:ILE:HG21	1:A:462:PHE:HA	1.91	0.51
2:E:75:C:H2'	2:E:76:A:O4'	2.09	0.51
1:B:203:VAL:HG13	1:B:231:TYR:CE1	2.46	0.51
1:D:130:TYR:HB2	1:D:155:PRO:HD2	1.93	0.51
1:C:393:ASP:O	1:C:397:LYS:HB3	2.10	0.51
2:G:66:C:H5"	2:E:50:G:H4'	1.93	0.51
1:B:421:TRP:CZ3	1:B:470:LYS:HG3	2.45	0.51
1:C:337:LYS:HG3	1:C:359:PHE:HE2	1.75	0.51
1:B:27:VAL:HG12	1:B:213:HIS:HB2	1.93	0.51
1:B:64:GLU:HG3	3:B:1001:GSU:H	1.74	0.51
1:D:62:ARG:NH1	1:D:205:ASP:HB2	2.26	0.51
1:D:251:ASP:OD2	1:D:253:THR:HB	2.10	0.51
1:D:369:LYS:HD2	2:H:36:G:N1	2.24	0.51
1:C:464:THR:O	1:C:468:LEU:HG	2.10	0.51
1:A:231:TYR:HD1	1:A:236:TRP:HB2	1.75	0.51
1:B:228:LEU:HA	1:B:231:TYR:HD2	1.75	0.51
1:C:259:HIS:HB3	1:A:259:HIS:O	2.10	0.51
1:A:284:LEU:O	1:A:286:TRP:N	2.44	0.51
1:A:421:TRP:CZ2	1:A:465:ILE:HG22	2.45	0.51
1:B:218:GLU:N	1:B:246:LEU:HD21	2.26	0.51
1:D:391:GLU:HG3	1:D:454:GLY:O	2.11	0.51
1:C:357:ARG:HG2	1:C:357:ARG:HH11	1.76	0.51
1:A:179:PHE:CD2	1:A:225:PRO:HG3	2.45	0.51
1:A:196:PRO:HG2	1:A:201:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:70:C:H2'	2:F:71:C:C6	2.46	0.51
2:G:40:C:H2'	2:G:41:C:C6	2.46	0.51
1:B:37:LEU:HD21	1:B:82:SER:CB	2.40	0.50
1:B:73:ARG:HH11	1:B:73:ARG:CA	2.24	0.50
1:B:120:VAL:HA	1:B:125:ALA:O	2.11	0.50
1:B:371:ASN:ND2	2:F:38:A:H5'	2.23	0.50
1:B:396:GLU:CB	1:D:73:ARG:HD3	2.41	0.50
1:A:213:HIS:HB3	1:A:215:PHE:CE1	2.46	0.50
2:H:38:A:H2'	2:H:39:U:H6	1.76	0.50
2:E:69:C:H2'	2:E:70:C:C6	2.46	0.50
1:D:407:VAL:HG11	1:D:447:LEU:HD12	1.92	0.50
1:C:30:ALA:HA	1:C:62:ARG:O	2.11	0.50
1:A:150:LYS:O	1:A:150:LYS:HD3	2.11	0.50
1:A:328:MET:HE3	1:A:373:LEU:HD23	1.93	0.50
1:A:458:THR:HB	1:A:459:PRO:HD2	1.93	0.50
2:E:1:U:H2'	2:E:2:G:H5'	1.93	0.50
1:A:251:ASP:O	1:A:253:THR:HG23	2.12	0.50
1:A:391:GLU:O	1:A:394:TYR:HB3	2.12	0.50
1:B:29:PHE:CD2	1:B:31:PRO:HG3	2.47	0.50
2:E:65:C:O2'	2:E:66:C:H5'	2.11	0.50
1:D:225:PRO:O	1:D:229:MET:HG3	2.10	0.50
1:D:257:LYS:HD2	1:D:257:LYS:N	2.27	0.50
1:A:193:ASN:OD1	1:A:195:PHE:HB2	2.11	0.50
1:A:395:VAL:HG12	1:A:400:LYS:HE3	1.93	0.50
2:F:59:G:C2'	2:F:60:U:H5'	2.41	0.50
1:B:98:GLY:HA3	1:B:103:TYR:CE2	2.46	0.50
1:D:215:PHE:CD1	1:D:242:MET:HB3	2.47	0.50
1:D:342:GLU:O	1:D:346:TYR:HB2	2.12	0.50
1:C:349:LYS:H	1:C:349:LYS:CD	2.24	0.50
1:C:63:ILE:O	1:C:105:GLN:HG2	2.11	0.50
1:C:226:LYS:HA	1:C:229:MET:CE	2.41	0.50
1:C:403:GLU:HA	1:C:406:ARG:HH12	1.76	0.50
1:D:169:PHE:CD2	1:D:228:LEU:HD11	2.47	0.50
1:C:223:ASN:HD21	2:G:76:A:H61	1.58	0.50
1:A:130:TYR:HB2	1:A:155:PRO:HD2	1.94	0.50
1:A:276:ALA:O	1:A:279:ASN:HB3	2.12	0.50
2:H:50:G:H2'	2:H:51:A:O4'	2.12	0.50
1:B:422:ASN:OD1	1:B:425:GLU:HG2	2.11	0.50
1:D:120:VAL:HG11	1:D:127:TYR:HE2	1.77	0.50
1:C:273:LEU:HD12	1:C:273:LEU:H	1.77	0.50
1:A:129:VAL:HG22	1:A:156:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:HIS:O	1:D:331:ILE:HG23	2.12	0.49
1:C:73:ARG:HH11	1:C:73:ARG:CB	2.25	0.49
1:C:120:VAL:N	1:C:125:ALA:HB3	2.27	0.49
1:A:408:LEU:HB2	1:A:481:LEU:HD21	1.94	0.49
2:F:22:G:O2'	2:F:23:G:H5'	2.12	0.49
1:B:43:ARG:CD	1:B:247:ILE:HD11	2.43	0.49
1:B:60:ILE:HG23	1:B:92:GLU:HB2	1.93	0.49
1:D:123:LYS:HD2	1:D:143:TYR:CE2	2.47	0.49
1:C:104:ARG:HG3	1:C:104:ARG:HH11	1.76	0.49
1:B:249:GLY:HA3	1:B:259:HIS:CD2	2.47	0.49
1:B:427:GLU:O	1:B:431:ARG:HG2	2.12	0.49
1:A:162:VAL:HG13	1:A:229:MET:SD	2.52	0.49
2:F:37:G:OP1	2:F:37:G:N3	2.46	0.49
2:G:53:G:H2'	2:G:54:U:C6	2.47	0.49
1:D:43:ARG:HD2	1:D:247:ILE:HD11	1.94	0.49
1:D:166:LYS:HG2	1:D:180:ASP:HA	1.95	0.49
1:C:440:SER:O	1:C:444:VAL:HG23	2.12	0.49
2:H:36:G:O2'	2:H:37:G:H5'	2.12	0.49
2:E:67:C:H2'	2:E:68:U:C6	2.47	0.49
1:C:26:ARG:HE	1:C:58:LYS:HB2	1.78	0.49
1:C:113:ARG:HH12	1:C:117:GLU:CD	2.15	0.49
1:A:273:LEU:H	1:A:273:LEU:HD12	1.78	0.49
2:G:53:G:O2'	2:G:54:U:H5'	2.12	0.49
1:B:29:PHE:CE2	1:B:31:PRO:HG3	2.48	0.49
1:B:200:PHE:O	1:B:204:VAL:HG23	2.12	0.49
1:A:135:PRO:HB3	1:A:155:PRO:HG2	1.94	0.49
1:A:334:GLU:O	1:A:338:ARG:HG3	2.12	0.49
1:A:458:THR:HB	1:A:459:PRO:CD	2.43	0.49
1:B:163:LEU:N	1:B:163:LEU:HD12	2.27	0.49
1:B:463:GLU:O	1:B:467:VAL:HG12	2.12	0.49
1:D:115:TYR:HE2	1:D:208:LEU:HD11	1.76	0.49
1:D:156:VAL:O	1:D:192:SER:HA	2.13	0.49
1:C:218:GLU:HG3	1:C:244:ILE:O	2.13	0.49
1:A:409:GLU:O	1:A:412:LYS:HB3	2.12	0.49
1:B:453:THR:CB	1:B:458:THR:HG21	2.43	0.49
1:D:179:PHE:CD2	1:D:225:PRO:HG2	2.48	0.49
1:D:216:ARG:HD2	1:D:243:HIS:NE2	2.28	0.49
1:D:398:PHE:HA	1:D:401:ARG:HG3	1.95	0.49
1:A:172:LEU:N	1:A:172:LEU:HD12	2.28	0.49
1:B:73:ARG:HA	1:B:73:ARG:HH11	1.78	0.49
1:B:226:LYS:HA	1:B:229:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ILE:HG22	1:B:459:PRO:CB	2.43	0.49
1:D:388:TYR:CE2	1:D:476:ARG:HD3	2.47	0.49
1:D:457:VAL:HA	2:H:35:U:O2	2.13	0.49
1:C:25:VAL:HB	1:C:57:GLY:HA3	1.95	0.49
1:C:28:ARG:HD3	1:C:28:ARG:N	2.28	0.49
1:A:213:HIS:HB3	1:A:215:PHE:HE1	1.77	0.49
1:D:53:ARG:HH12	1:D:58:LYS:HA	1.77	0.48
1:D:453:THR:O	1:D:455:LYS:HG3	2.13	0.48
1:C:108:ARG:HB2	1:C:112:TYR:CE2	2.48	0.48
1:C:309:SER:OG	1:C:311:LYS:HE3	2.13	0.48
1:A:112:TYR:CD2	1:A:196:PRO:HG3	2.48	0.48
1:A:244:ILE:HG23	1:A:308:ILE:CD1	2.43	0.48
1:D:421:TRP:HE1	1:D:465:ILE:HG22	1.79	0.48
1:C:342:GLU:O	1:C:345:LYS:HB3	2.13	0.48
1:C:463:GLU:HA	1:C:466:GLU:HB3	1.95	0.48
1:A:331:ILE:HD11	1:A:336:LEU:HD13	1.96	0.48
2:E:71:C:C3'	2:E:72:A:H5"	2.43	0.48
1:B:35:GLY:N	1:B:75:TYR:HB3	2.27	0.48
1:C:398:PHE:CD2	1:C:446:GLN:HB3	2.48	0.48
1:B:220:HIS:HA	1:B:223:ASN:HD22	1.77	0.48
1:D:381:TYR:N	1:D:382:PRO:HD2	2.28	0.48
1:C:25:VAL:HB	1:C:57:GLY:CA	2.44	0.48
1:C:108:ARG:HD3	1:C:112:TYR:OH	2.13	0.48
1:C:329:ARG:NH2	2:G:38:A:H4'	2.25	0.48
1:C:394:TYR:HE1	1:C:447:LEU:HA	1.78	0.48
1:A:120:VAL:HG11	1:A:127:TYR:CE2	2.49	0.48
2:F:67:C:H2'	2:F:68:U:C6	2.49	0.48
2:E:2:G:O2'	2:E:3:G:H5'	2.14	0.48
1:D:29:PHE:HB2	1:D:59:PHE:CZ	2.48	0.48
1:D:430:LEU:HG	1:D:433:LEU:HD12	1.95	0.48
1:D:464:THR:O	1:D:468:LEU:HG	2.13	0.48
1:A:135:PRO:HA	1:A:155:PRO:HG2	1.95	0.48
1:A:273:LEU:HD12	1:A:273:LEU:N	2.28	0.48
1:A:286:TRP:HB2	1:A:308:ILE:HA	1.96	0.48
1:A:333:LEU:HD23	1:A:333:LEU:O	2.13	0.48
1:A:369:LYS:HD2	2:E:36:G:C2	2.48	0.48
2:H:53:G:O2'	2:H:54:U:H5'	2.13	0.48
1:D:373:LEU:O	1:D:376:LEU:HB3	2.13	0.48
1:D:441:LYS:HB2	1:D:445:PHE:HE2	1.78	0.48
1:A:33:PRO:O	1:A:71:SER:HA	2.14	0.48
1:A:267:PHE:HB3	1:A:272:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LEU:CD2	1:B:244:ILE:HA	2.43	0.48
1:D:280:TYR:CZ	1:D:284:LEU:HD11	2.49	0.48
1:C:245:PRO:HG2	1:C:309:SER:O	2.13	0.48
1:C:352:PRO:O	1:C:354:VAL:HG13	2.13	0.48
1:B:49:TRP:HZ3	1:B:296:ILE:HG21	1.79	0.48
1:B:173:LEU:HD23	1:B:244:ILE:HA	1.96	0.48
1:C:340:PHE:O	1:C:343:TRP:HB3	2.14	0.48
1:A:123:LYS:NZ	1:A:123:LYS:HB3	2.28	0.48
1:B:37:LEU:HD23	1:B:37:LEU:N	2.25	0.48
1:D:252:ARG:CZ	1:D:314:ILE:HD11	2.44	0.48
1:D:388:TYR:HE2	1:D:476:ARG:HD3	1.78	0.48
1:D:471:GLU:O	1:D:475:LYS:HG3	2.13	0.48
1:C:167:THR:O	1:C:179:PHE:HB2	2.14	0.48
2:G:55:U:N3	2:G:57:G:H5''	2.28	0.48
1:D:422:ASN:HD21	1:D:425:GLU:HG2	1.79	0.47
1:A:28:ARG:NH2	1:A:214:VAL:HG13	2.29	0.47
2:F:55:U:N3	2:F:57:G:H5''	2.29	0.47
1:B:67:ASP:OD1	1:B:69:GLU:HB2	2.13	0.47
1:D:116:ALA:HB2	1:D:200:PHE:CZ	2.49	0.47
1:A:32:SER:O	1:A:34:THR:N	2.47	0.47
1:A:116:ALA:O	1:A:120:VAL:HG23	2.12	0.47
2:F:37:G:H3'	2:F:38:A:H8	1.79	0.47
1:D:94:PRO:HB3	1:D:102:PRO:HA	1.96	0.47
1:D:109:LEU:O	1:D:113:ARG:HG3	2.14	0.47
1:D:251:ASP:O	1:D:252:ARG:HB2	2.14	0.47
1:C:254:PRO:HD3	2:G:69:C:H4'	1.94	0.47
2:E:15:A:C2	2:E:21:A:H1'	2.49	0.47
1:B:198:TYR:O	1:B:202:VAL:HG23	2.14	0.47
1:B:369:LYS:HZ2	2:F:36:G:N2	2.12	0.47
1:B:485:LYS:H	1:B:485:LYS:CD	2.28	0.47
1:D:199:ASN:ND2	1:D:223:ASN:HD22	2.04	0.47
1:C:90:TRP:NE1	1:C:96:ILE:HD12	2.29	0.47
1:A:428:LYS:NZ	1:A:428:LYS:HB3	2.29	0.47
2:H:57:G:C2'	2:H:58:A:H5'	2.44	0.47
2:H:68:U:H2'	2:H:69:C:C6	2.50	0.47
1:B:37:LEU:HD21	1:B:82:SER:HB2	1.96	0.47
1:B:124:ARG:HG2	1:B:124:ARG:HH11	1.78	0.47
1:B:191:LYS:NZ	2:F:75:C:H5'	2.30	0.47
1:D:110:GLU:O	1:D:114:GLU:HG2	2.14	0.47
1:C:406:ARG:HD2	1:C:438:LEU:O	2.15	0.47
1:B:245:PRO:HB3	1:B:311:LYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:LYS:HA	1:B:329:ARG:NH1	2.29	0.47
1:D:198:TYR:O	1:D:202:VAL:HG23	2.15	0.47
1:D:368:GLU:O	1:D:369:LYS:HD3	2.14	0.47
1:C:273:LEU:HD12	1:C:273:LEU:N	2.29	0.47
1:C:390:TYR:HA	1:C:454:GLY:O	2.13	0.47
1:A:349:LYS:HD3	1:A:377:TYR:CE2	2.49	0.47
1:A:426:ILE:CG2	1:A:462:PHE:HA	2.45	0.47
1:B:35:GLY:H	1:B:75:TYR:CB	2.27	0.47
1:B:248:LEU:HD13	1:B:252:ARG:O	2.15	0.47
1:B:354:VAL:CG1	1:B:355:ASP:H	2.26	0.47
1:B:447:LEU:O	1:B:451:ALA:HB2	2.15	0.47
1:D:55:GLU:HG2	1:D:56:GLY:N	2.29	0.47
1:D:113:ARG:O	1:D:117:GLU:HB2	2.15	0.47
1:D:134:ASP:HB3	1:D:137:LYS:HB3	1.96	0.47
1:D:421:TRP:CZ3	1:D:470:LYS:HG3	2.50	0.47
1:C:250:SER:O	1:A:251:ASP:HB3	2.15	0.47
1:C:273:LEU:H	1:C:273:LEU:CD1	2.28	0.47
1:C:279:ASN:HD22	1:C:323:VAL:CG1	2.28	0.47
1:C:403:GLU:HB2	1:C:439:ALA:HB2	1.97	0.47
1:A:62:ARG:HH11	1:A:205:ASP:HB3	1.79	0.47
1:A:88:LEU:HD11	1:A:278:MET:HE1	1.97	0.47
1:A:338:ARG:NH1	1:A:338:ARG:HB2	2.30	0.47
1:A:395:VAL:HG12	1:A:400:LYS:HG3	1.97	0.47
1:A:421:TRP:HZ2	1:A:465:ILE:HG22	1.79	0.47
2:F:67:C:OP1	2:H:50:G:H5'	2.15	0.47
2:G:66:C:H2'	2:G:67:C:C6	2.50	0.47
1:C:126:TYR:HB2	1:C:142:THR:O	2.15	0.47
1:C:363:LEU:CD1	1:C:380:MET:HE1	2.45	0.47
1:A:283:LEU:HD11	1:A:292:GLU:HG2	1.96	0.47
1:A:482:GLN:HE22	1:A:485:LYS:NZ	2.13	0.47
2:H:2:G:H2'	2:H:3:G:H8	1.79	0.47
2:H:40:C:H2'	2:H:41:C:C6	2.50	0.47
1:B:148:GLU:HA	1:B:152:LYS:HZ2	1.79	0.47
1:B:354:VAL:HG21	1:B:384:MET:SD	2.54	0.47
1:D:271:GLY:CA	1:D:373:LEU:HB2	2.44	0.47
1:C:38:HIS:HE2	1:C:255:LEU:HG	1.79	0.47
1:C:86:CYS:HA	1:C:274:SER:HG	1.79	0.47
1:B:354:VAL:HG11	1:B:358:TYR:HD2	1.80	0.47
1:B:449:ARG:HG3	1:B:449:ARG:HH11	1.80	0.47
1:C:59:PHE:HD2	1:C:90:TRP:HA	1.80	0.47
1:C:248:LEU:C	1:C:255:LEU:HB2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:HD3	1:A:161:LYS:HZ1	1.80	0.47
2:G:28:C:O2'	2:G:29:G:H5'	2.15	0.47
1:B:376:LEU:HG	1:B:380:MET:HE1	1.96	0.46
1:D:47:PHE:CD2	1:D:244:ILE:HD11	2.50	0.46
1:C:27:VAL:CG1	1:C:213:HIS:HB2	2.45	0.46
1:C:271:GLY:CA	1:C:373:LEU:HB2	2.45	0.46
1:A:275:ARG:H	1:A:275:ARG:CD	2.28	0.46
1:A:399:LEU:HG	1:A:484:LEU:HD13	1.98	0.46
1:D:285:GLY:O	1:D:309:SER:HB2	2.16	0.46
1:D:361:GLU:O	1:D:365:ILE:HG13	2.15	0.46
1:C:212:SER:O	1:C:239:PRO:HB3	2.15	0.46
1:C:224:THR:O	1:C:228:LEU:HG	2.14	0.46
1:C:274:SER:O	1:C:278:MET:HG2	2.16	0.46
2:F:58:A:H2	2:F:60:U:HO2'	1.63	0.46
1:B:327:HIS:O	1:B:331:ILE:HG12	2.15	0.46
1:D:31:PRO:HD2	1:D:62:ARG:O	2.16	0.46
1:D:198:TYR:CD1	1:D:199:ASN:N	2.84	0.46
1:D:391:GLU:OE1	1:D:455:LYS:HA	2.15	0.46
1:D:422:ASN:ND2	1:D:425:GLU:HG2	2.31	0.46
1:C:86:CYS:HA	1:C:274:SER:OG	2.15	0.46
1:C:120:VAL:HA	1:C:125:ALA:O	2.15	0.46
1:D:218:GLU:HB3	1:D:246:LEU:HG	1.97	0.46
1:C:169:PHE:CD2	1:C:228:LEU:HD11	2.50	0.46
1:C:245:PRO:CG	1:C:310:ASN:HA	2.40	0.46
1:C:379:ILE:HD11	1:C:457:VAL:O	2.16	0.46
2:H:42:G:O2'	2:H:43:C:H5'	2.16	0.46
2:G:71:C:H5"	2:G:76:A:N1	2.31	0.46
1:B:159:LYS:HG2	1:B:188:ILE:HG12	1.97	0.46
1:B:370:VAL:HG21	1:B:376:LEU:HB2	1.98	0.46
1:B:395:VAL:HG22	1:B:399:LEU:HD23	1.97	0.46
1:D:434:SER:HB2	1:D:441:LYS:N	2.31	0.46
1:A:188:ILE:HD12	2:E:74:C:H5'	1.97	0.46
1:B:108:ARG:HB2	1:B:112:TYR:CE2	2.50	0.46
1:D:28:ARG:HH12	1:D:206:ASP:CG	2.19	0.46
1:D:369:LYS:CD	2:H:36:G:H22	2.24	0.46
1:C:215:PHE:HD1	1:C:242:MET:HB3	1.79	0.46
1:B:266:HIS:O	1:B:269:ARG:HB2	2.16	0.46
1:C:432:ASP:O	1:C:436:LYS:HG3	2.16	0.46
1:A:26:ARG:NH2	1:A:60:ILE:HD11	2.30	0.46
1:A:249:GLY:O	1:A:314:ILE:HG23	2.16	0.46
1:A:274:SER:O	1:A:278:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:C	1:A:287:ARG:HH21	2.18	0.46
1:A:423:MET:HG2	1:A:463:GLU:HA	1.98	0.46
2:H:9:C:O2	2:H:45:G:H2'	2.16	0.46
2:H:64:C:H2'	2:H:65:C:C6	2.51	0.46
2:E:24:A:H62	2:E:45:G:N2	2.13	0.46
1:B:129:VAL:CG1	1:B:139:LEU:HD12	2.41	0.46
1:B:313:VAL:HG23	1:B:313:VAL:O	2.16	0.46
1:D:95:ASP:OD2	1:D:96:ILE:HG12	2.15	0.46
1:D:163:LEU:H	1:D:163:LEU:CD2	2.27	0.46
1:D:457:VAL:HG11	2:H:37:G:C2	2.50	0.46
1:C:173:LEU:C	1:C:173:LEU:HD23	2.36	0.46
1:C:173:LEU:HD21	1:C:310:ASN:HB3	1.98	0.46
1:A:31:PRO:HD2	1:A:62:ARG:O	2.15	0.46
2:H:28:C:O2'	2:H:29:G:H5'	2.16	0.46
1:B:271:GLY:HA3	1:B:373:LEU:HB2	1.98	0.46
1:D:33:PRO:O	1:D:75:TYR:HB2	2.15	0.46
1:D:148:GLU:CD	1:D:148:GLU:H	2.19	0.46
1:D:275:ARG:HG2	1:D:275:ARG:HH11	1.81	0.46
1:D:344:ALA:HB1	1:D:350:GLU:HB3	1.98	0.46
1:A:369:LYS:CB	2:E:36:G:H22	2.27	0.46
1:D:168:SER:HB3	1:D:178:GLU:HA	1.98	0.45
1:D:335:ASP:CG	1:D:338:ARG:HH21	2.20	0.45
1:C:224:THR:N	1:C:225:PRO:CD	2.79	0.45
1:C:394:TYR:HA	1:C:398:PHE:HB2	1.99	0.45
1:B:125:ALA:HB1	1:B:158:ILE:CG2	2.45	0.45
1:B:269:ARG:HG2	1:B:346:TYR:HE2	1.81	0.45
1:D:46:LEU:O	1:D:50:MET:HE2	2.16	0.45
1:D:262:THR:C	1:D:264:VAL:H	2.19	0.45
1:D:429:THR:O	1:D:433:LEU:HG	2.16	0.45
1:C:73:ARG:HH11	1:C:73:ARG:CA	2.29	0.45
1:C:171:ASP:HB3	1:C:174:LYS:HB2	1.98	0.45
1:C:203:VAL:HG13	1:C:231:TYR:CD1	2.51	0.45
1:C:334:GLU:HB3	1:C:338:ARG:NH1	2.23	0.45
1:C:421:TRP:CH2	1:C:470:LYS:HA	2.51	0.45
1:A:63:ILE:CG1	1:A:94:PRO:HG3	2.45	0.45
1:B:403:GLU:N	1:B:403:GLU:OE2	2.47	0.45
1:B:62:ARG:HD2	1:B:105:GLN:NE2	2.32	0.45
1:B:161:LYS:HA	1:B:186:ASP:OD2	2.17	0.45
1:B:224:THR:O	1:B:228:LEU:HG	2.17	0.45
1:B:376:LEU:O	1:B:379:ILE:HG22	2.16	0.45
1:C:351:ILE:CG2	1:C:384:MET:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:MET:O	1:C:380:MET:HG2	2.16	0.45
1:A:295:THR:HB	1:A:298:GLU:HG2	1.98	0.45
2:F:28:C:O2'	2:F:29:G:H5'	2.16	0.45
2:E:67:C:H2'	2:E:68:U:H6	1.81	0.45
1:B:28:ARG:HD3	1:B:28:ARG:N	2.29	0.45
1:B:146:PRO:HB2	1:B:149:TYR:HB2	1.99	0.45
1:B:326:LYS:HA	1:B:329:ARG:HH11	1.81	0.45
1:D:94:PRO:HA	1:D:98:GLY:O	2.16	0.45
1:C:148:GLU:HB2	1:C:152:LYS:HE3	1.98	0.45
1:A:130:TYR:HE1	1:A:138:GLU:HG2	1.82	0.45
2:G:48:U:H3'	2:G:50:G:OP2	2.16	0.45
1:B:104:ARG:HG3	1:B:104:ARG:HH11	1.81	0.45
1:B:132:LYS:H	1:B:154:HIS:CE1	2.34	0.45
1:B:286:TRP:HE1	1:B:304:ASP:HB2	1.82	0.45
1:B:289:GLU:OE2	1:B:302:SER:HB2	2.17	0.45
1:B:334:GLU:O	1:B:338:ARG:HG3	2.16	0.45
1:D:94:PRO:CG	1:D:102:PRO:HA	2.47	0.45
1:D:351:ILE:CG1	1:D:385:ASN:HD21	2.12	0.45
1:C:352:PRO:HG2	1:C:385:ASN:OD1	2.16	0.45
1:A:96:ILE:HG13	1:A:97:GLY:N	2.31	0.45
1:B:330:ARG:HG2	1:B:330:ARG:HH11	1.81	0.45
1:B:333:LEU:O	1:B:333:LEU:HD23	2.16	0.45
1:B:395:VAL:HG12	1:B:400:LYS:HE3	1.99	0.45
1:B:412:LYS:O	1:B:416:LYS:HB2	2.17	0.45
1:D:27:VAL:CG2	1:D:52:ALA:HB2	2.46	0.45
1:C:148:GLU:OE1	1:C:148:GLU:N	2.50	0.45
1:A:130:TYR:HB2	1:A:155:PRO:HB2	1.98	0.45
2:H:1:U:H2'	2:H:2:G:C5'	2.47	0.45
1:B:477:LEU:O	1:B:481:LEU:HG	2.16	0.45
1:D:120:VAL:HG11	1:D:127:TYR:CE2	2.51	0.45
1:D:398:PHE:HB3	1:D:447:LEU:CD2	2.45	0.45
1:C:166:LYS:HB3	1:C:178:GLU:OE2	2.17	0.45
1:A:172:LEU:HD13	1:A:241:PHE:O	2.16	0.45
1:A:332:ASP:OD2	1:A:334:GLU:HB2	2.16	0.45
2:F:40:C:O2'	2:F:41:C:H5'	2.16	0.45
1:B:73:ARG:HH11	1:B:73:ARG:CB	2.30	0.45
1:D:328:MET:O	1:D:331:ILE:HG12	2.17	0.45
1:C:463:GLU:O	1:C:467:VAL:HG12	2.17	0.45
2:E:71:C:H2'	2:E:72:A:C4'	2.46	0.45
1:B:150:LYS:HD2	1:B:150:LYS:C	2.37	0.45
1:B:369:LYS:NZ	2:F:36:G:H22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ARG:NE	1:D:314:ILE:HD11	2.32	0.45
1:A:391:GLU:HG3	1:A:454:GLY:O	2.17	0.45
2:G:5:A:O2'	2:G:6:G:H5'	2.17	0.45
1:B:66:THR:HA	1:B:195:PHE:CE1	2.52	0.44
1:D:247:ILE:O	1:D:255:LEU:HG	2.17	0.44
1:C:43:ARG:O	1:C:46:LEU:HB3	2.17	0.44
1:A:248:LEU:HD22	1:A:252:ARG:O	2.16	0.44
1:A:443:VAL:HG12	1:A:443:VAL:O	2.16	0.44
1:B:84:ARG:HH11	1:B:84:ARG:HG2	1.81	0.44
1:B:407:VAL:HG22	1:B:438:LEU:HB3	1.99	0.44
1:B:426:ILE:HG21	1:B:465:ILE:HB	1.98	0.44
1:C:167:THR:HG21	1:C:225:PRO:HB3	1.99	0.44
1:A:58:LYS:HA	1:A:91:ASP:OD1	2.17	0.44
2:H:26:G:H2'	2:H:27:G:C8	2.51	0.44
1:B:284:LEU:HD12	2:F:12:C:H4'	1.99	0.44
1:B:397:LYS:O	1:B:401:ARG:HD2	2.18	0.44
1:D:61:LEU:HD11	1:D:63:ILE:HD11	1.98	0.44
1:D:216:ARG:HD3	1:D:220:HIS:CB	2.48	0.44
1:D:268:ARG:HG3	1:D:268:ARG:NH1	2.32	0.44
1:C:46:LEU:HD13	1:C:278:MET:CE	2.46	0.44
1:A:166:LYS:HZ3	1:A:180:ASP:HB2	1.82	0.44
1:D:299:LYS:O	1:D:303:PHE:HB2	2.17	0.44
1:C:255:LEU:HD21	1:C:262:THR:HG21	1.99	0.44
1:C:363:LEU:CD1	1:C:376:LEU:HD21	2.47	0.44
1:A:62:ARG:HH22	1:A:206:ASP:CG	2.21	0.44
1:A:340:PHE:CD1	1:A:376:LEU:HD23	2.52	0.44
2:G:41:C:H2'	2:G:42:G:H8	1.80	0.44
1:B:426:ILE:HD13	1:B:465:ILE:HG22	2.00	0.44
1:D:316:ASP:HB3	1:D:319:LYS:HB3	1.99	0.44
1:C:59:PHE:CD2	1:C:90:TRP:HA	2.53	0.44
1:C:457:VAL:HG11	2:G:37:G:C5	2.52	0.44
2:F:39:U:N3	2:F:40:C:N4	2.65	0.44
2:G:68:U:H2'	2:G:69:C:H6	1.79	0.44
1:B:172:LEU:HB3	1:B:242:MET:CB	2.43	0.44
1:D:105:GLN:O	1:D:106:SER:HB3	2.18	0.44
1:D:146:PRO:HA	1:D:148:GLU:OE2	2.18	0.44
1:D:148:GLU:O	1:D:151:GLU:HB3	2.18	0.44
1:A:300:LEU:C	1:A:302:SER:H	2.20	0.44
1:A:305:PRO:O	1:A:308:ILE:HG22	2.17	0.44
1:B:250:SER:C	1:B:252:ARG:H	2.21	0.44
1:D:83:LEU:HD23	1:D:83:LEU:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ARG:O	1:C:117:GLU:HG2	2.18	0.44
1:C:471:GLU:C	1:C:473:THR:H	2.21	0.44
1:A:84:ARG:HD3	1:A:84:ARG:C	2.38	0.44
1:A:204:VAL:O	1:A:207:HIS:HB3	2.17	0.44
1:A:395:VAL:HG13	1:A:399:LEU:HB3	1.99	0.44
1:D:180:ASP:OD2	1:D:182:SER:HB2	2.18	0.44
1:A:256:SER:C	1:A:258:ARG:H	2.20	0.44
2:E:10:G:H2'	2:E:11:U:C6	2.53	0.44
1:B:24:LEU:O	1:B:212:SER:HB3	2.18	0.44
1:B:35:GLY:H	1:B:75:TYR:HB3	1.82	0.44
1:B:47:PHE:CE1	1:B:308:ILE:HD11	2.53	0.44
1:D:78:GLN:HA	1:D:81:GLU:OE1	2.17	0.44
1:D:357:ARG:HG2	1:D:357:ARG:HH11	1.82	0.44
1:C:304:ASP:OD1	1:C:306:LYS:HB2	2.18	0.44
1:A:244:ILE:HG23	1:A:308:ILE:HD11	1.99	0.44
1:A:273:LEU:H	1:A:273:LEU:CD1	2.30	0.44
2:H:67:C:H2'	2:H:68:U:C6	2.53	0.44
1:C:100:PHE:CE1	1:C:210:ARG:HD3	2.53	0.43
1:C:262:THR:HG22	1:C:262:THR:O	2.18	0.43
1:C:279:ASN:ND2	1:C:323:VAL:HG11	2.33	0.43
2:E:8:U:H5'	2:E:49:G:OP2	2.18	0.43
1:B:434:SER:CB	1:B:441:LYS:HA	2.42	0.43
1:C:398:PHE:HD2	1:C:446:GLN:HB3	1.82	0.43
1:A:67:ASP:HB2	2:E:76:A:H5'	2.00	0.43
1:A:310:ASN:HD22	2:E:6:G:H5''	1.83	0.43
1:A:464:THR:O	1:A:468:LEU:HG	2.18	0.43
2:E:51:A:H2'	2:E:52:G:O4'	2.18	0.43
1:B:224:THR:HB	1:B:225:PRO:HD3	1.99	0.43
1:B:308:ILE:HG22	1:B:309:SER:N	2.33	0.43
1:B:445:PHE:HD1	1:B:461:LEU:HD23	1.82	0.43
1:B:484:LEU:HD13	1:B:484:LEU:C	2.39	0.43
1:C:149:TYR:O	1:C:154:HIS:HB2	2.18	0.43
1:C:355:ASP:HB3	1:C:358:TYR:CB	2.48	0.43
1:A:65:ASP:HA	1:A:71:SER:OG	2.18	0.43
2:E:63:U:O2'	2:E:64:C:H5'	2.19	0.43
1:B:171:ASP:OD1	1:B:242:MET:HA	2.19	0.43
1:B:306:LYS:HD3	1:B:306:LYS:N	2.32	0.43
1:B:385:ASN:N	1:B:385:ASN:HD22	2.15	0.43
1:D:61:LEU:HD13	1:D:61:LEU:C	2.39	0.43
2:G:42:G:H2'	2:G:43:C:H6	1.83	0.43
2:G:67:C:H2'	2:G:68:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:TYR:CD2	2:F:74:C:N4	2.87	0.43
1:B:366:CYS:SG	1:B:380:MET:HG2	2.58	0.43
1:B:388:TYR:O	1:B:479:ARG:NH2	2.51	0.43
1:C:375:GLN:O	1:C:379:ILE:HG22	2.18	0.43
1:A:60:ILE:HG23	1:A:92:GLU:HB2	2.00	0.43
1:A:288:VAL:HG11	1:A:292:GLU:HA	2.00	0.43
2:G:63:U:H2'	2:G:64:C:H6	1.83	0.43
2:G:66:C:H2'	2:G:67:C:H6	1.83	0.43
1:B:158:ILE:O	1:B:189:ILE:HG12	2.19	0.43
1:B:472:ARG:HA	1:B:475:LYS:CE	2.43	0.43
1:D:324:ASN:O	1:D:328:MET:HG3	2.18	0.43
2:G:24:A:N6	2:G:45:G:N2	2.65	0.43
1:B:122:ASP:HB2	1:B:124:ARG:HG3	1.99	0.43
1:B:448:ILE:HG21	1:B:465:ILE:HD11	2.00	0.43
1:D:37:LEU:HB3	1:D:264:VAL:HG22	2.01	0.43
1:D:65:ASP:HB2	1:D:71:SER:HB3	2.01	0.43
1:D:415:PHE:CZ	1:D:430:LEU:HD11	2.54	0.43
1:D:461:LEU:O	1:D:465:ILE:HG13	2.18	0.43
1:C:112:TYR:CG	1:C:196:PRO:HG3	2.53	0.43
1:C:179:PHE:CD2	1:C:225:PRO:HG3	2.54	0.43
1:C:234:PHE:HB3	1:C:236:TRP:CE2	2.54	0.43
1:A:288:VAL:HG22	1:A:290:GLY:N	2.26	0.43
1:B:422:ASN:O	1:B:426:ILE:HG13	2.19	0.43
1:D:343:TRP:CH2	1:D:349:LYS:HE3	2.54	0.43
1:C:28:ARG:HG2	1:C:28:ARG:HH11	1.83	0.43
2:G:63:U:O2'	2:G:64:C:H5'	2.19	0.43
1:B:242:MET:HE2	1:B:244:ILE:HG23	2.00	0.43
1:B:255:LEU:N	3:B:1001:GSU:HN61	2.17	0.43
1:B:322:TRP:CE2	2:F:25:C:H5"	2.54	0.43
1:D:118:LYS:HB3	1:D:118:LYS:HZ3	1.82	0.43
1:C:68:THR:HG21	1:C:195:PHE:CE2	2.53	0.43
1:C:473:THR:O	1:C:477:LEU:HG	2.18	0.43
1:A:224:THR:HB	1:A:225:PRO:HD3	2.01	0.43
1:A:228:LEU:O	1:A:232:GLU:HG3	2.19	0.43
1:B:104:ARG:HG3	1:B:104:ARG:NH1	2.34	0.43
1:B:113:ARG:HH22	1:B:194:GLY:CA	2.26	0.43
1:D:414:ALA:O	1:D:418:LEU:HG	2.18	0.43
1:C:393:ASP:OD1	1:A:72:SER:HB2	2.19	0.43
1:A:43:ARG:NH2	1:A:308:ILE:HD11	2.34	0.43
1:A:295:THR:HG22	1:A:297:GLU:H	1.83	0.43
2:H:13:U:H3	2:H:22:G:H1	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ARG:HH11	1:B:331:ILE:HG22	1.84	0.42
1:C:196:PRO:HB2	1:C:200:PHE:HD2	1.83	0.42
1:C:276:ALA:HB1	1:C:324:ASN:HA	2.01	0.42
1:C:431:ARG:HG2	1:C:431:ARG:HH11	1.83	0.42
1:A:379:ILE:HD11	1:A:459:PRO:HG3	2.01	0.42
1:D:273:LEU:HD12	1:D:273:LEU:N	2.35	0.42
1:C:226:LYS:HA	1:C:229:MET:HE3	2.01	0.42
1:C:363:LEU:HA	1:C:380:MET:CE	2.50	0.42
1:D:108:ARG:HA	1:A:164:PRO:CG	2.48	0.42
1:A:62:ARG:HH11	1:A:205:ASP:CB	2.33	0.42
1:A:115:TYR:HB3	1:A:234:PHE:CZ	2.54	0.42
1:A:394:TYR:HA	1:A:456:LEU:HD21	2.02	0.42
1:B:218:GLU:HB2	1:B:244:ILE:O	2.19	0.42
1:A:184:LEU:HD11	1:A:226:LYS:CG	2.49	0.42
1:A:248:LEU:HD22	1:A:252:ARG:C	2.40	0.42
1:D:113:ARG:HG2	1:D:190:MET:CE	2.50	0.42
1:D:118:LYS:HB3	1:D:118:LYS:HZ2	1.84	0.42
1:D:308:ILE:O	1:D:308:ILE:HG13	2.20	0.42
1:C:363:LEU:HA	1:C:380:MET:HE1	2.02	0.42
1:A:224:THR:N	1:A:225:PRO:CD	2.82	0.42
1:A:426:ILE:HD12	1:A:462:PHE:O	2.19	0.42
2:F:2:G:H2'	2:F:3:G:C8	2.54	0.42
2:F:26:G:H2'	2:F:27:G:O4'	2.19	0.42
2:F:67:C:H2'	2:F:68:U:H6	1.83	0.42
1:B:152:LYS:HD2	1:B:152:LYS:N	2.34	0.42
1:B:229:MET:O	1:B:233:ALA:HB2	2.19	0.42
1:C:478:GLU:OE2	1:C:482:GLN:HG2	2.19	0.42
1:A:67:ASP:OD1	1:A:69:GLU:HB2	2.18	0.42
1:A:426:ILE:HD13	1:A:465:ILE:HB	2.00	0.42
2:E:63:U:H2'	2:E:64:C:C6	2.55	0.42
1:B:271:GLY:CA	1:B:373:LEU:HB2	2.50	0.42
1:D:26:ARG:O	1:D:211:ILE:HG23	2.20	0.42
1:D:33:PRO:HA	1:D:79:ILE:CD1	2.50	0.42
1:D:134:ASP:N	1:D:135:PRO:HD3	2.35	0.42
1:D:173:LEU:HD23	1:D:243:HIS:O	2.19	0.42
1:D:321:GLU:HG2	1:D:371:ASN:HB3	2.01	0.42
3:D:1001:GSU:H2	2:H:76:A:C2'	2.32	0.42
1:C:104:ARG:HG3	1:C:104:ARG:NH1	2.34	0.42
1:C:313:VAL:HG11	2:G:13:U:OP1	2.19	0.42
1:C:327:HIS:O	1:C:331:ILE:HG12	2.20	0.42
2:E:5:A:O2'	2:E:6:G:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:HD13	1:B:278:MET:CE	2.48	0.42
1:B:222:SER:O	1:B:225:PRO:HD2	2.19	0.42
1:D:191:LYS:HE3	1:D:195:PHE:HB2	2.00	0.42
1:D:270:GLU:O	1:D:372:THR:HB	2.20	0.42
1:D:275:ARG:HG2	1:D:275:ARG:NH1	2.35	0.42
1:D:340:PHE:CD1	1:D:376:LEU:HD23	2.55	0.42
1:D:430:LEU:HA	1:D:433:LEU:HD12	2.01	0.42
1:C:369:LYS:O	2:G:37:G:H8	2.03	0.42
1:A:113:ARG:CA	1:A:190:MET:HE2	2.50	0.42
2:H:75:C:H2'	2:H:76:A:O4'	2.20	0.42
1:B:274:SER:O	1:B:278:MET:HG2	2.19	0.42
1:B:371:ASN:HD21	2:F:38:A:C5'	2.25	0.42
1:B:421:TRP:CD1	1:B:426:ILE:HD11	2.55	0.42
1:D:118:LYS:HA	1:D:121:GLU:OE1	2.20	0.42
1:D:168:SER:HB2	1:D:177:MET:O	2.20	0.42
1:D:205:ASP:C	1:D:207:HIS:H	2.23	0.42
1:D:215:PHE:HD1	1:D:242:MET:CB	2.32	0.42
1:D:351:ILE:HG12	1:D:377:TYR:OH	2.19	0.42
1:B:253:THR:OG1	1:B:259:HIS:NE2	2.52	0.42
1:B:365:ILE:HD13	1:B:463:GLU:HB3	2.02	0.42
1:B:369:LYS:HZ3	2:F:36:G:H22	1.67	0.42
1:B:485:LYS:N	1:B:485:LYS:CD	2.82	0.42
1:D:123:LYS:HA	1:D:143:TYR:CE1	2.55	0.42
1:D:191:LYS:CE	1:D:195:PHE:HB2	2.50	0.42
1:D:406:ARG:HG2	1:D:406:ARG:HH11	1.85	0.42
1:A:327:HIS:O	1:A:331:ILE:HG12	2.20	0.42
1:B:192:SER:OG	2:F:74:C:N3	2.47	0.41
1:C:43:ARG:HE	1:C:47:PHE:HE2	1.68	0.41
1:C:258:ARG:HG3	1:C:258:ARG:HH11	1.85	0.41
1:C:277:LEU:HA	1:C:320:LEU:HD11	2.01	0.41
1:C:357:ARG:HG2	1:C:357:ARG:NH1	2.34	0.41
1:A:406:ARG:HG2	1:A:406:ARG:HH11	1.86	0.41
1:B:73:ARG:NH1	1:B:73:ARG:CB	2.84	0.41
1:D:279:ASN:HD21	1:D:294:PHE:N	2.08	0.41
1:D:287:ARG:O	1:D:307:ASP:HB3	2.20	0.41
1:D:366:CYS:SG	1:D:380:MET:SD	3.17	0.41
1:C:380:MET:O	1:C:384:MET:HG2	2.19	0.41
1:A:50:MET:O	1:A:54:LYS:HB2	2.19	0.41
1:A:338:ARG:NH1	1:A:338:ARG:CB	2.83	0.41
1:A:357:ARG:NH1	1:A:357:ARG:HB2	2.35	0.41
1:B:62:ARG:HH11	1:B:205:ASP:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:ASN:ND2	1:C:425:GLU:HG2	2.35	0.41
1:A:120:VAL:N	1:A:125:ALA:HB3	2.35	0.41
1:A:401:ARG:HG2	1:A:401:ARG:HH11	1.86	0.41
1:B:322:TRP:O	1:B:326:LYS:HG3	2.20	0.41
1:D:319:LYS:HD3	2:H:25:C:H1'	2.01	0.41
1:D:363:LEU:HD23	1:D:380:MET:SD	2.60	0.41
1:C:122:ASP:O	1:C:124:ARG:HG3	2.19	0.41
1:C:131:ASP:CG	1:C:132:LYS:N	2.73	0.41
1:C:428:LYS:HG2	1:C:432:ASP:OD2	2.20	0.41
1:A:173:LEU:O	1:A:173:LEU:HD23	2.20	0.41
2:H:55:U:H3'	2:H:56:C:H5"	2.00	0.41
2:H:59:G:H2'	2:H:60:U:C5'	2.50	0.41
1:D:120:VAL:HA	1:D:125:ALA:HB3	2.03	0.41
1:D:252:ARG:HD3	1:D:314:ILE:HD11	2.02	0.41
1:D:395:VAL:HG13	1:D:399:LEU:HD23	2.01	0.41
1:C:369:LYS:CD	2:G:36:G:H22	2.34	0.41
2:G:29:G:H2'	2:G:30:G:O4'	2.21	0.41
2:E:26:G:H2'	2:E:27:G:C8	2.56	0.41
1:B:191:LYS:HZ1	2:F:75:C:H5'	1.84	0.41
1:D:228:LEU:HD21	1:D:241:PHE:HE2	1.85	0.41
1:D:286:TRP:HA	1:D:308:ILE:HA	2.01	0.41
1:C:397:LYS:HZ2	1:A:72:SER:HA	1.83	0.41
1:A:113:ARG:HH12	1:A:117:GLU:HG2	1.85	0.41
1:A:117:GLU:C	1:A:119:LEU:N	2.73	0.41
1:A:418:LEU:HD12	1:A:421:TRP:CE3	2.56	0.41
1:B:427:GLU:HG3	1:B:462:PHE:CE1	2.56	0.41
1:D:203:VAL:HG22	1:D:227:GLN:HB3	2.03	0.41
1:D:309:SER:C	1:D:311:LYS:H	2.24	0.41
1:C:66:THR:HB	2:G:76:A:OP1	2.21	0.41
1:C:365:ILE:HG22	1:C:459:PRO:HB3	2.03	0.41
1:C:411:ALA:HB1	1:C:477:LEU:HD13	2.01	0.41
1:A:280:TYR:O	1:A:284:LEU:HG	2.21	0.41
2:F:64:C:O2'	2:F:65:C:H5'	2.20	0.41
1:B:33:PRO:CB	1:B:76:GLU:HB2	2.43	0.41
1:B:167:THR:HG21	1:B:228:LEU:HB2	2.03	0.41
1:B:173:LEU:HD22	1:B:244:ILE:HG22	2.02	0.41
1:A:112:TYR:CG	1:A:196:PRO:HG3	2.55	0.41
1:A:355:ASP:HB3	1:A:358:TYR:CB	2.51	0.41
2:H:62:C:O2'	2:H:63:U:H5'	2.20	0.41
2:E:2:G:H2'	2:E:3:G:C8	2.55	0.41
1:B:64:GLU:OE1	1:B:105:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:HD2	1:B:195:PHE:HB3	2.02	0.41
1:B:368:GLU:O	1:B:369:LYS:HD3	2.20	0.41
1:B:378:ASP:O	1:B:455:LYS:HE2	2.21	0.41
1:B:482:GLN:OE1	1:B:482:GLN:N	2.54	0.41
1:D:28:ARG:HH11	1:D:28:ARG:HG2	1.85	0.41
1:D:74:GLU:OE1	1:D:74:GLU:HA	2.21	0.41
1:D:100:PHE:HD1	1:D:100:PHE:O	2.04	0.41
1:D:114:GLU:OE1	1:A:161:LYS:HE3	2.21	0.41
1:D:124:ARG:HG3	1:D:124:ARG:HH11	1.85	0.41
1:D:214:VAL:CG1	1:D:216:ARG:HE	2.33	0.41
1:D:218:GLU:HB2	1:D:244:ILE:O	2.21	0.41
1:D:294:PHE:HD1	1:D:295:THR:N	2.19	0.41
1:C:167:THR:HG21	1:C:225:PRO:HA	2.03	0.41
1:C:457:VAL:HG11	2:G:37:G:C6	2.55	0.41
1:C:468:LEU:HD13	1:C:472:ARG:O	2.21	0.41
1:A:102:PRO:HB2	1:A:107:GLU:OE1	2.20	0.41
1:A:216:ARG:HH12	1:A:227:GLN:HE22	1.69	0.41
1:A:460:GLY:O	1:A:461:LEU:HB2	2.20	0.41
2:F:63:U:H2'	2:F:64:C:C6	2.56	0.41
2:H:36:G:O2'	2:H:37:G:C5'	2.68	0.41
1:D:168:SER:HB3	1:D:178:GLU:HG3	2.02	0.41
1:C:363:LEU:HD11	1:C:376:LEU:HD21	2.02	0.41
1:A:94:PRO:HA	1:A:103:TYR:HB2	2.02	0.41
1:A:327:HIS:HA	1:A:330:ARG:HB3	2.03	0.41
1:A:357:ARG:NH1	1:A:357:ARG:CB	2.84	0.41
2:F:2:G:H2'	2:F:3:G:H8	1.85	0.41
1:C:100:PHE:CZ	1:C:210:ARG:HD3	2.55	0.40
1:C:112:TYR:CB	1:C:196:PRO:HG3	2.51	0.40
1:C:158:ILE:HD12	1:C:190:MET:HG3	2.02	0.40
1:A:47:PHE:CZ	1:A:305:PRO:HA	2.56	0.40
1:A:364:ARG:HG2	1:A:364:ARG:HH11	1.85	0.40
2:E:1:U:H2'	2:E:2:G:C5'	2.51	0.40
1:B:288:VAL:HG21	1:B:291:ASP:O	2.21	0.40
1:B:403:GLU:H	1:B:403:GLU:CD	2.23	0.40
1:D:223:ASN:HD21	2:H:76:A:H61	1.69	0.40
1:D:390:TYR:CD1	1:D:390:TYR:N	2.90	0.40
1:C:130:TYR:CD1	1:C:138:GLU:HA	2.56	0.40
1:A:297:GLU:O	1:A:299:LYS:N	2.54	0.40
1:A:358:TYR:O	1:A:362:THR:HG23	2.21	0.40
1:A:412:LYS:O	1:A:416:LYS:HB2	2.20	0.40
2:F:34:C:O2'	2:F:35:U:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:20:U:OP1	2:H:20:U:H3'	2.22	0.40
2:G:57:G:H2'	2:G:58:A:H5'	2.02	0.40
2:E:26:G:H22	2:E:44:U:H3	1.69	0.40
1:B:413:LYS:HA	1:B:416:LYS:NZ	2.35	0.40
1:D:30:ALA:HB2	1:D:62:ARG:HH21	1.87	0.40
1:D:128:VAL:HG22	1:D:159:LYS:HZ2	1.85	0.40
1:D:269:ARG:HH11	1:D:269:ARG:HG3	1.86	0.40
1:D:398:PHE:HB3	1:D:447:LEU:HD23	2.02	0.40
1:D:415:PHE:HZ	1:D:430:LEU:HD11	1.87	0.40
1:C:28:ARG:HG2	1:C:28:ARG:NH1	2.37	0.40
1:C:214:VAL:HG23	1:C:239:PRO:HB2	2.03	0.40
1:A:92:GLU:HB3	1:A:103:TYR:CZ	2.57	0.40
1:A:120:VAL:HA	1:A:125:ALA:HB3	2.03	0.40
1:A:363:LEU:CD2	1:A:376:LEU:HD21	2.52	0.40
2:H:71:C:H2'	2:H:72:A:C5'	2.51	0.40
2:G:53:G:H2'	2:G:54:U:H6	1.86	0.40
1:B:59:PHE:C	1:B:60:ILE:HD12	2.41	0.40
1:B:198:TYR:CD1	1:B:199:ASN:N	2.90	0.40
1:B:382:PRO:O	1:B:476:ARG:NH2	2.55	0.40
1:B:474:LEU:HA	1:B:477:LEU:HD12	2.03	0.40
1:D:391:GLU:O	1:D:395:VAL:HG23	2.22	0.40
1:C:26:ARG:HB3	1:C:211:ILE:HA	2.04	0.40
1:C:250:SER:H	1:C:259:HIS:HE1	1.66	0.40
1:C:410:GLU:OE2	1:C:414:ALA:HB2	2.22	0.40
1:A:124:ARG:HA	1:A:161:LYS:HZ2	1.86	0.40
1:A:162:VAL:HG13	1:A:181:ASN:HD22	1.86	0.40
2:F:72:A:P	2:F:75:C:H41	2.44	0.40
2:H:1:U:H2'	2:H:2:G:H5"	2.04	0.40
2:E:33:U:OP1	2:E:34:C:H3'	2.21	0.40
1:B:38:HIS:HA	1:B:263:SER:HA	2.03	0.40
1:B:168:SER:HB3	1:B:178:GLU:HA	2.02	0.40
1:B:352:PRO:CG	1:B:385:ASN:HD21	2.33	0.40
1:C:62:ARG:HD3	1:C:209:MET:SD	2.62	0.40
1:C:238:ALA:HA	1:C:239:PRO:HD3	1.83	0.40
1:C:397:LYS:HZ1	1:A:72:SER:HA	1.86	0.40
1:A:129:VAL:HA	1:A:155:PRO:O	2.21	0.40
1:A:196:PRO:CG	1:A:201:ALA:HB2	2.50	0.40
1:A:351:ILE:O	1:A:351:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	461/487 (95%)	394 (86%)	55 (12%)	12 (3%)	5	20
1	B	461/487 (95%)	375 (81%)	77 (17%)	9 (2%)	7	27
1	C	461/487 (95%)	367 (80%)	80 (17%)	14 (3%)	4	17
1	D	461/487 (95%)	375 (81%)	74 (16%)	12 (3%)	5	20
All	All	1844/1948 (95%)	1511 (82%)	286 (16%)	47 (2%)	5	21

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	106	SER
1	C	122	ASP
1	A	261	ALA
1	A	461	LEU
1	B	217	GLY
1	D	439	ALA
1	C	210	ARG
1	C	313	VAL
1	C	397	LYS
1	A	285	GLY
1	A	298	GLU
1	A	397	LYS
1	B	197	THR
1	B	308	ILE
1	D	92	GLU
1	C	300	LEU
1	C	303	PHE
1	A	262	THR
1	D	55	GLU
1	D	153	GLY
1	D	161	LYS
1	D	459	PRO

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Mol	Chain	Res	Type
1	C	83	LEU
1	C	352	PRO
1	C	472	ARG
1	A	33	PRO
1	B	105	GLN
1	B	257	LYS
1	B	298	GLU
1	B	352	PRO
1	D	95	ASP
1	D	100	PHE
1	C	254	PRO
1	C	299	LYS
1	D	97	GLY
1	D	305	PRO
1	C	459	PRO
1	A	260	GLY
1	A	443	VAL
1	D	469	GLY
1	C	111	ILE
1	B	459	PRO
1	B	31	PRO
1	C	202	VAL
1	A	153	GLY
1	A	459	PRO
1	A	444	VAL

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	415/436 (95%)	406 (98%)	9 (2%)	52	81
1	B	415/436 (95%)	408 (98%)	7 (2%)	60	86
1	C	415/436 (95%)	410 (99%)	5 (1%)	71	91
1	D	415/436 (95%)	408 (98%)	7 (2%)	60	86
All	All	1660/1744 (95%)	1632 (98%)	28 (2%)	60	86

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	28	ARG
1	B	145	TYR
1	B	186	ASP
1	B	195	PHE
1	B	206	ASP
1	B	330	ARG
1	B	482	GLN
1	D	28	ARG
1	D	55	GLU
1	D	100	PHE
1	D	148	GLU
1	D	206	ASP
1	D	267	PHE
1	D	346	TYR
1	C	28	ARG
1	C	148	GLU
1	C	265	GLU
1	C	307	ASP
1	C	349	LYS
1	A	28	ARG
1	A	65	ASP
1	A	139	LEU
1	A	186	ASP
1	A	275	ARG
1	A	287	ARG
1	A	301	GLN
1	A	403	GLU
1	A	471	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	HIS
1	B	48	ASN
1	B	199	ASN
1	B	223	ASN
1	B	279	ASN
1	B	375	GLN
1	B	385	ASN
1	D	105	GLN
1	D	223	ASN

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Mol	Chain	Res	Type
1	D	227	GLN
1	D	259	HIS
1	D	279	ASN
1	D	301	GLN
1	D	318	GLN
1	D	385	ASN
1	C	199	ASN
1	C	279	ASN
1	C	310	ASN
1	A	38	HIS
1	A	199	ASN
1	A	227	GLN
1	A	301	GLN
1	A	318	GLN
1	A	482	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	73/74 (98%)	15 (20%)	0
2	F	73/74 (98%)	12 (16%)	0
2	G	73/74 (98%)	13 (17%)	0
2	H	73/74 (98%)	14 (19%)	0
All	All	292/296 (98%)	54 (18%)	0

All (54) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	2	G
2	F	9	C
2	F	16	C
2	F	18	G
2	F	33	U
2	F	34	C
2	F	37	G
2	F	44	U
2	F	48	U
2	F	52	G
2	F	59	G
2	F	72	A
2	H	2	G

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Mol	Chain	Res	Type
2	H	9	C
2	H	16	C
2	H	18	G
2	H	33	U
2	H	34	C
2	H	37	G
2	H	44	U
2	H	48	U
2	H	56	C
2	H	57	G
2	H	58	A
2	H	61	C
2	H	72	A
2	G	2	G
2	G	9	C
2	G	16	C
2	G	18	G
2	G	19	G
2	G	20	U
2	G	33	U
2	G	34	C
2	G	37	G
2	G	52	G
2	G	59	G
2	G	61	C
2	G	72	A
2	E	2	G
2	E	9	C
2	E	16	C
2	E	18	G
2	E	33	U
2	E	34	C
2	E	37	G
2	E	48	U
2	E	56	C
2	E	57	G
2	E	59	G
2	E	61	C
2	E	72	A
2	E	74	C
2	E	75	C

There are no RNA pucker outliers to report.

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	GSU	C	1001	-	31,34,34	1.44	5 (16%)	34,50,50	1.61	5 (14%)
3	GSU	D	1001	-	31,34,34	1.44	5 (16%)	34,50,50	1.61	6 (17%)
3	GSU	B	1001	-	31,34,34	1.44	5 (16%)	34,50,50	1.61	6 (17%)
3	GSU	A	1001	-	31,34,34	1.41	5 (16%)	34,50,50	1.62	5 (14%)

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	GSU	C	1001	-	-	9/19/40/40	0/3/3/3
3	GSU	D	1001	-	-	7/19/40/40	0/3/3/3
3	GSU	B	1001	-	-	2/19/40/40	0/3/3/3
3	GSU	A	1001	-	-	6/19/40/40	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	GSU	S-N10	4.50	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	GSU	S-N10	4.33	1.67	1.59
3	D	1001	GSU	S-N10	4.25	1.67	1.59
3	D	1001	GSU	O4'-C1'	4.18	1.46	1.41
3	C	1001	GSU	O4'-C1'	4.16	1.46	1.41
3	A	1001	GSU	S-N10	4.15	1.67	1.59
3	B	1001	GSU	O4'-C1'	4.09	1.46	1.41
3	A	1001	GSU	O4'-C1'	4.05	1.46	1.41
3	D	1001	GSU	OE1-CD	-2.69	1.21	1.30
3	C	1001	GSU	OE1-CD	-2.67	1.21	1.30
3	B	1001	GSU	OE1-CD	-2.61	1.21	1.30
3	A	1001	GSU	OE1-CD	-2.57	1.22	1.30
3	C	1001	GSU	O5'-S	-2.40	1.54	1.59
3	D	1001	GSU	O5'-S	-2.38	1.54	1.59
3	A	1001	GSU	O5'-S	-2.37	1.54	1.59
3	B	1001	GSU	O5'-S	-2.34	1.54	1.59
3	D	1001	GSU	C8-N7	-2.24	1.30	1.34
3	B	1001	GSU	C8-N7	-2.21	1.30	1.34
3	C	1001	GSU	C8-N7	-2.20	1.30	1.34
3	A	1001	GSU	C8-N7	-2.18	1.30	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	GSU	N3-C2-N1	-4.68	121.37	128.68
3	D	1001	GSU	N3-C2-N1	-4.67	121.39	128.68
3	B	1001	GSU	N3-C2-N1	-4.65	121.41	128.68
3	C	1001	GSU	N3-C2-N1	-4.56	121.54	128.68
3	D	1001	GSU	C5'-O5'-S	-3.85	109.43	117.37
3	C	1001	GSU	C5'-O5'-S	-3.76	109.62	117.37
3	A	1001	GSU	C5'-O5'-S	-3.75	109.62	117.37
3	B	1001	GSU	C5'-O5'-S	-3.74	109.65	117.37
3	C	1001	GSU	C3'-C2'-C1'	2.90	105.34	100.98
3	B	1001	GSU	C3'-C2'-C1'	2.89	105.34	100.98
3	A	1001	GSU	C3'-C2'-C1'	2.87	105.30	100.98
3	D	1001	GSU	C3'-C2'-C1'	2.86	105.28	100.98
3	B	1001	GSU	O2S-S-O1S	2.22	124.21	120.76
3	A	1001	GSU	O2S-S-O1S	2.22	124.21	120.76
3	C	1001	GSU	O2S-S-O1S	2.21	124.20	120.76
3	D	1001	GSU	O2S-S-O1S	2.15	124.10	120.76
3	A	1001	GSU	C4-C5-N7	-2.11	107.20	109.40
3	D	1001	GSU	C4-C5-N7	-2.09	107.23	109.40
3	C	1001	GSU	C4-C5-N7	-2.08	107.23	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1001	GSU	C4-C5-N7	-2.04	107.28	109.40
3	B	1001	GSU	OE1-CD-CG	2.00	120.47	114.03
3	D	1001	GSU	O5'-C5'-C4'	2.00	111.36	107.62

There are no chirality outliers.
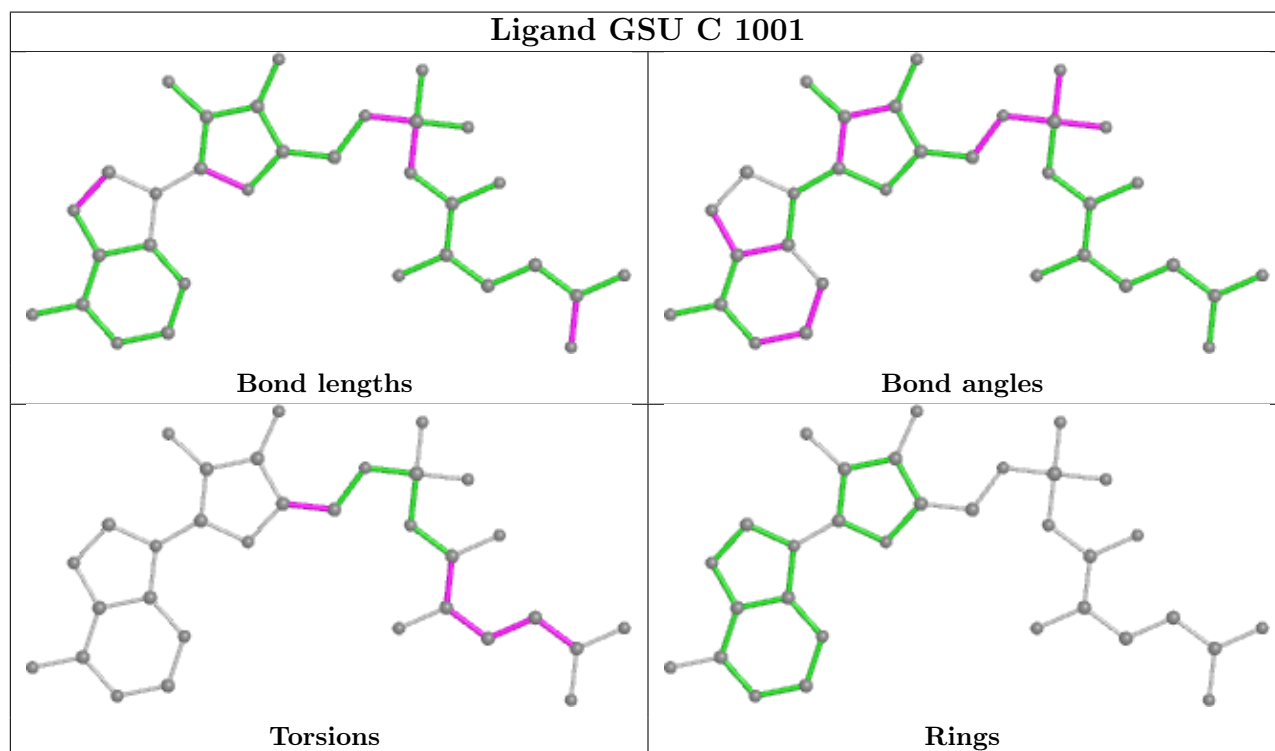
All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1001	GSU	N-CA-CB-CG
3	D	1001	GSU	C-CA-CB-CG
3	C	1001	GSU	N-CA-CB-CG
3	C	1001	GSU	C-CA-CB-CG
3	A	1001	GSU	N-CA-CB-CG
3	A	1001	GSU	C-CA-CB-CG
3	D	1001	GSU	N10-C-CA-N
3	C	1001	GSU	O-C-CA-N
3	C	1001	GSU	N10-C-CA-N
3	A	1001	GSU	N10-C-CA-N
3	C	1001	GSU	C3'-C4'-C5'-O5'
3	D	1001	GSU	O-C-CA-N
3	A	1001	GSU	O-C-CA-N
3	C	1001	GSU	CA-CB-CG-CD
3	B	1001	GSU	OE2-CD-CG-CB
3	B	1001	GSU	OE1-CD-CG-CB
3	D	1001	GSU	OE1-CD-CG-CB
3	D	1001	GSU	OE2-CD-CG-CB
3	A	1001	GSU	OE1-CD-CG-CB
3	C	1001	GSU	OE1-CD-CG-CB
3	C	1001	GSU	OE2-CD-CG-CB
3	D	1001	GSU	CA-CB-CG-CD
3	A	1001	GSU	OE2-CD-CG-CB
3	C	1001	GSU	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	GSU	2	0
3	D	1001	GSU	1	0
3	B	1001	GSU	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 GSU C 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand GSU D 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand GSU B 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand GSU A 1001

Bond lengths

Bond angles

Torsions

Rings
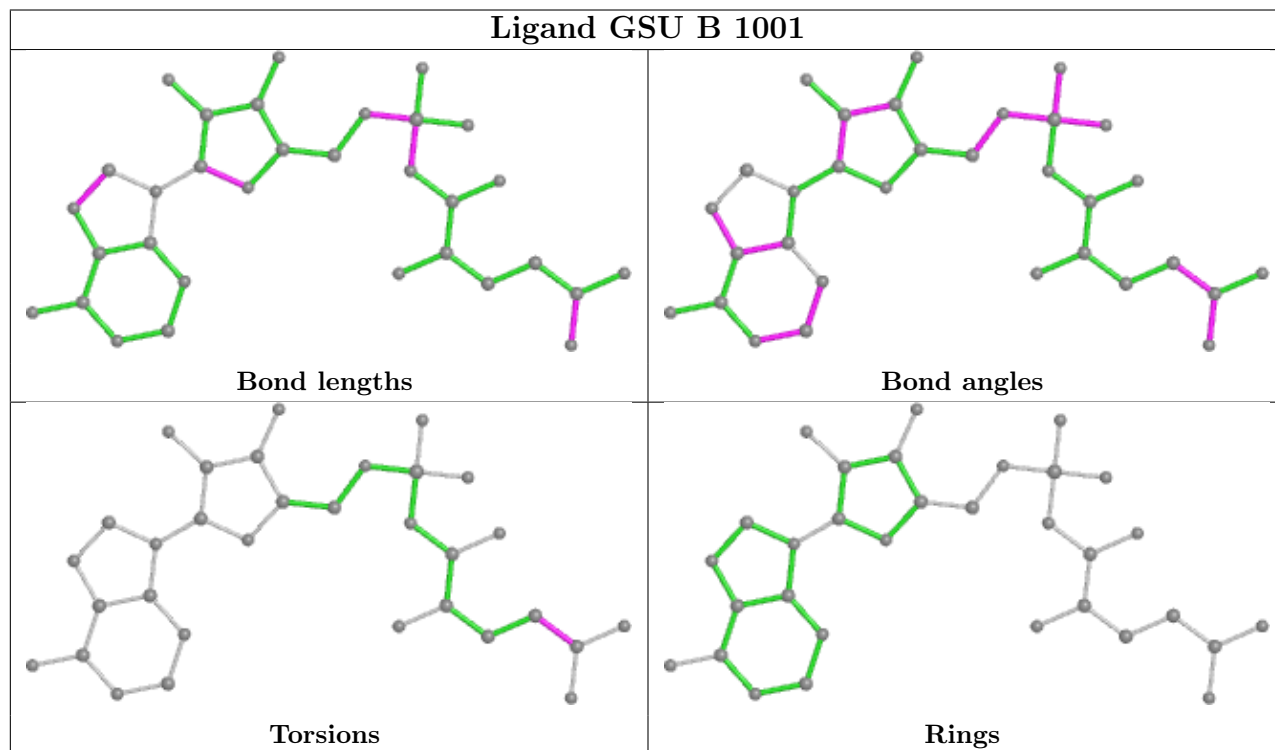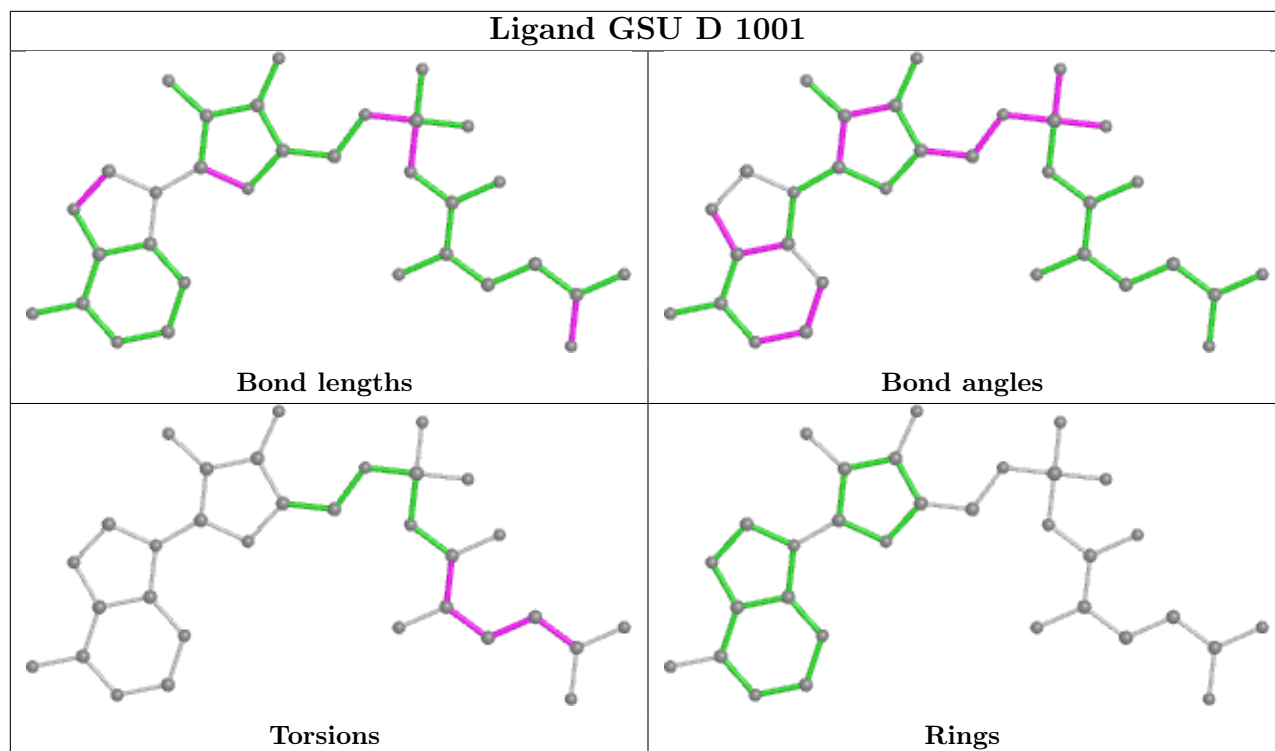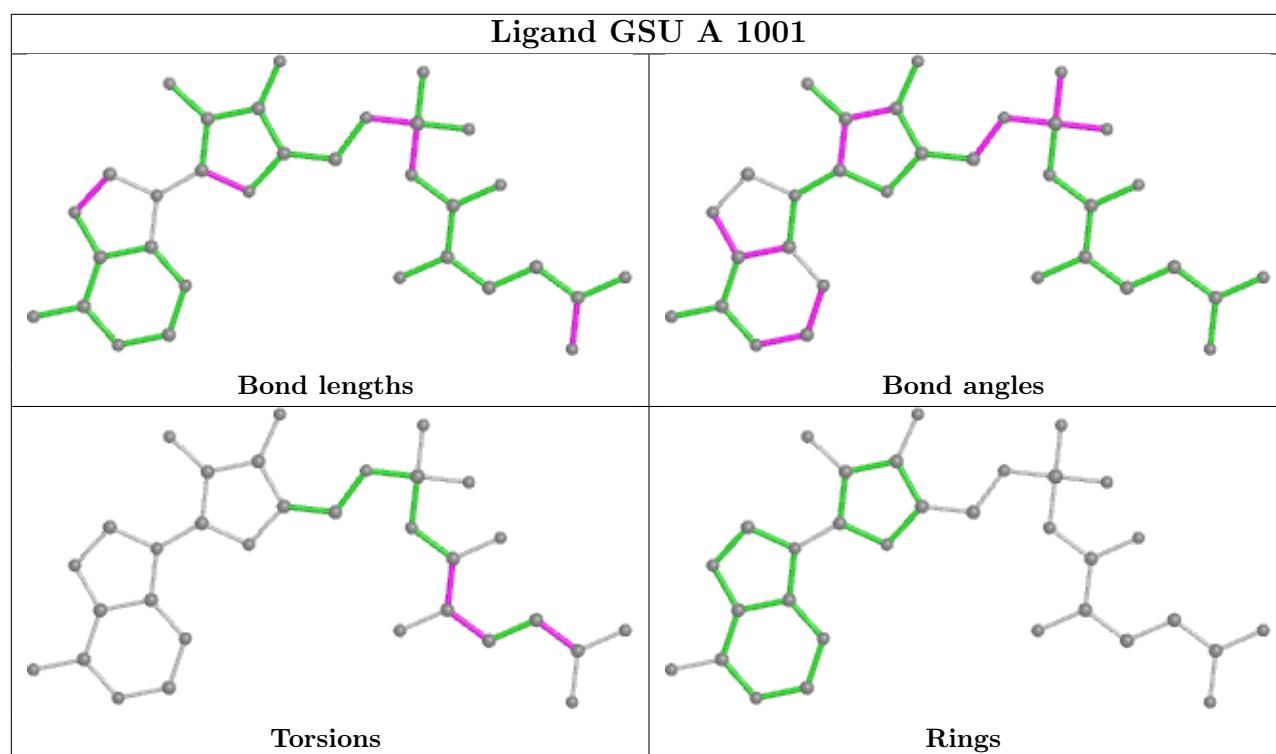
5.7 Other polymers ⓘ

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, 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	463/487 (95%)	0.13	7 (1%)	73	73	13, 41, 66, 86	0
1	B	463/487 (95%)	0.13	6 (1%)	77	77	15, 41, 65, 90	0
1	C	463/487 (95%)	0.37	25 (5%)	25	22	15, 48, 82, 100	0
1	D	463/487 (95%)	0.36	15 (3%)	47	43	18, 52, 80, 95	0
2	E	74/74 (100%)	0.08	1 (1%)	75	75	17, 37, 75, 97	0
2	F	74/74 (100%)	0.10	0	100	100	24, 44, 69, 74	0
2	G	74/74 (100%)	0.25	0	100	100	29, 53, 92, 101	0
2	H	74/74 (100%)	0.21	0	100	100	27, 56, 87, 92	0
All	All	2148/2244 (95%)	0.24	54 (2%)	57	55	13, 45, 80, 101	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	431	ARG	4.2
1	D	90	TRP	4.0
1	A	288	VAL	3.8
1	C	438	LEU	3.7
1	C	390	TYR	3.5
1	C	408	LEU	3.4
1	C	430	LEU	3.4
1	C	426	ILE	3.3
1	C	398	PHE	3.3
1	D	129	VAL	3.2
1	B	288	VAL	3.2
1	D	127	TYR	3.2
1	C	71	SER	3.2
1	C	484	LEU	3.1
1	D	353	SER	3.0
1	C	336	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	448	ILE	2.8
1	D	131	ASP	2.7
1	C	208	LEU	2.7
1	C	395	VAL	2.7
1	A	408	LEU	2.7
1	D	147	HIS	2.6
1	B	129	VAL	2.6
1	C	290	GLY	2.5
1	D	288	VAL	2.4
2	E	74	C	2.4
1	D	91	ASP	2.4
1	A	287	ARG	2.4
1	B	132	LYS	2.4
1	C	255	LEU	2.4
1	C	302	SER	2.4
1	D	83	LEU	2.3
1	C	257	LYS	2.3
1	A	286	TRP	2.3
1	D	421	TRP	2.3
1	C	433	LEU	2.3
1	C	256	SER	2.2
1	A	293	ILE	2.2
1	C	258	ARG	2.2
1	D	128	VAL	2.2
1	A	260	GLY	2.1
1	C	383	PHE	2.1
1	D	426	ILE	2.1
1	D	333	LEU	2.1
1	C	134	ASP	2.1
1	B	480	THR	2.1
1	D	140	PHE	2.1
1	B	136	SER	2.1
1	C	332	ASP	2.1
1	B	354	VAL	2.1
1	C	361	GLU	2.1
1	A	444	VAL	2.0
1	D	415	PHE	2.0
1	C	351	ILE	2.0

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GSU	C	1001	32/32	0.93	0.23	31,39,51,52	0
3	GSU	B	1001	32/32	0.95	0.20	7,36,38,39	0
3	GSU	D	1001	32/32	0.96	0.22	34,39,44,44	0
3	GSU	A	1001	32/32	0.96	0.19	30,36,38,40	0

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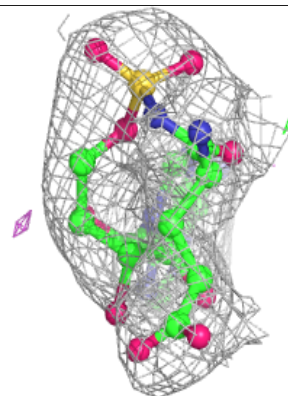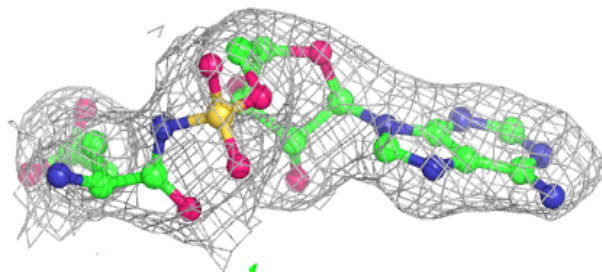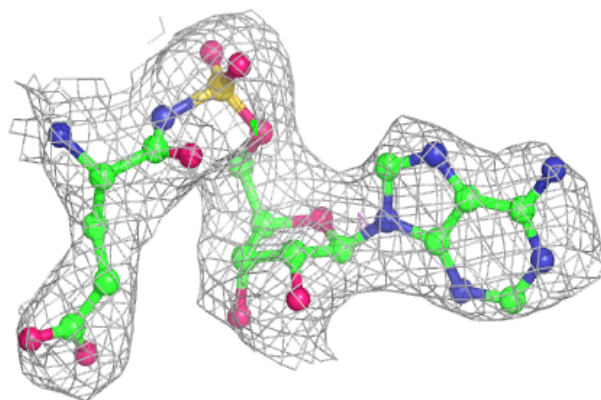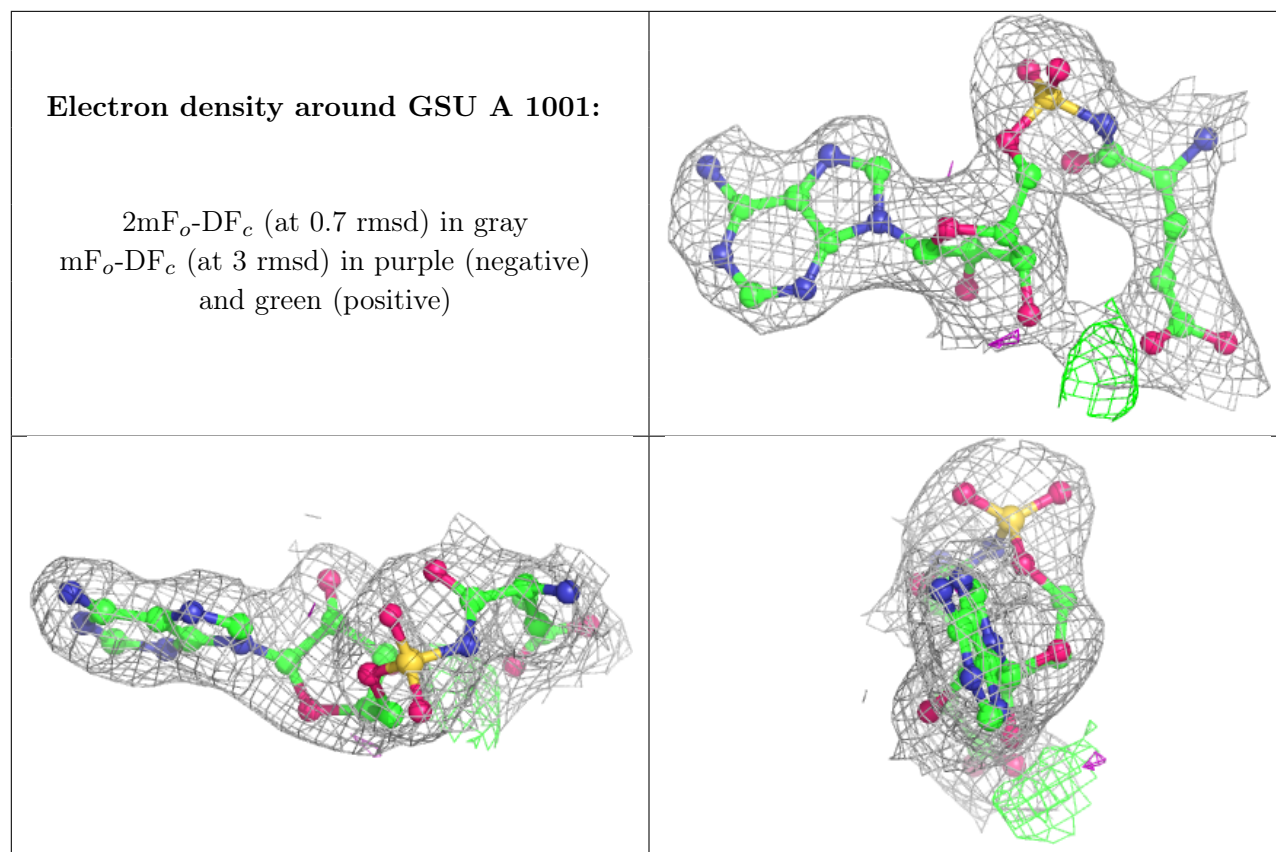

Electron density around GSU C 1001:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)
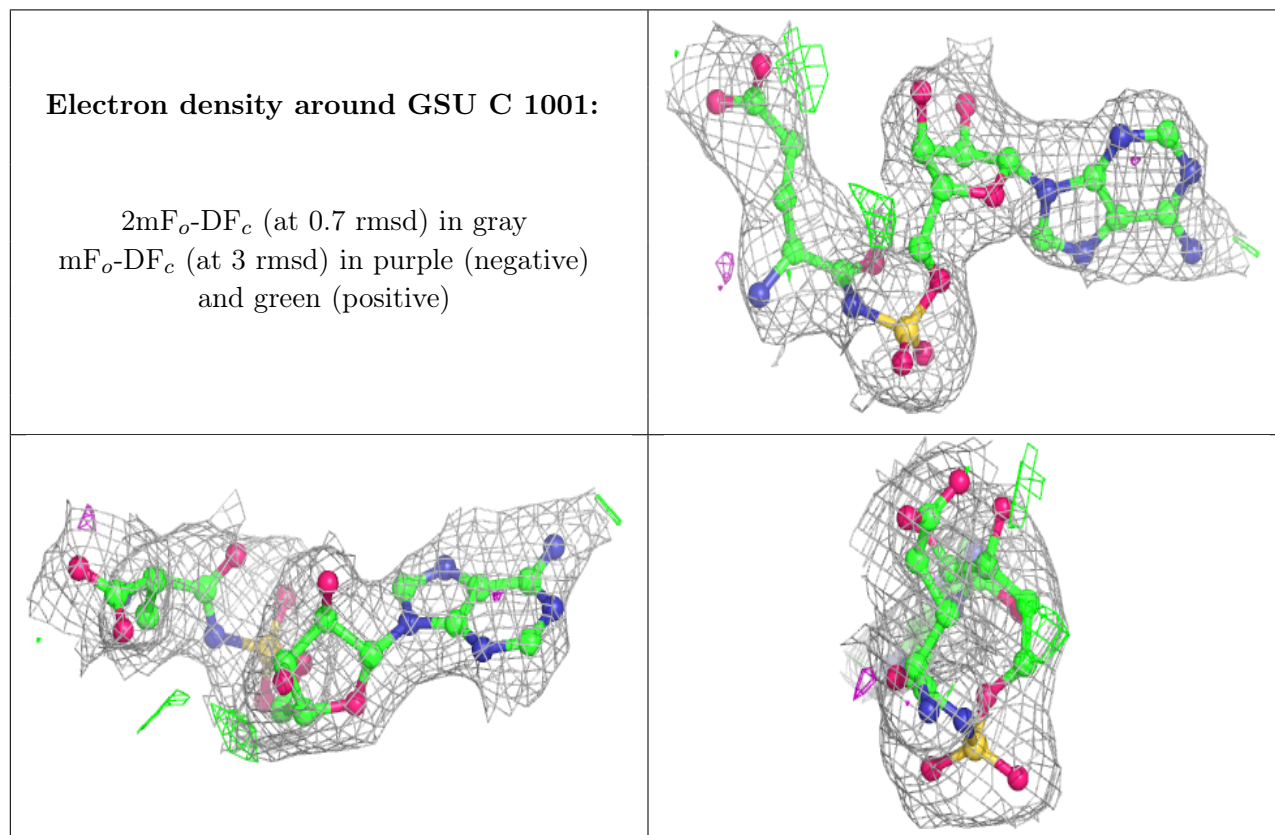
Electron density around GSU B 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
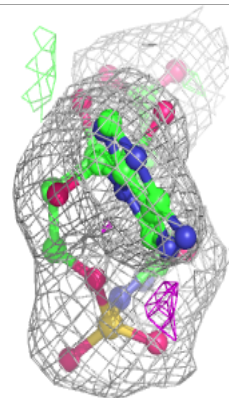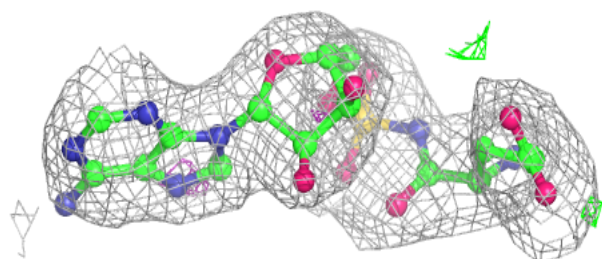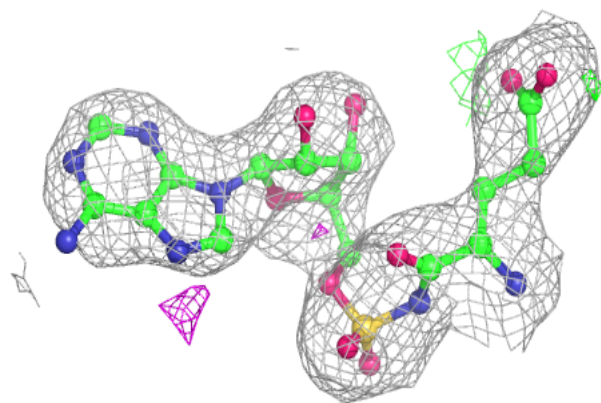
Electron density around GSU D 1001:

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

Electron density around GSU 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 ⓘ

There are no such residues in this entry.