Full wwPDB X-ray Structure Validation Report (i)

Jan 29, 2024 – 05:18 PM EST

PDB ID	:	1EQQ
Title	:	SINGLE STRANDED DNA BINDING PROTEIN AND SSDNA COMPLEX
Authors	:	Matsumoto, T.; Morimoto, Y.; Shibata, N.; Yasuoka, N.; Shimamoto, N.
Deposited on	:	2000-04-06
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

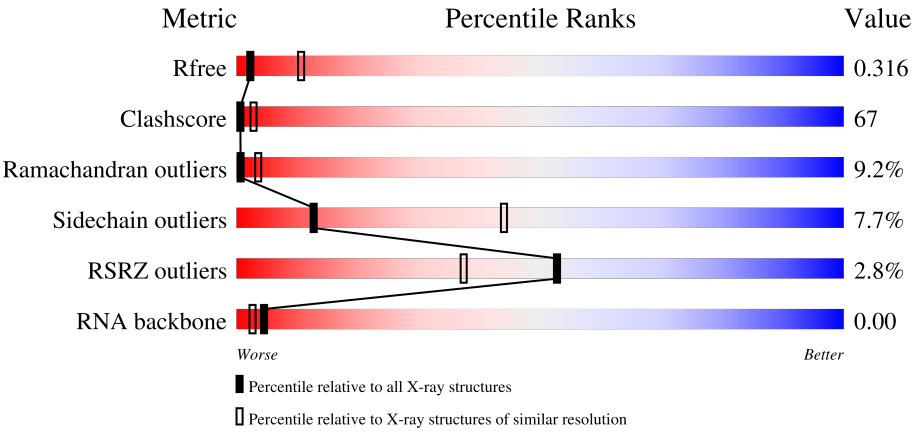
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 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	M	3	33% 67%
1	N	3	33% 67%
2	A	178	3% 16% 40% 7% • 36%
2	B	178	% 18% 43% 6% • 33%

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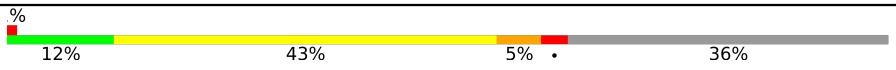
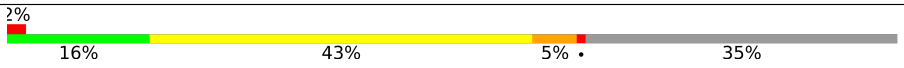
Mol	Chain	Length	Quality of chain
2	C	178	
2	D	178	

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
1	5MU	M	802	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3737 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 5'-R(*(5MU)P*(5MU)P*(5MU))-3'.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	M	3	Total C N O P 60 30 6 22 2	0	0	0
1	N	1	Total C N O 18 10 2 6	0	0	0

- Molecule 2 is a protein called SINGLE STRANDED DNA BINDING PROTEIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	A	114	Total C N O S 884 548 161 171 4	0	0	0
2	B	120	Total C N O S 921 568 171 178 4	0	0	0
2	C	114	Total C N O S 884 548 161 171 4	0	0	0
2	D	116	Total C N O S 904 559 167 174 4	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	1	Total O 1 1	0	0
3	A	20	Total O 20 20	0	0
3	B	15	Total O 15 15	0	0
3	C	17	Total O 17 17	0	0
3	D	13	Total O 13 13	0	0

3 Residue-property plots (i)

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

• Molecule 1: 5'-R(*(5MU)P*(5MU)P*(5MU))-3'

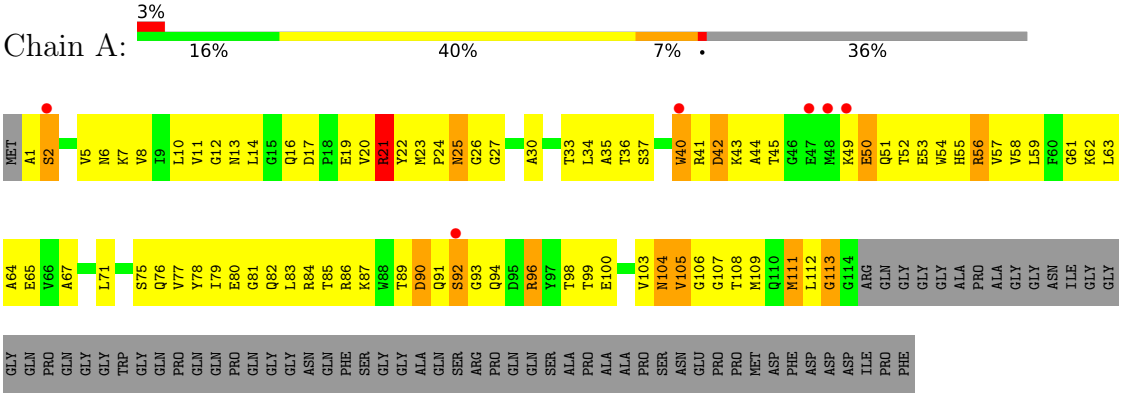
Chain M:

• Molecule 1: 5'-R(*(5MU)P*(5MU)P*(5MU))-3'

Chain N:

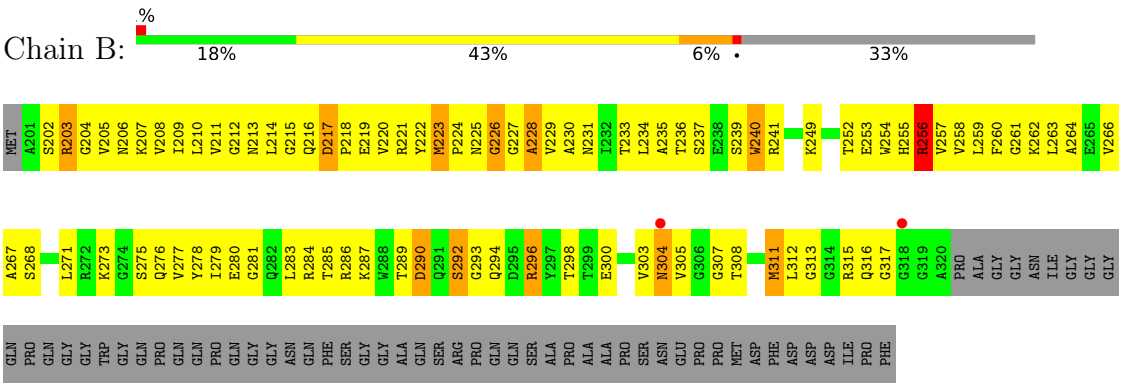
• Molecule 2: SINGLE STRANDED DNA BINDING PROTEIN

Chain A:



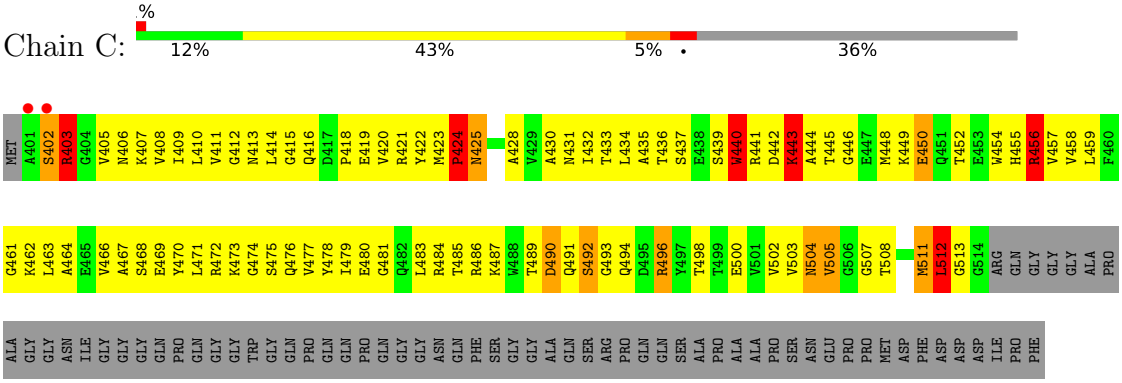
• Molecule 2: SINGLE STRANDED DNA BINDING PROTEIN

Chain B:



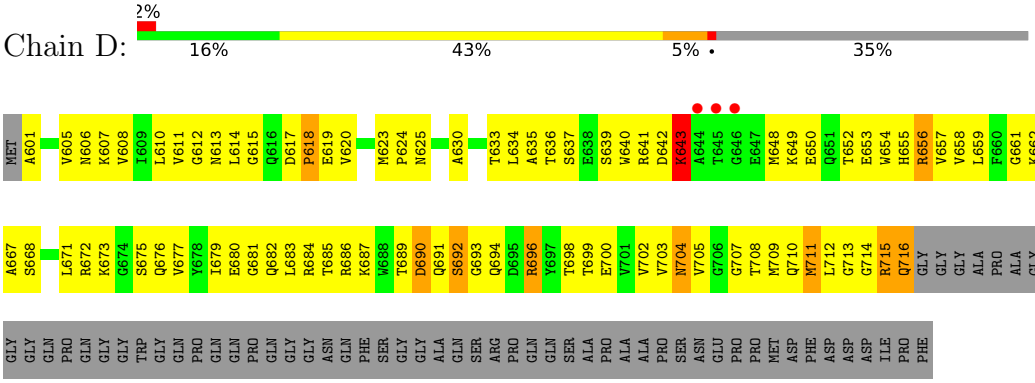
• Molecule 2: SINGLE STRANDED DNA BINDING PROTEIN

Chain C:



• Molecule 2: SINGLE STRANDED DNA BINDING PROTEIN

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.71Å 60.47Å 94.73Å 90.00° 112.60° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 14.89 – 3.20	Depositor EDS
% Data completeness (in resolution range)	82.5 (15.00-3.20) 82.5 (14.89-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	30.25 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.339 0.235 , 0.316	Depositor DCC
R_{free} test set	397 reflections (5.45%)	wwPDB-VP
Wilson B-factor (Å^2)	41.4	Xtriage
Anisotropy	0.933	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.052 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.055 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	3737	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU

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	$\#\|Z\| > 5$
2	A	0.52	0/897	0.89	3/1210 (0.2%)
2	B	0.51	0/934	0.89	3/1258 (0.2%)
2	C	0.52	0/897	0.89	3/1210 (0.2%)
2	D	0.51	0/917	0.87	3/1236 (0.2%)
All	All	0.51	0/3645	0.88	12/4914 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	456	ARG	NE-CZ-NH1	13.81	127.20	120.30
2	B	256	ARG	NE-CZ-NH1	13.41	127.01	120.30
2	A	56	ARG	NE-CZ-NH2	13.11	126.85	120.30
2	C	456	ARG	NE-CZ-NH2	-12.96	113.82	120.30
2	D	656	ARG	NE-CZ-NH1	-12.92	113.84	120.30
2	B	256	ARG	NE-CZ-NH2	-12.86	113.87	120.30
2	D	656	ARG	NE-CZ-NH2	12.80	126.70	120.30
2	A	56	ARG	NE-CZ-NH1	-12.77	113.92	120.30
2	D	656	ARG	CD-NE-CZ	7.10	133.54	123.60
2	C	456	ARG	CD-NE-CZ	6.91	133.28	123.60
2	A	56	ARG	CD-NE-CZ	6.91	133.27	123.60
2	B	256	ARG	CD-NE-CZ	6.86	133.21	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	60	0	37	16	0
1	N	18	0	13	1	0
2	A	884	0	880	145	0
2	B	921	0	912	133	0
2	C	884	0	877	146	0
2	D	904	0	898	132	0
3	A	20	0	0	13	0
3	B	15	0	0	11	0
3	C	17	0	0	6	0
3	D	13	0	0	2	0
3	N	1	0	0	0	0
All	All	3737	0	3617	486	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 67.

All (486) 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:A:7:LYS:HE2	2:C:407:LYS:HE2	1.25	1.14
2:C:483:LEU:HD21	2:D:683:LEU:HD21	1.32	1.11
2:B:207:LYS:HE2	2:D:607:LYS:HE2	1.36	1.04
2:A:23:MET:HB2	2:A:24:PRO:HD2	1.33	1.03
2:A:83:LEU:HD21	2:B:283:LEU:HD21	1.50	0.92
2:B:316:GLN:HG2	2:B:317:GLY:H	1.34	0.92
2:D:663:LEU:HD12	2:D:708:THR:CG2	2.02	0.89
2:B:223:MET:HA	2:B:225:ASN:H	1.38	0.89
2:C:470:TYR:HA	2:C:472:ARG:HH22	1.36	0.87
2:A:17:ASP:HA	3:A:1545:HOH:O	1.73	0.87
2:B:223:MET:O	2:B:227:GLY:HA3	1.77	0.85
1:M:803:5MU:H4'	2:A:87:LYS:H	1.41	0.85
2:C:463:LEU:HD12	2:C:508:THR:CG2	2.06	0.85
2:C:443:LYS:H	2:C:443:LYS:HD2	1.41	0.84
2:D:663:LEU:HD12	2:D:708:THR:HG22	1.60	0.84
2:C:413:ASN:ND2	2:C:476:GLN:HG3	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:89:THR:HG22	2:A:94:GLN:HG2	1.61	0.83
2:A:37:SER:O	2:B:203:ARG:HD3	1.78	0.82
2:A:63:LEU:HD12	2:A:108:THR:HG22	1.61	0.82
2:B:263:LEU:HD12	2:B:308:THR:CG2	2.10	0.82
2:C:435:ALA:HB2	2:C:454:TRP:CZ3	2.15	0.82
2:C:483:LEU:HD11	2:D:700:GLU:OE1	1.79	0.82
2:A:57:VAL:HA	2:A:100:GLU:HB2	1.61	0.81
2:B:235:ALA:HB2	2:B:254:TRP:CZ3	2.14	0.81
2:C:405:VAL:HB	2:D:611:VAL:HB	1.62	0.81
1:M:801:5MU:H3'	1:M:802:5MU:H5'	1.62	0.80
2:B:289:THR:HG22	2:B:294:GLN:HG2	1.61	0.80
2:C:489:THR:HG22	2:C:494:GLN:HG2	1.63	0.80
2:C:512:LEU:HG	2:C:513:GLY:H	1.46	0.80
2:B:263:LEU:HD12	2:B:308:THR:HG22	1.64	0.80
2:A:76:GLN:HE21	2:A:111:MET:HB2	1.47	0.80
2:B:208:VAL:HG11	2:B:300:GLU:OE1	1.83	0.79
2:D:689:THR:HG22	2:D:694:GLN:HG2	1.63	0.79
2:B:284:ARG:HH11	2:B:286:ARG:HD3	1.48	0.78
2:A:84:ARG:HH11	2:A:86:ARG:HD3	1.48	0.78
2:B:235:ALA:HA	3:B:1540:HOH:O	1.82	0.78
2:C:484:ARG:NH1	2:C:486:ARG:HD3	1.99	0.78
2:C:500:GLU:OE1	2:D:683:LEU:HD11	1.84	0.77
2:A:84:ARG:NH1	2:A:86:ARG:HD3	1.99	0.76
2:B:293:GLY:HA3	3:B:1549:HOH:O	1.84	0.76
2:B:284:ARG:NH1	2:B:286:ARG:HD3	2.00	0.76
2:C:476:GLN:HE21	2:C:511:MET:HB2	1.50	0.76
2:B:276:GLN:HE21	2:B:311:MET:HB2	1.49	0.76
2:C:484:ARG:HH11	2:C:486:ARG:HD3	1.50	0.76
2:C:463:LEU:HD12	2:C:508:THR:HG22	1.68	0.76
2:B:257:VAL:HA	2:B:300:GLU:HB2	1.67	0.75
2:D:684:ARG:HH11	2:D:686:ARG:HD3	1.50	0.75
2:D:623:MET:HB2	2:D:624:PRO:HD2	1.68	0.75
2:A:20:VAL:HG12	2:A:21:ARG:H	1.50	0.75
2:A:100:GLU:OE1	2:B:283:LEU:HD11	1.86	0.75
2:A:23:MET:CB	2:A:24:PRO:HD2	2.13	0.75
2:D:649:LYS:HA	2:D:649:LYS:HE2	1.68	0.74
2:A:111:MET:HG3	2:D:676:GLN:OE1	1.87	0.74
2:B:287:LYS:HD3	3:B:1544:HOH:O	1.87	0.74
2:A:8:VAL:HG11	2:A:100:GLU:OE1	1.87	0.74
2:D:676:GLN:HE21	2:D:711:MET:HB2	1.52	0.74
2:D:684:ARG:NH1	2:D:686:ARG:HD3	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:87:LYS:HB2	3:A:1512:HOH:O	1.87	0.74
2:D:617:ASP:OD1	2:D:672:ARG:HA	1.88	0.74
2:A:76:GLN:OE1	2:D:711:MET:HG3	1.88	0.73
2:A:58:VAL:N	2:A:100:GLU:O	2.22	0.72
2:D:657:VAL:HA	2:D:700:GLU:HB2	1.72	0.71
2:A:112:LEU:O	2:A:112:LEU:HD23	1.89	0.71
1:M:801:5MU:H2'	2:B:254:TRP:HE1	1.56	0.71
2:C:406:ASN:HB2	2:D:636:THR:HG21	1.73	0.71
2:C:457:VAL:HA	2:C:500:GLU:HB2	1.73	0.70
2:A:85:THR:HA	2:A:98:THR:HA	1.72	0.70
2:D:667:ALA:HB1	2:D:671:LEU:HD12	1.71	0.70
2:C:413:ASN:HD21	2:C:476:GLN:HG3	1.57	0.70
2:C:507:GLY:HA3	3:C:1501:HOH:O	1.92	0.70
2:C:414:LEU:HD13	2:C:475:SER:HB2	1.74	0.69
2:A:36:THR:HG21	2:B:206:ASN:HB2	1.74	0.69
2:C:485:THR:HA	2:C:498:THR:HA	1.74	0.69
2:A:7:LYS:HE2	2:C:407:LYS:CE	2.16	0.69
2:A:20:VAL:HG12	2:A:21:ARG:N	2.07	0.69
2:B:285:THR:HA	2:B:298:THR:HA	1.73	0.69
2:D:608:VAL:HG11	2:D:700:GLU:OE1	1.93	0.69
2:B:271:LEU:HD21	2:B:277:VAL:CG1	2.22	0.69
2:A:25:ASN:N	2:A:25:ASN:HD22	1.91	0.68
2:C:402:SER:C	2:D:637:SER:HB2	2.14	0.68
2:A:78:TYR:HB2	3:A:1551:HOH:O	1.93	0.68
2:C:420:VAL:HG21	2:C:468:SER:HB2	1.76	0.68
2:A:13:ASN:HA	2:A:75:SER:O	1.94	0.68
2:C:420:VAL:HG21	2:C:468:SER:CB	2.23	0.67
2:C:430:ALA:HB3	2:C:459:LEU:HB2	1.75	0.67
2:A:24:PRO:C	2:A:26:GLY:H	1.96	0.67
1:M:802:5MU:HN3	2:A:96:ARG:HG3	1.59	0.67
2:A:113:GLY:HA3	3:A:1516:HOH:O	1.92	0.67
2:D:667:ALA:O	2:D:671:LEU:HB2	1.93	0.67
2:D:685:THR:HA	2:D:698:THR:HA	1.76	0.67
2:D:707:GLY:HA3	3:D:1524:HOH:O	1.93	0.67
2:C:406:ASN:HA	2:D:610:LEU:HD23	1.78	0.66
2:C:463:LEU:HD12	2:C:508:THR:HG23	1.76	0.66
1:M:803:5MU:H5'	2:A:87:LYS:HB3	1.77	0.66
2:D:635:ALA:HB2	2:D:654:TRP:CZ3	2.31	0.66
2:C:470:TYR:HA	2:C:472:ARG:NH2	2.10	0.65
2:C:442:ASP:HB3	2:C:445:THR:OG1	1.96	0.65
2:C:418:PRO:HB3	2:C:432:ILE:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:469:GLU:C	2:C:472:ARG:HH12	2.01	0.65
2:A:63:LEU:HD12	2:A:108:THR:CG2	2.27	0.65
2:B:207:LYS:CE	2:D:607:LYS:HE2	2.20	0.65
2:B:267:ALA:O	2:B:271:LEU:HB2	1.97	0.65
2:C:442:ASP:HB2	2:C:449:LYS:HE2	1.79	0.64
2:B:215:GLY:HA3	2:B:254:TRP:CZ3	2.32	0.64
2:C:511:MET:C	2:C:512:LEU:HD23	2.18	0.64
2:C:470:TYR:N	2:C:472:ARG:HH12	1.96	0.64
2:B:207:LYS:HE2	2:D:607:LYS:CE	2.21	0.64
2:C:483:LEU:HD12	2:D:655:HIS:HD2	1.62	0.63
2:A:23:MET:HB2	2:A:24:PRO:CD	2.18	0.63
2:A:7:LYS:CE	2:C:407:LYS:HE2	2.16	0.63
2:B:214:LEU:HD13	2:B:275:SER:HB2	1.78	0.63
2:B:316:GLN:HG2	2:B:317:GLY:N	2.11	0.63
2:A:30:ALA:HB3	2:A:59:LEU:HB2	1.81	0.63
2:D:667:ALA:CB	2:D:671:LEU:HD12	2.27	0.63
2:B:208:VAL:CG2	2:B:283:LEU:HG	2.28	0.62
2:B:233:THR:HG21	2:B:256:ARG:HH21	1.64	0.62
2:A:5:VAL:HB	2:B:211:VAL:HB	1.81	0.62
2:B:223:MET:HA	2:B:225:ASN:N	2.11	0.62
2:D:630:ALA:HB3	2:D:659:LEU:HB2	1.81	0.62
2:A:99:THR:HG21	3:A:1507:HOH:O	2.00	0.62
2:A:24:PRO:C	2:A:25:ASN:HD22	2.02	0.62
2:A:7:LYS:HE3	2:A:80:GLU:HG2	1.82	0.61
2:A:22:TYR:HA	2:A:27:GLY:O	2.01	0.61
2:C:408:VAL:HG11	2:C:500:GLU:OE1	2.01	0.61
2:C:479:ILE:HG22	2:C:481:GLY:H	1.66	0.61
2:A:79:ILE:HG22	2:A:81:GLY:H	1.66	0.61
2:C:467:ALA:HA	2:C:471:LEU:HG	1.83	0.61
2:A:67:ALA:HA	2:A:71:LEU:HD12	1.82	0.60
2:B:219:GLU:HB3	2:B:231:ASN:HB2	1.83	0.60
2:A:5:VAL:O	2:B:210:LEU:HA	2.01	0.60
2:B:234:LEU:HD11	2:B:277:VAL:HG23	1.84	0.60
2:C:405:VAL:O	2:D:610:LEU:HA	2.01	0.60
2:B:253:GLU:O	3:B:1540:HOH:O	2.16	0.60
2:A:67:ALA:HA	2:A:71:LEU:CD1	2.32	0.60
2:B:226:GLY:C	2:B:228:ALA:H	2.05	0.60
2:A:10:LEU:HA	2:B:205:VAL:O	2.01	0.60
2:B:315:ARG:HD2	2:B:315:ARG:N	2.15	0.60
2:C:405:VAL:CB	2:D:611:VAL:HB	2.31	0.60
2:D:679:ILE:HG22	2:D:681:GLY:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:615:GLY:O	2:D:673:LYS:HE2	2.02	0.59
2:D:607:LYS:HE3	2:D:680:GLU:HG2	1.85	0.59
2:B:307:GLY:CA	3:B:1517:HOH:O	2.51	0.59
2:C:411:VAL:HB	2:D:605:VAL:HB	1.83	0.59
2:A:107:GLY:HA3	3:A:1503:HOH:O	2.03	0.59
2:D:643:LYS:HD2	2:D:643:LYS:N	2.18	0.59
2:C:484:ARG:HA	2:D:653:GLU:CD	2.23	0.58
2:B:263:LEU:HD12	2:B:308:THR:HG23	1.83	0.58
2:C:463:LEU:H	2:C:463:LEU:HD22	1.68	0.58
2:C:423:MET:HB3	2:C:424:PRO:HD2	1.85	0.58
2:A:11:VAL:HB	2:B:205:VAL:HB	1.84	0.58
2:A:83:LEU:HD11	2:B:300:GLU:OE1	2.04	0.58
2:A:50:GLU:OE2	2:A:52:THR:HG23	2.03	0.57
2:A:112:LEU:O	2:A:113:GLY:O	2.21	0.57
2:B:215:GLY:O	2:B:273:LYS:HE3	2.04	0.57
2:C:435:ALA:HB2	2:C:454:TRP:CE3	2.39	0.57
2:D:639:SER:HA	2:D:650:GLU:HA	1.86	0.57
2:B:218:PRO:HG2	2:B:271:LEU:O	2.04	0.57
2:A:8:VAL:HG11	2:A:100:GLU:CD	2.24	0.57
2:A:109:MET:CE	2:C:403:ARG:HG2	2.35	0.57
2:B:223:MET:CA	2:B:225:ASN:H	2.12	0.57
2:C:437:SER:CB	2:C:452:THR:HG22	2.35	0.57
2:B:278:TYR:CD2	2:D:605:VAL:HG21	2.39	0.57
2:B:235:ALA:HB2	2:B:254:TRP:CE3	2.39	0.57
2:C:413:ASN:HA	2:C:475:SER:O	2.04	0.56
2:C:432:ILE:HG13	3:C:1562:HOH:O	2.04	0.56
2:D:663:LEU:HD12	2:D:708:THR:HG23	1.85	0.56
2:A:30:ALA:HB3	2:A:59:LEU:HD12	1.86	0.56
2:C:419:GLU:HB3	2:C:431:ASN:HB2	1.87	0.56
2:A:35:ALA:HB2	2:A:54:TRP:CZ3	2.40	0.56
2:A:37:SER:HB3	2:A:52:THR:HG22	1.87	0.56
2:A:37:SER:CB	2:A:52:THR:HG22	2.35	0.56
2:B:279:ILE:HG22	2:B:281:GLY:H	1.70	0.56
2:C:405:VAL:HB	2:D:611:VAL:CB	2.32	0.56
2:C:434:LEU:HG	3:C:1562:HOH:O	2.04	0.56
2:B:258:VAL:N	2:B:300:GLU:O	2.37	0.56
2:C:408:VAL:CG2	2:C:483:LEU:HG	2.35	0.56
2:C:436:THR:HG21	2:D:606:ASN:HB2	1.88	0.56
2:C:512:LEU:CG	2:C:513:GLY:H	2.14	0.56
2:C:455:HIS:HD2	2:D:683:LEU:HD12	1.70	0.55
2:B:221:ARG:O	2:B:228:ALA:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:663:LEU:H	2:D:663:LEU:HD22	1.71	0.55
2:B:214:LEU:HD12	2:B:214:LEU:H	1.72	0.55
2:D:617:ASP:O	2:D:618:PRO:O	2.25	0.55
2:B:220:VAL:HG21	2:B:268:SER:HB2	1.89	0.55
2:C:433:THR:HG21	2:C:456:ARG:HH21	1.72	0.55
2:D:703:VAL:O	2:D:703:VAL:HG13	2.07	0.55
2:A:35:ALA:HB2	2:A:54:TRP:CE3	2.42	0.54
2:A:10:LEU:HD23	2:B:206:ASN:HA	1.89	0.54
2:A:103:VAL:O	2:A:103:VAL:HG13	2.07	0.54
2:A:109:MET:HE1	2:C:403:ARG:HG2	1.89	0.54
1:M:801:5MU:O4	2:B:256:ARG:NH2	2.41	0.54
2:D:619:GLU:OE1	2:D:619:GLU:HA	2.07	0.54
2:D:667:ALA:HA	2:D:671:LEU:HG	1.89	0.54
2:A:90:ASP:C	2:A:92:SER:H	2.12	0.54
2:B:213:ASN:HA	2:B:275:SER:O	2.08	0.54
2:C:413:ASN:HD21	2:D:601:ALA:HA	1.72	0.54
2:C:442:ASP:C	2:C:444:ALA:H	2.11	0.54
2:D:690:ASP:C	2:D:692:SER:H	2.11	0.54
2:B:263:LEU:H	2:B:263:LEU:HD22	1.73	0.54
2:D:658:VAL:N	2:D:700:GLU:O	2.41	0.54
2:A:6:ASN:HA	2:B:210:LEU:HD23	1.89	0.53
2:A:41:ARG:O	2:A:42:ASP:HB2	2.06	0.53
2:C:410:LEU:O	2:C:478:TYR:HA	2.08	0.53
2:C:419:GLU:OE2	2:C:421:ARG:HD3	2.08	0.53
2:C:512:LEU:HG	2:C:513:GLY:N	2.22	0.53
2:A:33:THR:HG21	2:A:56:ARG:HH21	1.73	0.53
2:C:437:SER:HB3	2:C:452:THR:HG22	1.90	0.53
2:A:10:LEU:O	2:A:78:TYR:HA	2.08	0.53
2:B:316:GLN:CG	2:B:317:GLY:H	2.14	0.53
2:C:498:THR:HB	2:D:698:THR:HB	1.91	0.53
2:D:663:LEU:CD1	2:D:708:THR:HG22	2.36	0.53
2:D:714:GLY:C	2:D:716:GLN:H	2.11	0.53
2:A:24:PRO:C	2:A:26:GLY:N	2.61	0.53
2:A:63:LEU:H	2:A:63:LEU:HD22	1.73	0.53
2:D:707:GLY:CA	3:D:1524:HOH:O	2.53	0.53
2:B:303:VAL:HG13	2:B:303:VAL:O	2.09	0.53
2:D:608:VAL:CG2	2:D:683:LEU:HG	2.38	0.52
1:M:802:5MU:N3	2:A:96:ARG:NE	2.58	0.52
2:B:284:ARG:NH1	3:B:1520:HOH:O	2.42	0.52
2:D:634:LEU:HD11	2:D:677:VAL:HG23	1.91	0.52
2:D:640:TRP:N	2:D:649:LYS:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:41:ARG:O	2:A:42:ASP:CB	2.57	0.52
2:D:659:LEU:HD13	2:D:667:ALA:HB2	1.92	0.52
2:B:290:ASP:C	2:B:292:SER:H	2.13	0.52
2:B:307:GLY:HA3	3:B:1517:HOH:O	2.10	0.52
2:A:55:HIS:HD2	2:B:283:LEU:HD12	1.74	0.52
2:B:237:SER:HB3	2:B:252:THR:HG22	1.90	0.52
2:C:511:MET:SD	2:C:511:MET:N	2.82	0.52
2:B:259:LEU:HD13	2:B:267:ALA:HB2	1.91	0.51
2:C:402:SER:O	2:D:637:SER:HB2	2.10	0.51
2:C:406:ASN:HA	2:D:610:LEU:CD2	2.39	0.51
2:C:476:GLN:OE1	2:D:601:ALA:HB2	2.10	0.51
1:M:802:5MU:H4'	1:M:802:5MU:OP1	2.09	0.51
2:B:280:GLU:OE2	2:D:607:LYS:HD2	2.10	0.51
2:D:656:ARG:HB2	2:D:699:THR:HG22	1.91	0.51
2:A:2:SER:O	2:B:237:SER:HB2	2.11	0.51
2:C:414:LEU:HD12	2:C:414:LEU:H	1.74	0.51
2:C:415:GLY:O	2:C:416:GLN:HB3	2.10	0.51
2:A:33:THR:HG22	2:A:54:TRP:HE3	1.75	0.51
2:A:67:ALA:HA	2:A:71:LEU:HG	1.92	0.51
2:B:213:ASN:ND2	2:B:276:GLN:HG3	2.25	0.51
2:A:25:ASN:N	2:A:25:ASN:ND2	2.59	0.51
2:B:208:VAL:HG11	2:B:300:GLU:CD	2.31	0.51
2:C:490:ASP:C	2:C:492:SER:H	2.14	0.51
2:C:420:VAL:CG2	2:C:468:SER:HB2	2.40	0.51
2:B:203:ARG:NE	2:D:709:MET:HE1	2.25	0.51
2:C:503:VAL:HG13	2:C:503:VAL:O	2.10	0.50
2:C:442:ASP:O	2:C:444:ALA:N	2.44	0.50
2:C:459:LEU:HD13	2:C:467:ALA:HB2	1.94	0.50
2:D:612:GLY:C	2:D:634:LEU:HD22	2.31	0.50
2:A:56:ARG:HB2	2:A:99:THR:HG22	1.93	0.50
2:B:227:GLY:O	2:B:229:VAL:HG23	2.11	0.50
2:A:14:LEU:HD12	2:A:14:LEU:H	1.74	0.50
2:C:483:LEU:CD1	2:D:655:HIS:HD2	2.23	0.50
2:A:67:ALA:CB	2:A:71:LEU:HD12	2.42	0.50
2:B:276:GLN:HE21	2:B:311:MET:CB	2.23	0.50
2:C:415:GLY:HA3	2:C:454:TRP:CZ3	2.47	0.50
2:C:416:GLN:HA	2:C:473:LYS:HG3	1.93	0.50
1:M:801:5MU:H2'	2:B:254:TRP:NE1	2.26	0.49
2:A:59:LEU:HD13	2:A:67:ALA:HB2	1.92	0.49
2:A:111:MET:HB3	2:D:676:GLN:HE22	1.77	0.49
2:D:608:VAL:HG11	2:D:700:GLU:CD	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:61:GLY:O	2:A:64:ALA:HB3	2.13	0.49
2:D:687:LYS:NZ	2:D:696:ARG:NH2	2.60	0.49
2:D:690:ASP:OD2	2:D:692:SER:N	2.45	0.49
2:A:20:VAL:CG1	2:A:21:ARG:H	2.23	0.49
2:A:87:LYS:NZ	2:A:96:ARG:NH2	2.60	0.49
2:A:99:THR:CG2	3:A:1507:HOH:O	2.60	0.49
2:B:203:ARG:CD	2:D:709:MET:HE1	2.43	0.49
2:A:36:THR:CG2	2:B:206:ASN:HB2	2.41	0.49
2:A:20:VAL:O	2:A:21:ARG:HB2	2.13	0.49
2:B:222:TYR:HB3	2:B:225:ASN:C	2.33	0.49
2:C:439:SER:O	2:C:440:TRP:HB3	2.13	0.49
2:B:237:SER:CB	2:B:252:THR:HG22	2.41	0.49
2:C:448:MET:HB2	3:C:1539:HOH:O	2.13	0.49
2:D:614:LEU:H	2:D:614:LEU:HD12	1.77	0.49
2:D:635:ALA:HB2	2:D:654:TRP:CE3	2.47	0.49
2:D:613:ASN:HA	2:D:675:SER:O	2.13	0.49
2:B:208:VAL:HG21	2:B:300:GLU:OE1	2.12	0.49
1:M:803:5MU:O2'	2:A:86:ARG:HB2	2.13	0.48
2:A:87:LYS:NZ	2:A:96:ARG:HH22	2.11	0.48
2:C:403:ARG:NH2	2:D:639:SER:OG	2.46	0.48
2:B:215:GLY:HA3	2:B:254:TRP:CH2	2.49	0.48
2:C:442:ASP:CG	2:C:445:THR:HG23	2.33	0.48
2:D:637:SER:HB3	2:D:652:THR:HG22	1.95	0.48
2:D:711:MET:N	2:D:711:MET:SD	2.87	0.48
2:A:57:VAL:HG22	2:A:100:GLU:HB2	1.96	0.48
2:A:83:LEU:HD12	2:B:255:HIS:HD2	1.78	0.48
2:A:90:ASP:OD2	2:A:92:SER:N	2.47	0.48
2:B:222:TYR:O	2:B:225:ASN:HA	2.14	0.48
1:M:801:5MU:O5'	1:M:802:5MU:H5'	2.13	0.48
2:A:12:GLY:C	2:A:34:LEU:HD22	2.34	0.48
2:A:50:GLU:HG2	2:A:51:GLN:N	2.29	0.48
2:A:67:ALA:HA	2:A:71:LEU:CG	2.44	0.48
2:B:278:TYR:CZ	2:D:605:VAL:HG11	2.49	0.48
2:A:16:GLN:HE22	2:A:19:GLU:CD	2.18	0.48
2:A:33:THR:HG23	3:A:1509:HOH:O	2.14	0.48
2:B:215:GLY:HA3	2:B:254:TRP:HZ3	1.79	0.48
2:B:223:MET:O	2:B:227:GLY:CA	2.56	0.48
2:B:311:MET:SD	2:B:311:MET:N	2.87	0.48
2:C:498:THR:CB	2:D:698:THR:HB	2.44	0.48
2:D:690:ASP:OD2	2:D:693:GLY:N	2.47	0.48
2:D:703:VAL:HG22	2:D:704:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:THR:CG2	2:B:294:GLN:HG2	2.39	0.47
2:D:687:LYS:NZ	2:D:696:ARG:HH22	2.12	0.47
1:M:802:5MU:HN3	2:A:96:ARG:CG	2.27	0.47
2:A:107:GLY:CA	3:A:1503:HOH:O	2.61	0.47
1:M:802:5MU:H2'	3:A:1512:HOH:O	2.14	0.47
2:B:240:TRP:CZ2	2:B:249:LYS:HD3	2.49	0.47
2:C:483:LEU:O	2:D:653:GLU:HG3	2.14	0.47
2:D:649:LYS:HA	2:D:649:LYS:CE	2.39	0.47
2:B:214:LEU:HD12	2:B:214:LEU:N	2.28	0.47
2:C:450:GLU:OE2	2:C:452:THR:HG23	2.14	0.47
2:C:406:ASN:HB2	2:D:636:THR:CG2	2.43	0.47
2:A:24:PRO:O	2:A:25:ASN:HB2	2.15	0.47
2:B:271:LEU:HD11	2:B:277:VAL:HG11	1.95	0.47
2:C:443:LYS:H	2:C:443:LYS:CD	2.10	0.47
2:C:498:THR:HB	2:D:698:THR:CB	2.45	0.47
2:B:230:ALA:HB3	2:B:259:LEU:HB2	1.96	0.47
2:D:608:VAL:HG21	2:D:700:GLU:OE1	2.15	0.47
2:D:614:LEU:HD13	2:D:675:SER:HB2	1.96	0.47
1:M:801:5MU:H3'	1:M:802:5MU:C5'	2.38	0.46
2:A:90:ASP:OD2	2:A:93:GLY:N	2.48	0.46
2:C:413:ASN:ND2	2:C:413:ASN:N	2.63	0.46
2:B:203:ARG:HG2	2:B:203:ARG:HH21	1.80	0.46
2:A:21:ARG:HG2	2:A:21:ARG:HH11	1.81	0.46
2:A:35:ALA:HA	2:A:53:GLU:O	2.15	0.46
2:A:36:THR:OG1	2:B:206:ASN:HB2	2.16	0.46
2:A:76:GLN:HE21	2:A:111:MET:CB	2.23	0.46
2:B:271:LEU:HD21	2:B:277:VAL:HG13	1.98	0.46
2:C:413:ASN:ND2	2:D:601:ALA:HA	2.31	0.46
2:C:503:VAL:O	2:C:505:VAL:N	2.49	0.46
2:C:434:LEU:HD11	2:C:477:VAL:HG23	1.98	0.46
2:C:415:GLY:O	2:C:473:LYS:HE3	2.16	0.46
2:C:437:SER:HA	2:C:452:THR:HG22	1.98	0.46
2:D:714:GLY:H	2:D:716:GLN:NE2	2.13	0.46
2:B:216:GLN:HG3	2:B:217:ASP:O	2.16	0.46
2:B:263:LEU:CD1	2:B:308:THR:HG22	2.42	0.46
1:M:802:5MU:H2'	1:M:802:5MU:O2	2.15	0.46
2:A:14:LEU:HD12	2:A:14:LEU:N	2.30	0.46
2:A:37:SER:HB2	2:B:202:SER:C	2.36	0.46
2:B:207:LYS:HE3	2:B:280:GLU:HG2	1.97	0.45
2:B:290:ASP:OD2	2:B:292:SER:N	2.49	0.45
2:A:106:GLY:HA2	3:A:1534:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:111:MET:SD	2:A:111:MET:N	2.89	0.45
2:D:657:VAL:HG12	2:D:658:VAL:N	2.31	0.45
2:A:13:ASN:N	2:A:13:ASN:ND2	2.62	0.45
2:D:649:LYS:HE2	2:D:649:LYS:CA	2.44	0.45
2:A:5:VAL:HG21	2:C:478:TYR:CD2	2.51	0.45
2:B:257:VAL:HG12	2:B:258:VAL:N	2.31	0.45
2:B:312:LEU:HD21	2:B:316:GLN:HE22	1.81	0.45
2:C:490:ASP:OD2	2:C:492:SER:N	2.50	0.45
2:D:633:THR:HG21	2:D:656:ARG:HH21	1.80	0.45
1:M:803:5MU:H5"	1:M:803:5MU:H6	1.82	0.45
2:C:483:LEU:CD2	2:D:683:LEU:HD21	2.24	0.45
2:A:20:VAL:CG1	2:A:21:ARG:N	2.77	0.45
2:A:57:VAL:HG12	2:A:58:VAL:N	2.32	0.45
2:C:463:LEU:CD1	2:C:508:THR:HG22	2.43	0.45
2:C:487:LYS:NZ	2:C:496:ARG:NH2	2.65	0.45
2:A:89:THR:CG2	2:A:94:GLN:HG2	2.37	0.45
2:B:287:LYS:NZ	2:B:296:ARG:NH2	2.65	0.45
2:A:67:ALA:CA	2:A:71:LEU:HD12	2.46	0.45
2:A:103:VAL:HG22	2:A:104:ASN:OD1	2.16	0.45
2:B:263:LEU:HD23	3:B:1506:HOH:O	2.16	0.45
2:C:458:VAL:N	2:C:500:GLU:O	2.50	0.44
2:C:461:GLY:O	2:C:464:ALA:HB3	2.17	0.44
2:B:261:GLY:O	2:B:264:ALA:HB3	2.17	0.44
2:B:212:GLY:C	2:B:234:LEU:HD22	2.38	0.44
2:D:613:ASN:N	2:D:613:ASN:ND2	2.65	0.44
2:D:662:LYS:O	2:D:666:VAL:HG23	2.17	0.44
2:B:239:SER:C	2:B:240:TRP:HE3	2.20	0.44
2:B:255:HIS:ND1	3:B:1540:HOH:O	2.27	0.44
2:B:278:TYR:CG	2:D:605:VAL:HG21	2.52	0.44
2:A:6:ASN:ND2	2:A:82:GLN:HB2	2.33	0.44
2:A:87:LYS:HZ3	2:A:96:ARG:NH2	2.14	0.44
2:A:34:LEU:O	2:A:55:HIS:N	2.45	0.44
2:C:416:GLN:HA	2:C:473:LYS:CG	2.47	0.44
2:B:290:ASP:OD2	2:B:293:GLY:N	2.51	0.44
2:C:413:ASN:HD22	2:C:476:GLN:HG3	1.79	0.44
2:C:423:MET:SD	3:C:1556:HOH:O	2.60	0.44
2:D:637:SER:CB	2:D:652:THR:HG22	2.47	0.44
2:D:715:ARG:HG2	2:D:715:ARG:HH11	1.83	0.44
2:B:203:ARG:HB3	2:B:204:GLY:H	1.47	0.43
2:B:263:LEU:HB3	2:B:308:THR:HG22	2.00	0.43
2:C:414:LEU:HD12	2:C:414:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:503:VAL:HG22	2:C:504:ASN:OD1	2.18	0.43
2:A:12:GLY:C	2:A:13:ASN:HD22	2.22	0.43
2:A:55:HIS:HD2	2:B:283:LEU:CD1	2.31	0.43
2:C:487:LYS:HZ3	2:C:496:ARG:NH2	2.16	0.43
2:C:457:VAL:HG12	2:C:458:VAL:N	2.34	0.43
2:C:410:LEU:HD23	2:D:606:ASN:HA	1.99	0.43
2:C:436:THR:OG1	2:C:455:HIS:HE1	2.00	0.43
2:C:489:THR:CG2	2:C:494:GLN:HG2	2.40	0.43
2:D:687:LYS:HZ1	2:D:696:ARG:HH22	1.65	0.43
2:D:689:THR:CG2	2:D:694:GLN:HG2	2.41	0.43
2:B:262:LYS:O	2:B:266:VAL:HG23	2.18	0.43
2:B:287:LYS:NZ	2:B:296:ARG:HH22	2.17	0.43
2:C:487:LYS:NZ	2:C:496:ARG:HH22	2.17	0.43
2:D:614:LEU:HD12	2:D:614:LEU:N	2.33	0.43
2:D:661:GLY:O	2:D:664:ALA:HB3	2.19	0.43
2:D:690:ASP:C	2:D:690:ASP:OD2	2.57	0.43
2:A:34:LEU:HD23	2:A:34:LEU:HA	1.75	0.43
2:A:62:LYS:O	2:A:65:GLU:N	2.51	0.43
2:A:89:THR:HA	2:A:94:GLN:HA	1.99	0.43
2:A:5:VAL:HB	2:B:211:VAL:CB	2.46	0.43
2:A:21:ARG:HD3	2:A:22:TYR:H	1.83	0.43
2:B:234:LEU:HA	2:B:234:LEU:HD23	1.75	0.43
2:D:633:THR:HG22	2:D:654:TRP:HE3	1.83	0.43
2:A:40:TRP:O	2:A:40:TRP:CD1	2.72	0.43
2:B:303:VAL:O	2:B:305:VAL:N	2.52	0.43
2:C:490:ASP:C	2:C:490:ASP:OD2	2.57	0.43
2:C:467:ALA:O	2:C:471:LEU:HB2	2.18	0.42
2:A:36:THR:OG1	2:A:55:HIS:HE1	2.02	0.42
2:A:76:GLN:HE22	2:D:711:MET:HB3	1.83	0.42
2:C:415:GLY:HA3	2:C:454:TRP:HZ3	1.84	0.42
2:C:422:TYR:HA	2:C:428:ALA:HA	2.00	0.42
2:C:459:LEU:CD1	2:C:467:ALA:HB2	2.49	0.42
2:B:227:GLY:O	2:B:228:ALA:C	2.57	0.42
2:C:442:ASP:C	2:C:444:ALA:N	2.73	0.42
2:D:710:GLN:NE2	2:D:714:GLY:HA2	2.34	0.42
2:A:5:VAL:CB	2:B:211:VAL:HB	2.47	0.42
2:A:8:VAL:HG21	2:A:100:GLU:OE1	2.20	0.42
2:C:434:LEU:HD23	2:C:434:LEU:HA	1.76	0.42
2:C:471:LEU:HD11	2:C:477:VAL:HG11	2.01	0.42
1:N:900:5MU:H1'	2:B:260:PHE:HB3	2.02	0.42
2:B:303:VAL:HG22	2:B:304:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:489:THR:HA	2:C:494:GLN:HA	2.02	0.42
2:A:1:ALA:O	2:A:2:SER:CB	2.68	0.42
2:B:213:ASN:ND2	2:B:213:ASN:N	2.64	0.42
2:C:442:ASP:OD2	2:C:445:THR:HG23	2.20	0.42
2:A:103:VAL:HG23	3:A:1541:HOH:O	2.19	0.42
2:C:490:ASP:OD2	2:C:493:GLY:N	2.53	0.42
2:C:441:ARG:NE	2:C:446:GLY:O	2.42	0.42
2:D:641:ARG:HB3	2:D:648:MET:CE	2.50	0.42
2:A:103:VAL:O	2:A:105:VAL:N	2.52	0.41
2:C:407:LYS:HE3	2:C:480:GLU:HG2	2.00	0.41
2:C:423:MET:HA	3:C:1556:HOH:O	2.20	0.41
2:D:606:ASN:ND2	2:D:682:GLN:HB2	2.34	0.41
2:A:57:VAL:CA	2:A:100:GLU:HB2	2.40	0.41
2:C:462:LYS:O	2:C:466:VAL:HG23	2.20	0.41
2:A:10:LEU:HD11	2:A:100:GLU:HG3	2.03	0.41
2:A:76:GLN:NE2	2:A:111:MET:HB2	2.24	0.41
2:B:289:THR:HA	2:B:294:GLN:HA	2.01	0.41
2:C:405:VAL:N	2:D:611:VAL:HB	2.35	0.41
2:D:630:ALA:HB3	2:D:659:LEU:HD12	2.01	0.41
2:A:41:ARG:O	2:A:42:ASP:OD2	2.39	0.41
2:B:209:ILE:CD1	2:C:409:ILE:HD12	2.51	0.41
2:B:216:GLN:HB2	3:B:1533:HOH:O	2.20	0.41
2:B:236:THR:OG1	2:B:255:HIS:HE1	2.03	0.41
2:D:667:ALA:HA	2:D:671:LEU:CG	2.49	0.41
2:A:58:VAL:HG23	2:A:99:THR:HB	2.01	0.41
2:A:11:VAL:HA	2:A:77:VAL:O	2.21	0.41
2:A:13:ASN:N	2:A:13:ASN:HD22	2.18	0.41
2:B:235:ALA:CA	3:B:1540:HOH:O	2.54	0.41
2:B:312:LEU:HD21	2:B:316:GLN:NE2	2.36	0.41
2:C:406:ASN:CB	2:D:636:THR:HG21	2.48	0.41
2:C:436:THR:HG23	2:C:455:HIS:CE1	2.55	0.41
2:D:703:VAL:O	2:D:705:VAL:N	2.54	0.41
2:D:714:GLY:C	2:D:716:GLN:N	2.73	0.41
2:B:235:ALA:HB2	2:B:254:TRP:CH2	2.55	0.41
2:D:659:LEU:CD1	2:D:667:ALA:HB2	2.50	0.41
2:D:689:THR:HA	2:D:694:GLN:HA	2.02	0.41
2:C:410:LEU:CD2	2:D:606:ASN:HA	2.50	0.41
2:D:623:MET:HG3	2:D:625:ASN:HB3	2.02	0.41
2:A:8:VAL:CG2	2:A:83:LEU:HG	2.51	0.41
2:A:59:LEU:CD1	2:A:67:ALA:HB2	2.50	0.41
2:C:405:VAL:HB	2:D:611:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:612:GLY:C	2:D:613:ASN:HD22	2.24	0.41
2:D:634:LEU:HD23	2:D:634:LEU:HA	1.76	0.41
2:C:405:VAL:N	2:D:611:VAL:O	2.46	0.41
2:D:662:LYS:O	2:D:665:GLU:N	2.54	0.41
2:A:90:ASP:C	2:A:90:ASP:OD2	2.60	0.40
2:B:259:LEU:CD1	2:B:267:ALA:HB2	2.51	0.40
2:C:425:ASN:H	2:C:425:ASN:HD22	1.69	0.40
2:C:476:GLN:CD	2:D:601:ALA:HB2	2.41	0.40
2:A:111:MET:HG2	3:A:1521:HOH:O	2.21	0.40
2:B:287:LYS:HZ3	2:B:296:ARG:NH2	2.19	0.40
2:C:412:GLY:C	2:C:413:ASN:HD22	2.24	0.40
2:C:473:LYS:HG2	2:C:474:GLY:N	2.36	0.40
2:C:483:LEU:HD21	2:D:683:LEU:CD2	2.24	0.40
2:C:403:ARG:HA	2:D:637:SER:HB2	2.03	0.40
2:A:87:LYS:HZ3	2:A:96:ARG:CZ	2.35	0.40
2:B:221:ARG:HH21	2:B:229:VAL:CG1	2.35	0.40
2:C:412:GLY:O	2:C:477:VAL:N	2.45	0.40
2:C:434:LEU:HD21	2:C:477:VAL:HG22	2.03	0.40
2:D:620:VAL:HG21	2:D:668:SER:OG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	112/178 (63%)	82 (73%)	16 (14%)	14 (12%)	0	1
2	B	118/178 (66%)	96 (81%)	14 (12%)	8 (7%)	1	9
2	C	112/178 (63%)	89 (80%)	12 (11%)	11 (10%)	0	3
2	D	114/178 (64%)	93 (82%)	12 (10%)	9 (8%)	1	6
All	All	456/712 (64%)	360 (79%)	54 (12%)	42 (9%)	1	3

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	2	SER
2	A	42	ASP
2	A	92	SER
2	A	113	GLY
2	B	292	SER
2	C	492	SER
2	C	512	LEU
2	D	618	PRO
2	D	692	SER
2	A	43	LYS
2	A	44	ALA
2	A	49	LYS
2	B	228	ALA
2	C	443	LYS
2	D	712	LEU
2	A	40	TRP
2	A	90	ASP
2	B	290	ASP
2	C	402	SER
2	C	424	PRO
2	A	21	ARG
2	A	104	ASN
2	B	224	PRO
2	B	226	GLY
2	B	240	TRP
2	C	490	ASP
2	C	504	ASN
2	D	690	ASP
2	A	45	THR
2	A	91	GLN
2	B	304	ASN
2	C	403	ARG
2	C	440	TRP
2	D	643	LYS
2	D	704	ASN
2	D	715	ARG
2	C	491	GLN
2	D	691	GLN
2	D	713	GLY
2	A	105	VAL
2	C	505	VAL
2	B	313	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	93/136 (68%)	88 (95%)	5 (5%)	22 58
2	B	95/136 (70%)	88 (93%)	7 (7%)	13 46
2	C	93/136 (68%)	82 (88%)	11 (12%)	5 23
2	D	95/136 (70%)	89 (94%)	6 (6%)	18 52
All	All	376/544 (69%)	347 (92%)	29 (8%)	13 44

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	21	ARG
2	A	25	ASN
2	A	50	GLU
2	A	96	ARG
2	A	111	MET
2	B	203	ARG
2	B	217	ASP
2	B	223	MET
2	B	241	ARG
2	B	256	ARG
2	B	296	ARG
2	B	311	MET
2	C	403	ARG
2	C	424	PRO
2	C	425	ASN
2	C	440	TRP
2	C	443	LYS
2	C	450	GLU
2	C	456	ARG
2	C	496	ARG
2	C	502	VAL
2	C	511	MET
2	C	512	LEU
2	D	642	ASP

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Mol	Chain	Res	Type
2	D	643	LYS
2	D	696	ARG
2	D	702	VAL
2	D	711	MET
2	D	716	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	13	ASN
2	A	16	GLN
2	A	25	ASN
2	A	55	HIS
2	A	76	GLN
2	B	213	ASN
2	B	276	GLN
2	B	316	GLN
2	C	413	ASN
2	C	416	GLN
2	C	425	ASN
2	C	455	HIS
2	C	476	GLN
2	D	613	ASN
2	D	676	GLN
2	D	716	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	M	2/3 (66%)	2 (100%)	0
1	N	0/3	-	-
All	All	2/6 (33%)	2 (100%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	M	802	5MU
1	M	803	5MU

There are no RNA pucker outliers to report.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	5MU	M	803	1	19,22,23	0.34	0	28,32,35	0.52	0
1	5MU	M	801	1	19,19,23	0.28	0	28,28,35	0.26	0
1	5MU	M	802	1	19,22,23	0.29	0	28,32,35	0.43	0
1	5MU	N	900	-	19,19,23	0.37	0	28,28,35	0.45	0

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
1	5MU	M	803	1	-	1/7/25/26	0/2/2/2
1	5MU	M	801	1	-	0/6/22/26	0/2/2/2
1	5MU	M	802	1	-	4/7/25/26	0/2/2/2
1	5MU	N	900	-	-	0/6/22/26	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	M	802	5MU	C4'-C5'-O5'-P
1	M	802	5MU	C2'-C1'-N1-C2
1	M	802	5MU	C2'-C1'-N1-C6
1	M	803	5MU	O4'-C4'-C5'-O5'
1	M	802	5MU	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	803	5MU	4	0
1	M	801	5MU	6	0
1	M	802	5MU	9	0
1	N	900	5MU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	M	0/3	-	-			-	-
1	N	0/3	-	-			-	-
2	A	114/178 (64%)	-0.03	6 (5%)	26	14	3, 19, 74, 83	0
2	B	120/178 (67%)	-0.23	2 (1%)	70	57	2, 20, 59, 65	0
2	C	114/178 (64%)	-0.15	2 (1%)	68	55	2, 18, 49, 61	0
2	D	116/178 (65%)	-0.15	3 (2%)	56	40	2, 20, 63, 80	0
All	All	464/718 (64%)	-0.14	13 (2%)	53	37	2, 19, 61, 83	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	646	GLY	4.5
2	D	645	THR	4.4
2	A	48	MET	4.1
2	D	644	ALA	3.7
2	A	2	SER	3.7
2	B	304	ASN	3.6
2	B	318	GLY	3.3
2	C	402	SER	2.9
2	C	401	ALA	2.8
2	A	40	TRP	2.6
2	A	49	LYS	2.2
2	A	47	GLU	2.0
2	A	92	SER	2.0

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

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
1	5MU	M	803	21/22	0.71	0.32	85,87,88,89	0
1	5MU	M	802	21/22	0.72	0.34	73,87,92,92	0
1	5MU	N	900	18/22	0.74	0.38	47,48,52,52	0
1	5MU	M	801	18/22	0.77	0.31	72,73,75,76	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.