Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:03 PM GMT

PDB ID	:	1NB7
Title	:	HC-J4 RNA polymerase complexed with short RNA template strand
Authors	:	O'Farrell, D.J.; Trowbridge, R.; Rowlands, D.J.; Jaeger, J.
Deposited on	:	2002-12-02
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

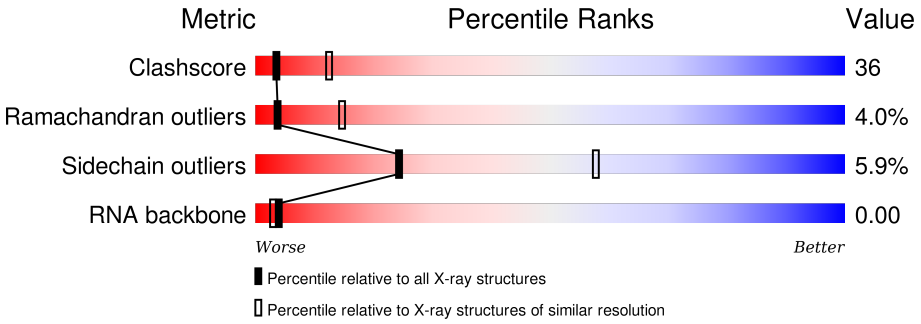
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	4	75% 25%
1	F	4	75% 25%
2	A	570	44% 51% 5% •
2	B	570	44% 50% 5% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8927 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(*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			
1	F	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 2 is a protein called polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	566	Total	C	N	O	S	0	0	0
			4388	2763	777	816	32			
2	B	565	Total	C	N	O	S	0	0	0
			4381	2758	776	815	32			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mn	0	0
			2	2		
3	A	2	Total	Mn	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: 5'-R(*UP*UP*UP*U)-3'

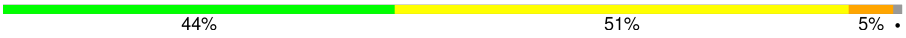
Chain E:

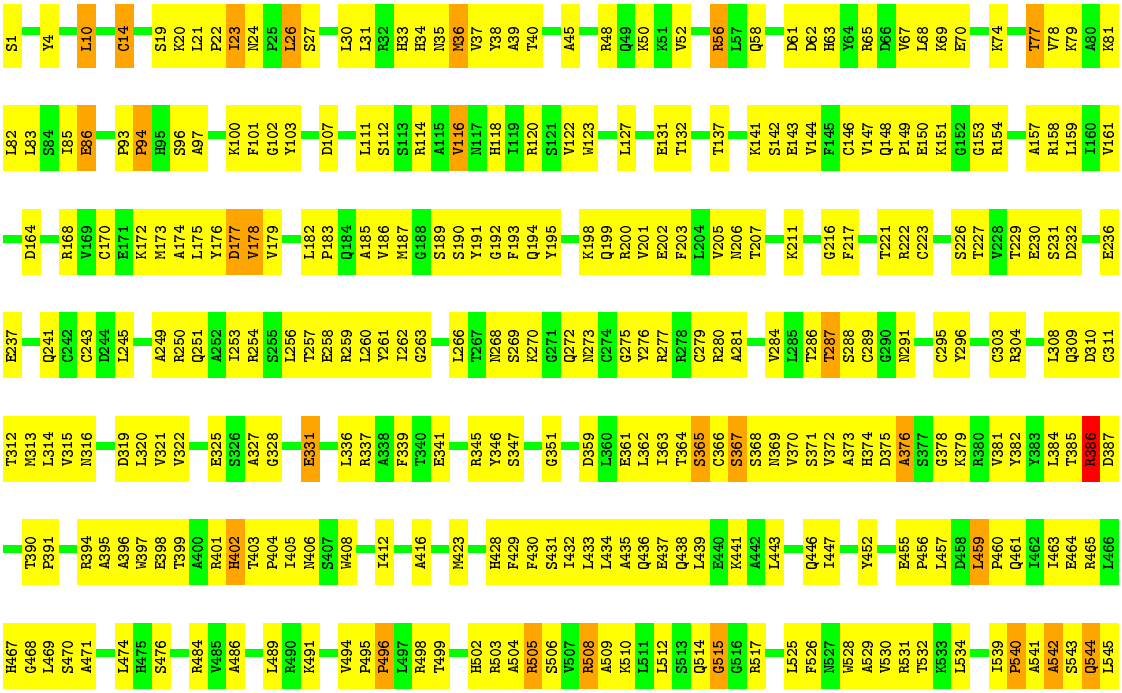
- Molecule 1: 5'-R(*UP*UP*UP*U)-3'

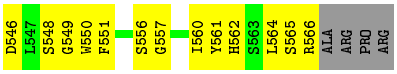
Chain F:

- Molecule 2: polyprotein

Chain A:

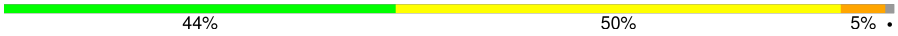


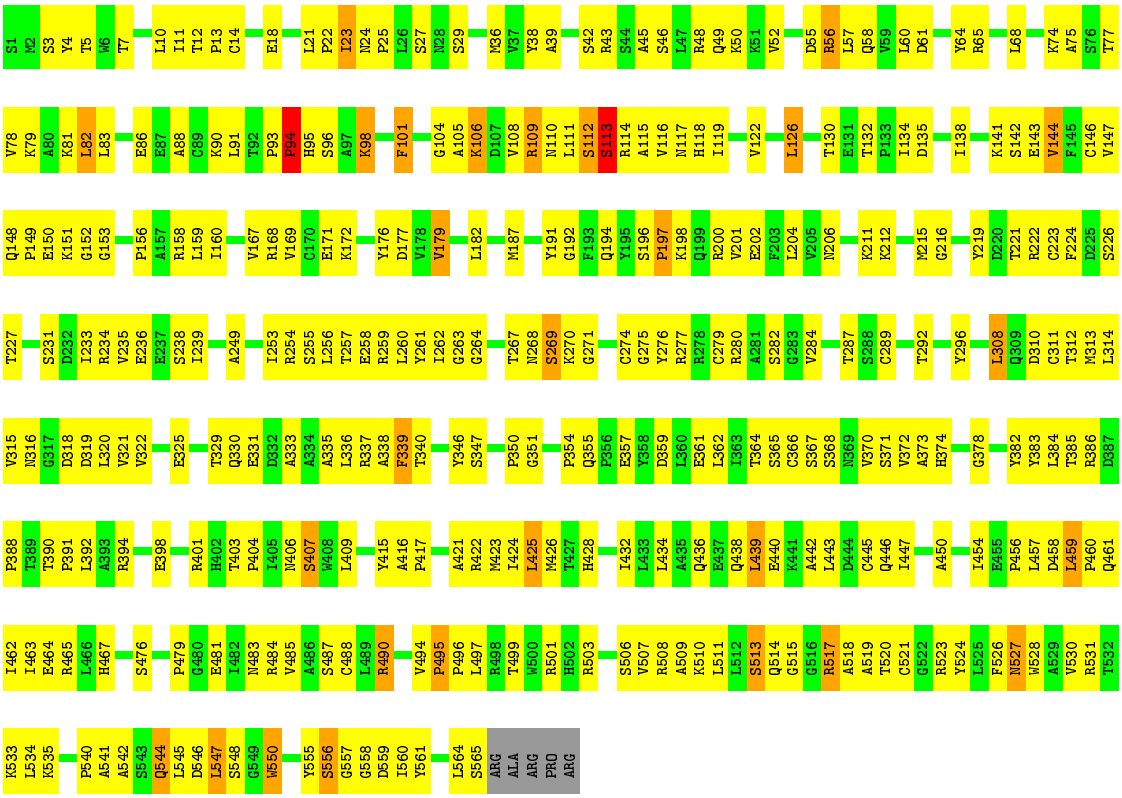




• Molecule 2: polyprotein

Chain B:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.66Å 108.50Å 134.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (22.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8927	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	E	1.39	0/84	1.33	2/128 (1.6%)
1	F	1.23	0/84	1.44	1/128 (0.8%)
2	A	0.49	0/4484	0.74	1/6087 (0.0%)
2	B	0.52	1/4477 (0.0%)	0.73	0/6077
All	All	0.53	1/9129 (0.0%)	0.75	4/12420 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	142	SER	CB-OG	7.89	1.52	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	3	U	O4'-C1'-N1	7.28	114.03	108.20
1	E	4	U	C2'-C3'-O3'	5.29	122.17	113.70
2	A	351	GLY	N-CA-C	-5.12	100.29	113.10
1	E	4	U	N1-C1'-C2'	5.03	120.53	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	4	U	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	77	0	42	22	0
1	F	77	0	42	23	0
2	A	4388	0	4383	326	0
2	B	4381	0	4374	302	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	8927	0	8841	641	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 36.

All (641) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:GLY:HA2	2:B:519:ALA:HB2	1.33	1.06
2:B:144:VAL:HG22	2:B:394:ARG:HG2	1.35	1.03
2:B:160:ILE:HD12	2:B:282:SER:HG	1.27	1.00
1:F:1:U:HO5'	1:F:1:U:H6	1.03	1.00
2:A:195:TYR:HB3	2:A:199:GLN:HB2	1.43	1.00
2:A:268:ASN:HD21	2:A:272:GLN:HE21	1.01	0.98
2:A:531:ARG:HH22	2:B:198:LYS:NZ	1.62	0.97
2:A:191:TYR:HB3	2:A:194:GLN:HE21	1.25	0.96
2:B:56:ARG:HH21	2:B:279:CYS:HB3	1.32	0.95
2:B:126:LEU:HD21	2:B:256:LEU:HD21	1.49	0.94
2:A:268:ASN:HD21	2:A:272:GLN:HB2	1.34	0.93
2:B:18:GLU:HG2	2:B:401:ARG:NH2	1.85	0.92
2:B:86:GLU:HG3	2:B:111:LEU:HD11	1.51	0.92
2:A:367:SER:O	2:A:386:ARG:HG3	1.69	0.91
2:A:10:LEU:H	2:A:10:LEU:HD12	1.36	0.91
1:E:1:U:H2'	1:E:2:U:C5	2.06	0.91
2:B:313:MET:HB3	2:B:322:VAL:HG22	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:112:SER:O	2:A:116:VAL:HG13	1.72	0.90
2:A:394:ARG:O	2:A:398:GLU:HG3	1.72	0.89
2:B:160:ILE:HD12	2:B:282:SER:OG	1.72	0.88
2:A:268:ASN:HD21	2:A:272:GLN:NE2	1.70	0.88
2:B:148:GLN:HE21	2:B:153:GLY:HA3	1.38	0.88
2:B:398:GLU:OE2	2:B:407:SER:HB3	1.74	0.88
2:B:52:VAL:HG23	2:B:226:SER:OG	1.75	0.87
2:A:56:ARG:HB2	2:A:56:ARG:HH11	1.41	0.85
2:A:508:ARG:HG3	2:A:526:PHE:HB2	1.59	0.84
2:A:56:ARG:HB2	2:A:56:ARG:NH1	1.92	0.84
2:A:182:LEU:HD12	2:A:243:CYS:SG	2.17	0.84
2:A:457:LEU:HD12	2:A:517:ARG:HH21	1.43	0.84
2:A:268:ASN:ND2	2:A:272:GLN:HE21	1.75	0.83
2:B:236:GLU:OE1	2:B:280:ARG:NH2	2.11	0.83
1:F:4:U:H4'	2:B:141:LYS:NZ	1.94	0.83
2:A:132:THR:O	2:A:259:ARG:HD2	1.79	0.82
2:A:361:GLU:HG3	2:A:370:VAL:O	1.80	0.82
2:A:439:LEU:HD22	2:A:439:LEU:H	1.45	0.81
2:B:18:GLU:HG2	2:B:401:ARG:CZ	2.10	0.81
2:A:268:ASN:ND2	2:A:272:GLN:HB2	1.95	0.81
2:A:390:THR:HB	2:A:391:PRO:HD3	1.64	0.79
2:A:489:LEU:HD22	2:A:494:VAL:HB	1.63	0.79
2:B:515:GLY:CA	2:B:519:ALA:HB2	2.12	0.79
2:A:141:LYS:HD2	2:A:158:ARG:HH12	1.44	0.79
2:A:74:LYS:O	2:A:77:THR:HB	1.83	0.78
1:F:3:U:C4	2:B:93:PRO:HB2	2.17	0.78
2:B:113:SER:O	2:B:116:VAL:HG22	1.83	0.78
2:A:531:ARG:NH2	2:B:198:LYS:NZ	2.31	0.78
2:B:409:LEU:HD23	2:B:445:CYS:HB3	1.65	0.77
2:A:148:GLN:HG2	2:A:150:GLU:H	1.50	0.77
2:B:106:LYS:HB2	2:B:106:LYS:NZ	1.99	0.76
2:B:555:TYR:CB	2:B:560:ILE:HG13	2.15	0.76
2:A:144:VAL:HG13	2:A:394:ARG:HG2	1.68	0.76
2:B:24:ASN:HD22	2:B:27:SER:H	1.34	0.76
1:F:1:U:H2'	1:F:2:U:C5	2.20	0.76
2:A:245:LEU:HD13	2:A:253:ILE:HD12	1.69	0.74
2:A:33:HIS:CE1	2:B:212:LYS:HE2	2.24	0.73
2:A:179:VAL:HG13	2:A:289:CYS:HB2	1.70	0.73
2:A:175:LEU:HD13	2:A:286:THR:CG2	2.18	0.73
2:B:388:PRO:HG2	2:B:488:CYS:SG	2.29	0.73
2:B:158:ARG:HB3	2:B:158:ARG:HH11	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:374:HIS:ND1	2:A:476:SER:HB2	2.04	0.73
2:A:509:ALA:HA	2:A:512:LEU:HD12	1.71	0.72
2:B:528:TRP:HA	2:B:533:LYS:HE3	1.71	0.72
2:B:21:LEU:HD12	2:B:22:PRO:HD2	1.72	0.71
2:A:191:TYR:HB3	2:A:194:GLN:NE2	2.04	0.71
1:E:3:U:C2'	1:E:4:U:OP2	2.37	0.71
2:A:439:LEU:HB3	2:A:457:LEU:HG	1.72	0.71
2:B:82:LEU:HD12	2:B:82:LEU:H	1.55	0.71
2:B:308:LEU:HB3	2:B:311:CYS:SG	2.30	0.71
2:A:328:GLY:HA3	2:A:331:GLU:HG2	1.73	0.71
2:A:428:HIS:O	2:A:432:ILE:HG12	1.90	0.71
2:B:158:ARG:HB3	2:B:158:ARG:NH1	2.07	0.70
1:F:3:U:O2'	1:F:4:U:OP2	2.08	0.70
1:E:1:U:H2'	1:E:2:U:H5	1.56	0.70
2:B:374:HIS:HD2	2:B:378:GLY:O	1.74	0.70
2:B:144:VAL:CG2	2:B:394:ARG:HG2	2.16	0.70
2:A:148:GLN:OE1	2:A:153:GLY:HA3	1.92	0.69
2:A:368:SER:HB2	2:A:385:THR:O	1.92	0.69
2:B:116:VAL:HG23	2:B:117:ASN:N	2.08	0.69
2:A:79:LYS:HE2	2:A:81:LYS:HE2	1.75	0.68
2:B:555:TYR:CG	2:B:560:ILE:HG13	2.28	0.68
2:A:223:CYS:O	2:A:227:THR:HG23	1.93	0.68
2:A:461:GLN:HG3	2:A:539:ILE:HG21	1.76	0.68
1:E:2:U:H2'	2:A:97:ALA:H	1.58	0.68
2:A:460:PRO:HB2	2:A:461:GLN:OE1	1.94	0.67
2:B:234:ARG:NH2	2:B:262:ILE:HD11	2.09	0.67
2:A:22:PRO:O	2:A:24:ASN:N	2.26	0.67
2:B:148:GLN:NE2	2:B:153:GLY:HA3	2.09	0.67
2:B:390:THR:HB	2:B:391:PRO:HD3	1.75	0.67
2:A:58:GLN:HB2	2:A:347:SER:HB3	1.77	0.67
2:A:313:MET:HE2	2:A:322:VAL:HB	1.77	0.67
2:B:219:TYR:HE1	2:B:221:THR:HG22	1.60	0.67
2:A:82:LEU:HD13	2:A:249:ALA:HB2	1.76	0.66
2:A:504:ALA:O	2:A:506:SER:N	2.28	0.66
2:B:61:ASP:O	2:B:65:ARG:HG3	1.95	0.66
2:A:432:ILE:CG2	2:A:436:GLN:HE22	2.08	0.66
2:B:446:GLN:C	2:B:447:ILE:HD12	2.16	0.66
2:A:369:ASN:O	2:A:384:LEU:HD22	1.97	0.65
2:B:308:LEU:CD1	2:B:335:ALA:HB1	2.26	0.65
2:B:3:SER:HB3	2:B:56:ARG:NE	2.11	0.65
2:B:508:ARG:NE	2:B:530:VAL:HG11	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:327:ALA:O	2:A:331:GLU:HG3	1.97	0.65
2:A:386:ARG:NE	2:A:387:ASP:O	2.29	0.65
2:A:263:GLY:HA2	2:A:277:ARG:NH1	2.12	0.65
2:B:506:SER:O	2:B:510:LYS:HG3	1.97	0.65
2:B:255:SER:O	2:B:259:ARG:HB2	1.96	0.65
2:B:86:GLU:CG	2:B:111:LEU:HD11	2.27	0.65
2:A:172:LYS:HE3	2:A:560:ILE:HD13	1.77	0.65
2:A:254:ARG:HH11	2:A:254:ARG:HA	1.60	0.65
2:A:24:ASN:ND2	2:A:27:SER:N	2.45	0.64
2:A:438:GLN:NE2	2:A:441:LYS:HD2	2.13	0.64
1:F:3:U:C5	2:B:93:PRO:HB2	2.32	0.64
1:E:1:U:C2'	1:E:2:U:C5	2.80	0.64
2:B:191:TYR:O	2:B:194:GLN:HG2	1.98	0.64
2:B:442:ALA:O	2:B:443:LEU:HD23	1.97	0.64
2:B:465:ARG:HH21	2:B:546:ASP:CB	2.09	0.64
2:B:219:TYR:HB3	2:B:320:LEU:HD23	1.81	0.63
2:B:13:PRO:HB3	2:B:42:SER:OG	1.98	0.63
2:A:36:MET:HE3	2:A:491:LYS:HG2	1.80	0.63
2:B:93:PRO:HB3	2:B:561:TYR:HB2	1.80	0.63
2:B:126:LEU:HA	2:B:259:ARG:NH2	2.14	0.63
2:A:30:LEU:HB2	2:A:428:HIS:CD2	2.34	0.63
2:A:508:ARG:CZ	2:A:512:LEU:HD11	2.29	0.63
2:B:526:PHE:C	2:B:528:TRP:H	2.02	0.63
2:B:126:LEU:HD21	2:B:256:LEU:CD2	2.26	0.62
2:B:224:PHE:CD2	2:B:318:ASP:HB3	2.33	0.62
2:B:4:TYR:CE2	2:B:52:VAL:HG22	2.35	0.62
2:A:457:LEU:CD1	2:A:517:ARG:HH21	2.12	0.62
2:A:216:GLY:HA3	2:A:363:ILE:HD11	1.79	0.62
1:E:4:U:OP1	2:A:556:SER:HA	1.99	0.62
2:A:359:ASP:HB3	2:A:362:LEU:HB2	1.82	0.62
2:A:191:TYR:O	2:A:194:GLN:HG2	2.00	0.62
2:B:313:MET:CB	2:B:322:VAL:HG22	2.27	0.62
2:B:501:ARG:HH12	2:B:528:TRP:HE3	1.48	0.62
2:B:526:PHE:O	2:B:528:TRP:N	2.31	0.62
2:B:254:ARG:HH22	2:B:258:GLU:HG2	1.64	0.62
2:B:24:ASN:HB3	2:B:27:SER:OG	2.00	0.61
2:B:93:PRO:HD2	2:B:559:ASP:HB3	1.82	0.61
2:B:182:LEU:HD11	2:B:239:ILE:HG22	1.82	0.61
2:A:217:PHE:CE1	2:A:322:VAL:HG22	2.35	0.61
2:A:86:GLU:HG3	2:A:111:LEU:HD21	1.81	0.61
2:B:108:VAL:O	2:B:110:ASN:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:217:PHE:CE1	2:A:336:LEU:HD11	2.35	0.61
2:A:321:VAL:HG13	2:A:321:VAL:O	2.00	0.60
2:A:328:GLY:HA3	2:A:331:GLU:CG	2.31	0.60
2:A:256:LEU:HB3	2:A:261:TYR:CE2	2.36	0.60
2:B:56:ARG:NH2	2:B:279:CYS:HB3	2.09	0.60
2:B:82:LEU:N	2:B:82:LEU:HD12	2.16	0.60
2:A:102:GLY:HA3	2:A:114:ARG:HH21	1.66	0.60
2:A:423:MET:HA	2:A:528:TRP:CZ2	2.36	0.60
2:B:423:MET:HA	2:B:528:TRP:CZ2	2.37	0.60
2:A:387:ASP:HA	2:A:484:ARG:HD3	1.83	0.60
1:E:2:U:H4'	1:E:3:U:O5'	2.01	0.60
2:A:102:GLY:HA3	2:A:114:ARG:NH2	2.16	0.59
2:B:81:LYS:HG2	2:B:177:ASP:OD2	2.01	0.59
2:A:48:ARG:HG2	2:A:159:LEU:HG	1.85	0.59
2:A:508:ARG:HG3	2:A:526:PHE:CB	2.32	0.59
2:A:398:GLU:HB3	2:A:403:THR:HG22	1.84	0.59
2:B:46:SER:O	2:B:50:LYS:HG2	2.02	0.59
2:B:254:ARG:NH2	2:B:258:GLU:HG2	2.16	0.59
2:B:5:THR:O	2:B:275:GLY:HA3	2.01	0.59
2:B:490:ARG:HA	2:B:490:ARG:HE	1.68	0.59
2:B:108:VAL:C	2:B:110:ASN:H	2.04	0.59
2:A:254:ARG:NH2	2:A:258:GLU:HG2	2.17	0.59
2:B:254:ARG:NH2	2:B:258:GLU:CG	2.66	0.59
2:A:287:THR:HG23	2:A:288:SER:N	2.17	0.59
2:B:179:VAL:HG22	2:B:289:CYS:CB	2.33	0.59
1:E:3:U:H2'	1:E:4:U:OP2	2.02	0.59
2:B:101:PHE:CD1	2:B:118:HIS:CE1	2.91	0.59
2:B:284:VAL:O	2:B:287:THR:HG22	2.03	0.58
2:B:126:LEU:HA	2:B:259:ARG:HH21	1.68	0.58
1:E:4:U:H6	2:A:556:SER:HG	1.49	0.58
2:A:439:LEU:N	2:A:439:LEU:HD22	2.16	0.58
2:B:21:LEU:HD12	2:B:22:PRO:CD	2.34	0.58
2:A:36:MET:HA	2:A:147:VAL:HG22	1.84	0.58
2:A:308:LEU:HB2	2:A:311:CYS:SG	2.44	0.58
2:A:337:ARG:O	2:A:341:GLU:HG3	2.03	0.58
1:E:4:U:P	2:A:557:GLY:H	2.26	0.58
2:A:254:ARG:HH22	2:A:258:GLU:HG2	1.69	0.58
2:A:287:THR:CG2	2:A:288:SER:N	2.66	0.58
2:B:264:GLY:HA2	2:B:276:TYR:CZ	2.38	0.58
2:A:386:ARG:HG2	2:A:387:ASP:N	2.17	0.58
2:B:403:THR:HB	2:B:404:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ALA:O	2:B:253:ILE:HG13	2.03	0.58
1:F:4:U:H2'	2:B:282:SER:O	2.03	0.58
2:A:38:TYR:O	2:A:144:VAL:HG23	2.03	0.58
2:A:232:ASP:O	2:A:236:GLU:HG3	2.04	0.57
2:A:34:HIS:O	2:A:37:VAL:HG23	2.05	0.57
2:A:1:SER:O	2:A:56:ARG:NH1	2.37	0.57
2:B:106:LYS:HB2	2:B:106:LYS:HZ2	1.68	0.57
2:A:423:MET:HA	2:A:528:TRP:CH2	2.39	0.57
2:A:374:HIS:O	2:A:474:LEU:HA	2.04	0.57
2:B:483:ASN:O	2:B:487:SER:HB3	2.04	0.57
2:A:268:ASN:ND2	2:A:272:GLN:NE2	2.44	0.57
2:B:386:ARG:HG2	2:B:415:TYR:CE1	2.39	0.57
2:A:201:VAL:HG13	2:A:202:GLU:N	2.20	0.57
2:A:192:GLY:HA3	2:A:316:ASN:OD1	2.04	0.57
2:A:187:MET:HB3	2:A:190:SER:HB2	1.86	0.57
2:A:182:LEU:O	2:A:186:VAL:HG23	2.04	0.57
2:B:555:TYR:HB2	2:B:560:ILE:HG13	1.86	0.57
2:A:74:LYS:HB2	2:A:186:VAL:HA	1.86	0.57
2:B:45:ALA:O	2:B:49:GLN:HG3	2.04	0.57
2:B:148:GLN:HG2	2:B:152:GLY:O	2.04	0.57
1:F:2:U:OP1	1:F:2:U:C6	2.58	0.56
2:B:74:LYS:O	2:B:77:THR:HG22	2.04	0.56
2:A:195:TYR:CB	2:A:199:GLN:HB2	2.29	0.56
2:B:547:LEU:HD12	2:B:547:LEU:H	1.70	0.56
2:A:211:LYS:HA	2:A:325:GLU:OE2	2.06	0.56
2:B:416:ALA:HB3	2:B:417:PRO:HD3	1.87	0.56
2:B:234:ARG:NH2	2:B:262:ILE:CD1	2.68	0.56
2:A:310:ASP:OD2	2:A:325:GLU:HG3	2.05	0.56
2:A:198:LYS:HA	2:A:201:VAL:HG12	1.87	0.56
2:A:20:LYS:O	2:A:22:PRO:HD3	2.05	0.56
2:B:116:VAL:CG2	2:B:117:ASN:N	2.69	0.56
2:A:465:ARG:HD3	2:A:543:SER:HA	1.87	0.56
2:B:330:GLN:HA	2:B:330:GLN:OE1	2.05	0.56
2:B:222:ARG:HG3	2:B:351:GLY:HA3	1.87	0.56
2:A:295:CYS:SG	2:A:320:LEU:HB2	2.45	0.56
2:A:531:ARG:NH2	2:B:198:LYS:HZ1	2.02	0.56
2:B:179:VAL:HG22	2:B:289:CYS:HB2	1.88	0.56
2:A:506:SER:O	2:A:509:ALA:N	2.38	0.55
2:A:399:THR:OG1	2:A:428:HIS:CE1	2.58	0.55
2:A:217:PHE:CD1	2:A:336:LEU:HD11	2.42	0.55
2:B:333:ALA:O	2:B:337:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:U:O2'	2:A:158:ARG:NH2	2.39	0.55
2:A:432:ILE:HG22	2:A:436:GLN:HE22	1.70	0.55
2:A:505:ARG:CG	2:A:529:ALA:O	2.55	0.55
2:B:336:LEU:O	2:B:337:ARG:C	2.44	0.55
2:A:195:TYR:HB3	2:A:199:GLN:CB	2.29	0.55
2:B:83:LEU:HD21	2:B:176:TYR:CD2	2.41	0.55
2:B:423:MET:HA	2:B:528:TRP:CH2	2.42	0.55
2:A:45:ALA:O	2:A:48:ARG:HB3	2.07	0.55
2:A:216:GLY:HA3	2:A:363:ILE:CD1	2.37	0.55
2:B:461:GLN:HB3	2:B:542:ALA:HA	1.89	0.54
2:A:237:GLU:HG3	2:A:257:THR:OG1	2.07	0.54
2:A:189:SER:HB2	2:A:203:PHE:CE1	2.42	0.54
2:B:372:VAL:HG12	2:B:373:ALA:H	1.72	0.54
2:B:3:SER:HB3	2:B:56:ARG:HE	1.72	0.54
2:B:236:GLU:O	2:B:239:ILE:HB	2.07	0.54
2:A:26:LEU:HD21	2:A:432:ILE:HD11	1.89	0.54
2:B:296:TYR:HB2	2:B:315:VAL:HG21	1.89	0.54
2:A:118:HIS:O	2:A:122:VAL:HG23	2.08	0.54
2:B:86:GLU:HA	2:B:111:LEU:HD21	1.88	0.54
2:A:461:GLN:HB3	2:A:542:ALA:HA	1.89	0.54
2:A:452:TYR:HA	2:A:562:HIS:O	2.07	0.54
2:A:93:PRO:HB3	2:A:561:TYR:HB2	1.89	0.54
1:E:4:U:H6	2:A:556:SER:OG	1.91	0.54
2:A:23:ILE:HG13	2:A:23:ILE:O	2.08	0.54
2:A:320:LEU:HD11	2:A:322:VAL:HG12	1.90	0.53
2:A:148:GLN:CG	2:A:150:GLU:HG2	2.38	0.53
2:A:531:ARG:HH22	2:B:198:LYS:HZ3	1.53	0.53
2:B:254:ARG:HH22	2:B:258:GLU:CG	2.21	0.53
2:A:101:PHE:CD1	2:A:101:PHE:N	2.77	0.53
1:F:4:U:H4'	2:B:141:LYS:HZ1	1.69	0.53
2:A:141:LYS:HD2	2:A:158:ARG:NH1	2.20	0.53
2:A:314:LEU:HB3	2:A:321:VAL:CG1	2.38	0.53
2:A:361:GLU:HG3	2:A:371:SER:HA	1.91	0.53
2:B:528:TRP:CA	2:B:533:LYS:HE3	2.39	0.53
2:A:123:TRP:CH2	2:A:174:ALA:HB2	2.43	0.53
2:B:359:ASP:OD2	2:B:362:LEU:HD13	2.09	0.53
2:B:436:GLN:HB2	2:B:438:GLN:HG2	1.91	0.53
2:A:432:ILE:HG23	2:A:436:GLN:HE22	1.72	0.53
2:A:303:CYS:SG	2:A:339:PHE:HE2	2.31	0.53
2:B:372:VAL:HG12	2:B:373:ALA:N	2.24	0.53
2:B:508:ARG:CZ	2:B:530:VAL:HG11	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:93:PRO:HG2	2:A:96:SER:HB2	1.90	0.53
2:A:137:THR:O	2:A:161:VAL:HA	2.09	0.53
2:B:310:ASP:HB2	2:B:325:GLU:HG2	1.90	0.52
2:B:365:SER:O	2:B:366:CYS:HB2	2.09	0.52
2:A:430:PHE:O	2:A:434:LEU:HB3	2.09	0.52
2:A:78:VAL:HG21	2:A:182:LEU:HA	1.92	0.52
2:B:223:CYS:O	2:B:227:THR:HG23	2.10	0.52
2:B:234:ARG:CZ	2:B:262:ILE:HD11	2.40	0.52
2:B:422:ARG:HA	2:B:426:MET:SD	2.49	0.52
1:E:3:U:O2'	1:E:4:U:OP2	2.28	0.52
2:A:564:LEU:O	2:A:566:ARG:N	2.43	0.52
2:A:506:SER:O	2:A:510:LYS:HG3	2.10	0.52
2:A:464:GLU:O	2:A:468:GLY:N	2.41	0.52
2:B:132:THR:O	2:B:259:ARG:HD2	2.09	0.52
2:A:245:LEU:CD1	2:A:253:ILE:HD12	2.37	0.52
2:B:13:PRO:HB3	2:B:42:SER:HG	1.75	0.52
2:B:461:GLN:HB3	2:B:542:ALA:CB	2.40	0.52
2:A:375:ASP:OD1	2:A:379:LYS:N	2.43	0.52
2:A:142:SER:O	2:A:143:GLU:HG2	2.10	0.52
2:A:56:ARG:HD2	2:A:226:SER:O	2.10	0.51
2:A:470:SER:O	2:A:474:LEU:HG	2.10	0.51
2:B:374:HIS:HB2	2:B:476:SER:CB	2.39	0.51
2:A:254:ARG:HH11	2:A:254:ARG:CA	2.22	0.51
2:B:254:ARG:HA	2:B:254:ARG:HH11	1.75	0.51
2:B:101:PHE:HD2	2:B:101:PHE:N	2.08	0.51
2:B:547:LEU:HB3	2:B:550:TRP:CD1	2.46	0.51
2:B:75:ALA:C	2:B:77:THR:H	2.13	0.51
2:A:21:LEU:HD11	2:A:397:TRP:HA	1.92	0.51
2:B:11:ILE:HD13	2:B:159:LEU:HD22	1.92	0.51
2:A:452:TYR:CE2	2:A:562:HIS:HB2	2.45	0.51
2:A:182:LEU:HD23	2:A:182:LEU:C	2.31	0.51
2:A:489:LEU:HD22	2:A:494:VAL:CB	2.39	0.51
2:B:534:LEU:HD12	2:B:535:LYS:H	1.75	0.51
2:A:164:ASP:O	2:A:168:ARG:HG3	2.11	0.51
2:A:508:ARG:NH1	2:A:530:VAL:HG11	2.25	0.51
2:A:148:GLN:C	2:A:150:GLU:H	2.14	0.51
2:B:88:ALA:HA	2:B:91:LEU:HD12	1.92	0.51
1:F:1:U:H5'	2:B:14:CYS:SG	2.50	0.51
2:B:196:SER:O	2:B:197:PRO:C	2.49	0.51
2:B:235:VAL:O	2:B:238:SER:OG	2.28	0.51
2:B:198:LYS:O	2:B:202:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:ARG:NH1	2:B:528:TRP:HE3	2.09	0.51
2:A:548:SER:OG	2:A:549:GLY:N	2.43	0.51
2:A:504:ALA:O	2:A:505:ARG:C	2.50	0.50
2:A:148:GLN:CD	2:A:150:GLU:HG2	2.31	0.50
2:A:539:ILE:HG23	2:A:540:PRO:HD2	1.94	0.50
2:A:21:LEU:CD1	2:A:397:TRP:HA	2.41	0.50
2:B:446:GLN:HB2	2:B:450:ALA:O	2.11	0.50
2:B:130:THR:O	2:B:130:THR:CG2	2.59	0.50
2:A:395:ALA:HB1	2:A:429:PHE:HZ	1.75	0.50
2:A:229:THR:O	2:A:232:ASP:N	2.44	0.50
2:B:461:GLN:HB3	2:B:542:ALA:HB2	1.94	0.50
2:A:399:THR:OG1	2:A:428:HIS:HE1	1.94	0.50
2:B:440:GLU:HG2	2:B:457:LEU:HD12	1.94	0.50
2:B:39:ALA:HA	2:B:143:GLU:O	2.12	0.50
2:A:505:ARG:HG2	2:A:529:ALA:O	2.11	0.50
2:B:547:LEU:CD1	2:B:547:LEU:H	2.20	0.50
2:B:101:PHE:CD2	2:B:101:PHE:N	2.78	0.50
2:B:534:LEU:HD12	2:B:535:LYS:N	2.27	0.50
2:B:211:LYS:NZ	2:B:312:THR:OG1	2.45	0.50
2:A:439:LEU:CD2	2:A:439:LEU:H	2.20	0.50
2:A:432:ILE:HG22	2:A:436:GLN:NE2	2.27	0.50
2:B:438:GLN:HA	2:B:438:GLN:OE1	2.11	0.50
2:B:544:GLN:O	2:B:545:LEU:C	2.49	0.50
2:B:330:GLN:O	2:B:333:ALA:HB3	2.12	0.50
2:A:372:VAL:HG12	2:A:373:ALA:N	2.27	0.50
2:A:61:ASP:O	2:A:65:ARG:NH1	2.44	0.50
2:B:454:ILE:HG21	2:B:462:ILE:CD1	2.41	0.50
2:B:147:VAL:HB	2:B:152:GLY:HA2	1.94	0.49
2:B:10:LEU:HD22	2:B:10:LEU:N	2.27	0.49
2:A:24:ASN:ND2	2:A:27:SER:H	2.11	0.49
2:B:460:PRO:O	2:B:464:GLU:HB2	2.12	0.49
2:B:499:THR:O	2:B:503:ARG:HG3	2.12	0.49
2:B:520:THR:HG23	2:B:524:TYR:CD1	2.47	0.49
2:B:108:VAL:C	2:B:110:ASN:N	2.65	0.49
2:A:403:THR:OG1	2:A:404:PRO:HD2	2.12	0.49
2:A:502:HIS:HA	2:A:505:ARG:HD2	1.95	0.49
2:A:506:SER:OG	2:A:510:LYS:HD2	2.12	0.49
2:A:148:GLN:HG2	2:A:150:GLU:N	2.25	0.49
2:A:459:LEU:N	2:A:460:PRO:CD	2.75	0.49
2:A:78:VAL:HG12	2:A:79:LYS:N	2.26	0.49
2:A:154:ARG:HG3	2:A:154:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:ALA:HA	2:B:425:LEU:HB2	1.93	0.49
2:B:5:THR:O	2:B:275:GLY:CA	2.60	0.49
2:A:455:GLU:HG3	2:A:566:ARG:O	2.12	0.49
1:F:1:U:H5	2:B:98:LYS:HZ3	1.57	0.49
2:A:284:VAL:HG23	2:A:287:THR:N	2.27	0.49
2:B:366:CYS:C	2:B:368:SER:H	2.14	0.49
2:B:461:GLN:N	2:B:461:GLN:OE1	2.39	0.49
2:B:361:GLU:HG2	2:B:370:VAL:O	2.13	0.49
2:B:7:THR:HG23	2:B:274:CYS:C	2.33	0.49
2:A:107:ASP:HB3	2:A:112:SER:OG	2.12	0.49
1:E:1:U:O4'	2:A:14:CYS:SG	2.71	0.49
2:A:24:ASN:HD21	2:A:26:LEU:HB3	1.78	0.49
2:A:429:PHE:O	2:A:433:LEU:HB2	2.11	0.49
2:B:390:THR:HG22	2:B:394:ARG:HD2	1.94	0.48
2:A:144:VAL:CG1	2:A:394:ARG:HG2	2.42	0.48
2:A:328:GLY:CA	2:A:331:GLU:HG2	2.41	0.48
2:A:207:THR:HG23	2:A:312:THR:HG21	1.95	0.48
2:B:434:LEU:HD13	2:B:511:LEU:CD2	2.43	0.48
2:B:507:VAL:O	2:B:508:ARG:C	2.50	0.48
2:A:36:MET:CE	2:A:491:LYS:HG2	2.44	0.48
2:B:518:ALA:O	2:B:521:CYS:HB2	2.13	0.48
2:B:526:PHE:C	2:B:528:TRP:N	2.67	0.48
2:A:216:GLY:CA	2:A:363:ILE:HD11	2.42	0.48
2:A:346:TYR:O	2:A:347:SER:OG	2.25	0.48
2:A:544:GLN:O	2:A:546:ASP:N	2.37	0.48
2:A:260:LEU:O	2:A:277:ARG:NH2	2.44	0.48
2:A:38:TYR:O	2:A:144:VAL:HA	2.14	0.48
2:A:79:LYS:HE2	2:A:81:LYS:CE	2.42	0.48
2:A:280:ARG:HD2	2:A:291:ASN:OD1	2.13	0.48
2:B:267:THR:HG23	2:B:271:GLY:O	2.13	0.48
2:A:463:ILE:HD12	2:A:525:LEU:HD21	1.96	0.48
2:A:368:SER:HB2	2:A:384:LEU:HD11	1.96	0.48
2:B:109:ARG:HG3	2:B:109:ARG:HH11	1.78	0.48
2:B:423:MET:HE1	2:B:497:LEU:HB3	1.96	0.47
1:E:2:U:OP1	1:E:2:U:C6	2.67	0.47
2:A:175:LEU:HA	2:A:178:VAL:HG23	1.96	0.47
2:B:501:ARG:HH11	2:B:501:ARG:HG3	1.79	0.47
2:B:461:GLN:HB3	2:B:542:ALA:CA	2.44	0.47
2:B:93:PRO:CB	2:B:561:TYR:HB2	2.44	0.47
2:B:38:TYR:HE1	2:B:147:VAL:HA	1.79	0.47
2:A:447:ILE:CD1	2:A:550:TRP:CZ3	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:LYS:HZ3	2:B:106:LYS:HB2	1.76	0.47
2:A:123:TRP:HB2	2:A:170:CYS:SG	2.54	0.47
2:A:4:TYR:CE1	2:A:279:CYS:SG	3.07	0.47
1:F:1:U:C5	2:B:98:LYS:HG2	2.49	0.47
1:E:1:U:C2'	1:E:2:U:H5	2.23	0.47
2:B:96:SER:HB3	2:B:168:ARG:NH2	2.30	0.47
2:B:119:ILE:HD13	2:B:169:VAL:HG11	1.96	0.47
2:B:115:ALA:O	2:B:119:ILE:HG13	2.15	0.47
2:A:148:GLN:HB3	2:A:153:GLY:O	2.15	0.47
2:B:461:GLN:CB	2:B:542:ALA:HB2	2.45	0.47
2:A:385:THR:HG23	2:A:386:ARG:N	2.28	0.47
2:B:490:ARG:NE	2:B:490:ARG:HA	2.30	0.47
2:B:201:VAL:HG21	2:B:383:TYR:HA	1.96	0.47
1:F:2:U:C2	2:B:95:HIS:O	2.68	0.47
2:A:375:ASP:HB3	2:A:381:VAL:HG21	1.97	0.47
2:B:12:THR:OG1	2:B:269:SER:HB3	2.15	0.47
2:B:501:ARG:NH1	2:B:528:TRP:CE3	2.83	0.47
2:A:505:ARG:HG3	2:A:529:ALA:O	2.15	0.46
2:B:219:TYR:CE1	2:B:221:THR:HG22	2.46	0.46
2:B:465:ARG:NH2	2:B:547:LEU:HD12	2.31	0.46
2:B:481:GLU:OE1	2:B:484:ARG:NH2	2.46	0.46
2:B:52:VAL:HG23	2:B:226:SER:HG	1.78	0.46
2:B:336:LEU:HD23	2:B:354:PRO:HB2	1.96	0.46
2:A:438:GLN:O	2:A:441:LYS:HB3	2.14	0.46
2:B:463:ILE:HG23	2:B:467:HIS:CD2	2.50	0.46
2:A:486:ALA:O	2:A:489:LEU:HB2	2.16	0.46
2:A:175:LEU:HD13	2:A:286:THR:HG23	1.94	0.46
2:A:116:VAL:O	2:A:120:ARG:HG3	2.15	0.46
2:A:175:LEU:HA	2:A:178:VAL:CG2	2.45	0.46
2:B:506:SER:O	2:B:509:ALA:HB3	2.15	0.46
2:A:24:ASN:HB3	2:A:27:SER:CB	2.46	0.46
2:B:368:SER:HB3	2:B:415:TYR:OH	2.15	0.46
2:B:556:SER:OG	2:B:557:GLY:N	2.47	0.46
1:E:4:U:C5	2:A:556:SER:HB3	2.51	0.46
2:A:245:LEU:HD13	2:A:253:ILE:CD1	2.43	0.46
2:A:227:THR:HB	2:A:347:SER:O	2.16	0.46
1:E:4:U:C6	2:A:556:SER:HB3	2.51	0.46
2:A:281:ALA:O	2:A:284:VAL:HG22	2.15	0.46
2:A:123:TRP:HH2	2:A:174:ALA:HB2	1.80	0.46
2:A:40:THR:HB	2:A:157:ALA:HA	1.97	0.46
2:B:134:ILE:HG13	2:B:259:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:HIS:HB2	2:B:476:SER:HB3	1.96	0.46
2:B:372:VAL:HG22	2:B:382:TYR:CD1	2.51	0.46
2:B:114:ARG:O	2:B:115:ALA:C	2.54	0.46
2:B:233:ILE:HD13	2:B:261:TYR:O	2.15	0.46
2:B:141:LYS:NZ	2:B:158:ARG:HH22	2.14	0.46
2:B:385:THR:OG1	2:B:386:ARG:N	2.49	0.46
2:B:361:GLU:HG2	2:B:371:SER:HA	1.98	0.46
2:B:346:TYR:O	2:B:347:SER:HB3	2.16	0.46
2:B:48:ARG:O	2:B:52:VAL:HG12	2.16	0.46
2:A:30:LEU:HD23	2:A:396:ALA:HA	1.98	0.46
2:A:447:ILE:HD11	2:A:550:TRP:CZ3	2.51	0.46
2:B:463:ILE:HG23	2:B:467:HIS:HD2	1.81	0.46
2:A:211:LYS:HD2	2:A:211:LYS:N	2.31	0.45
2:A:266:LEU:N	2:A:275:GLY:O	2.46	0.45
2:A:100:LYS:HE3	2:A:100:LYS:HB2	1.85	0.45
2:B:388:PRO:O	2:B:392:LEU:HG	2.16	0.45
2:A:540:PRO:HG2	2:A:541:ALA:H	1.80	0.45
1:F:2:U:O2'	1:F:3:U:P	2.74	0.45
2:B:4:TYR:CE2	2:B:52:VAL:CG2	2.99	0.45
2:A:175:LEU:O	2:A:176:TYR:C	2.55	0.45
2:B:540:PRO:O	2:B:541:ALA:C	2.54	0.45
2:B:331:GLU:H	2:B:331:GLU:CD	2.17	0.45
2:A:201:VAL:CG1	2:A:202:GLU:N	2.79	0.45
2:A:254:ARG:HH22	2:A:258:GLU:CG	2.29	0.45
2:A:467:HIS:HB2	2:A:471:ALA:HB2	1.98	0.45
2:B:78:VAL:CG1	2:B:79:LYS:N	2.79	0.45
2:B:256:LEU:O	2:B:260:LEU:N	2.49	0.45
2:A:385:THR:OG1	2:A:386:ARG:N	2.47	0.45
1:E:4:U:H6	2:A:556:SER:CB	2.29	0.45
2:A:175:LEU:HD23	2:A:178:VAL:HG21	1.98	0.45
2:B:335:ALA:O	2:B:338:ALA:HB3	2.16	0.45
2:B:11:ILE:HD12	2:B:45:ALA:HB1	1.99	0.45
2:A:93:PRO:HA	2:A:94:PRO:HD3	1.86	0.45
2:A:27:SER:O	2:A:31:LEU:N	2.50	0.45
2:A:30:LEU:O	2:A:494:VAL:HG22	2.17	0.45
2:B:374:HIS:CD2	2:B:378:GLY:O	2.63	0.45
2:A:10:LEU:HD12	2:A:10:LEU:N	2.16	0.45
2:A:52:VAL:HG13	2:A:226:SER:OG	2.16	0.45
2:A:177:ASP:O	2:A:178:VAL:C	2.54	0.45
2:A:65:ARG:O	2:A:69:LYS:HG3	2.16	0.45
2:A:50:LYS:HD3	2:A:50:LYS:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:555:TYR:O	2:B:556:SER:O	2.34	0.45
2:A:24:ASN:HD21	2:A:399:THR:HG22	1.82	0.45
2:B:374:HIS:HB2	2:B:476:SER:HB2	1.99	0.45
2:A:365:SER:O	2:A:366:CYS:HB2	2.17	0.45
2:B:192:GLY:HA2	2:B:314:LEU:HD11	1.98	0.45
2:B:138:ILE:HG23	2:B:138:ILE:O	2.17	0.45
2:B:428:HIS:O	2:B:432:ILE:HG12	2.17	0.45
2:B:144:VAL:HG21	2:B:394:ARG:HA	1.97	0.45
2:A:313:MET:HB3	2:A:322:VAL:HB	1.99	0.45
2:A:284:VAL:HG23	2:A:287:THR:H	1.82	0.45
2:B:434:LEU:HD13	2:B:511:LEU:HD23	1.98	0.45
2:B:260:LEU:O	2:B:277:ARG:NH2	2.50	0.45
1:E:3:U:H2'	2:A:446:GLN:HE22	1.81	0.45
2:A:319:ASP:CG	2:A:366:CYS:SG	2.96	0.44
2:B:93:PRO:CD	2:B:559:ASP:HB3	2.46	0.44
2:A:313:MET:HE2	2:A:313:MET:HB3	1.53	0.44
2:A:287:THR:CG2	2:A:288:SER:H	2.30	0.44
2:B:168:ARG:O	2:B:171:GLU:HB2	2.16	0.44
2:A:127:LEU:HD23	2:A:251:GLN:HG2	1.99	0.44
2:A:387:ASP:C	2:A:387:ASP:OD2	2.56	0.44
2:B:233:ILE:HG22	2:B:233:ILE:O	2.17	0.44
2:A:345:ARG:HB2	2:A:345:ARG:CZ	2.47	0.44
2:B:112:SER:O	2:B:113:SER:C	2.56	0.44
2:A:172:LYS:HE3	2:A:560:ILE:CD1	2.46	0.44
2:B:109:ARG:HG3	2:B:109:ARG:NH1	2.32	0.44
2:A:78:VAL:CG1	2:A:79:LYS:N	2.80	0.44
2:A:198:LYS:O	2:A:201:VAL:HG12	2.18	0.44
2:A:514:GLN:O	2:A:515:GLY:O	2.35	0.44
1:E:1:U:C3'	1:E:2:U:H5	2.31	0.44
2:A:67:VAL:O	2:A:70:GLU:HB2	2.18	0.44
2:B:216:GLY:O	2:B:357:GLU:N	2.47	0.44
2:B:106:LYS:CB	2:B:106:LYS:NZ	2.78	0.44
2:A:102:GLY:O	2:A:103:TYR:HB3	2.18	0.44
2:B:141:LYS:HZ2	2:B:158:ARG:HH22	1.64	0.43
2:B:93:PRO:CA	2:B:561:TYR:HB2	2.48	0.43
2:B:215:MET:HA	2:B:357:GLU:O	2.17	0.43
2:B:187:MET:SD	2:B:292:THR:HG22	2.57	0.43
2:A:194:GLN:HA	2:A:551:PHE:O	2.18	0.43
2:B:315:VAL:HG12	2:B:316:ASN:N	2.32	0.43
2:B:104:GLY:O	2:B:105:ALA:C	2.56	0.43
2:B:508:ARG:NE	2:B:530:VAL:CG1	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:LEU:O	2:B:339:PHE:HB3	2.18	0.43
2:A:314:LEU:HB3	2:A:321:VAL:HG13	1.99	0.43
2:B:202:GLU:O	2:B:206:ASN:OD1	2.36	0.43
2:A:229:THR:C	2:A:231:SER:N	2.71	0.43
2:A:187:MET:HG2	2:A:296:TYR:CD1	2.53	0.43
1:F:4:U:C6	2:B:556:SER:HB2	2.52	0.43
2:B:56:ARG:C	2:B:57:LEU:HD22	2.39	0.43
2:B:485:VAL:O	2:B:488:CYS:HB3	2.17	0.43
2:A:541:ALA:O	2:A:542:ALA:C	2.57	0.43
2:B:118:HIS:O	2:B:122:VAL:HG23	2.18	0.43
2:B:94:PRO:O	2:B:95:HIS:ND1	2.49	0.43
2:B:263:GLY:HA2	2:B:277:ARG:CZ	2.48	0.43
2:A:398:GLU:OE2	2:A:403:THR:HG21	2.18	0.43
2:A:254:ARG:NH2	2:A:258:GLU:CG	2.81	0.43
2:A:441:LYS:HE2	2:A:443:LEU:CD2	2.49	0.43
2:B:458:ASP:O	2:B:462:ILE:HG13	2.18	0.43
2:B:454:ILE:HG23	2:B:565:SER:O	2.19	0.43
1:F:2:U:HO2'	1:F:3:U:P	2.42	0.43
2:A:435:ALA:HB3	2:A:436:GLN:OE1	2.18	0.43
2:A:148:GLN:NE2	2:A:150:GLU:HG2	2.34	0.43
2:B:219:TYR:CD2	2:B:339:PHE:HE1	2.37	0.43
2:B:340:THR:CG2	2:B:350:PRO:HG3	2.48	0.43
2:A:103:TYR:C	2:A:103:TYR:CD1	2.92	0.43
2:A:296:TYR:HD1	2:A:315:VAL:HG21	1.84	0.43
2:A:39:ALA:HA	2:A:143:GLU:O	2.19	0.43
2:B:457:LEU:CD1	2:B:517:ARG:HH12	2.31	0.43
2:A:401:ARG:O	2:A:402:HIS:C	2.57	0.43
2:B:94:PRO:C	2:B:95:HIS:ND1	2.72	0.43
2:A:514:GLN:HB3	2:A:514:GLN:HE21	1.68	0.43
2:A:376:ALA:C	2:A:378:GLY:H	2.21	0.43
1:F:3:U:O2'	1:F:4:U:P	2.76	0.43
2:A:86:GLU:OE1	2:A:86:GLU:N	2.51	0.43
2:B:257:THR:HA	2:B:261:TYR:HB2	2.00	0.43
2:A:70:GLU:OE2	2:A:304:ARG:NH2	2.48	0.43
2:B:45:ALA:C	2:B:49:GLN:HG3	2.40	0.42
2:B:446:GLN:O	2:B:447:ILE:HD12	2.17	0.42
2:A:531:ARG:NH2	2:B:198:LYS:HZ2	2.16	0.42
2:A:489:LEU:HD23	2:A:489:LEU:HA	1.72	0.42
2:A:310:ASP:HB2	2:A:325:GLU:HG2	2.01	0.42
2:B:459:LEU:O	2:B:463:ILE:HG13	2.19	0.42
2:B:60:LEU:HD13	2:B:64:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:ARG:O	2:B:527:ASN:HB2	2.18	0.42
2:B:339:PHE:O	2:B:340:THR:C	2.57	0.42
2:B:336:LEU:HD23	2:B:354:PRO:HG2	2.01	0.42
2:A:36:MET:HA	2:A:147:VAL:CG2	2.49	0.42
2:A:372:VAL:HG22	2:A:382:TYR:CD1	2.53	0.42
2:B:36:MET:O	2:B:146:CYS:HA	2.19	0.42
2:B:172:LYS:HE2	2:B:559:ASP:O	2.19	0.42
2:A:368:SER:HB2	2:A:384:LEU:CD1	2.50	0.42
2:B:530:VAL:HG23	2:B:533:LYS:HD3	2.02	0.42
2:B:45:ALA:O	2:B:46:SER:C	2.58	0.42
2:A:236:GLU:CD	2:A:280:ARG:HH22	2.18	0.42
2:B:83:LEU:HD12	2:B:83:LEU:N	2.33	0.42
2:B:86:GLU:OE2	2:B:90:LYS:NZ	2.50	0.42
2:B:150:GLU:CD	2:B:150:GLU:H	2.23	0.42
2:B:23:ILE:O	2:B:23:ILE:HG23	2.20	0.42
2:A:205:VAL:O	2:A:206:ASN:C	2.57	0.42
2:A:230:GLU:HG2	2:A:262:ILE:O	2.19	0.42
2:A:504:ALA:C	2:A:506:SER:N	2.73	0.42
2:A:24:ASN:HD22	2:A:27:SER:HB2	1.84	0.42
2:A:495:PRO:HA	2:A:496:PRO:HD3	1.83	0.42
2:A:499:THR:CG2	2:A:503:ARG:NH2	2.82	0.42
2:B:424:ILE:HD13	2:B:494:VAL:HG11	2.01	0.42
2:B:495:PRO:HA	2:B:496:PRO:HD3	1.80	0.42
1:F:4:U:H2'	1:F:4:U:O2	2.19	0.42
2:A:48:ARG:CG	2:A:159:LEU:HG	2.49	0.42
2:A:433:LEU:HA	2:A:433:LEU:HD12	1.75	0.42
2:A:405:ILE:O	2:A:405:ILE:HG23	2.20	0.42
2:A:456:PRO:HA	2:A:459:LEU:CD2	2.50	0.42
2:A:254:ARG:NH1	2:A:254:ARG:O	2.53	0.42
2:A:201:VAL:O	2:A:205:VAL:HG23	2.20	0.42
2:B:83:LEU:CD1	2:B:83:LEU:N	2.83	0.42
2:A:385:THR:O	2:A:386:ARG:HB2	2.20	0.41
2:A:541:ALA:O	2:A:544:GLN:N	2.53	0.41
2:A:372:VAL:HG22	2:A:382:TYR:CE1	2.55	0.41
2:B:10:LEU:CD2	2:B:10:LEU:N	2.82	0.41
1:F:4:U:C6	2:B:556:SER:CB	3.03	0.41
2:A:26:LEU:HD11	2:A:432:ILE:HD12	2.02	0.41
2:A:499:THR:HG22	2:A:503:ARG:NH2	2.35	0.41
2:A:408:TRP:O	2:A:412:ILE:HG13	2.20	0.41
2:B:4:TYR:HE2	2:B:52:VAL:HG22	1.84	0.41
2:B:434:LEU:HD12	2:B:439:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:498:ARG:HD3	2:B:206:ASN:HD21	1.85	0.41
2:A:280:ARG:HG3	2:A:281:ALA:N	2.35	0.41
2:B:494:VAL:HA	2:B:495:PRO:HD2	1.84	0.41
2:B:401:ARG:HH11	2:B:401:ARG:HG2	1.84	0.41
2:A:368:SER:CB	2:A:385:THR:O	2.67	0.41
1:F:3:U:O3'	2:B:556:SER:O	2.39	0.41
2:A:316:ASN:HB2	2:A:319:ASP:HB3	2.02	0.41
2:B:321:VAL:O	2:B:321:VAL:HG13	2.20	0.41
2:B:423:MET:HG2	2:B:528:TRP:CZ3	2.56	0.41
2:A:365:SER:O	2:A:366:CYS:CB	2.68	0.41
2:A:241:GLN:OE1	2:A:250:ARG:HG3	2.20	0.41
2:A:368:SER:CB	2:A:384:LEU:HD11	2.51	0.41
2:A:386:ARG:HG2	2:A:387:ASP:H	1.82	0.41
2:B:48:ARG:NH2	2:B:156:PRO:HG2	2.36	0.41
2:A:201:VAL:HG23	2:A:370:VAL:HG22	2.03	0.41
2:A:222:ARG:O	2:A:223:CYS:C	2.59	0.41
2:A:336:LEU:O	2:A:339:PHE:HB3	2.21	0.41
2:B:329:THR:HG22	2:B:330:GLN:N	2.35	0.41
2:A:321:VAL:O	2:A:321:VAL:CG1	2.67	0.41
2:B:366:CYS:O	2:B:367:SER:HB2	2.21	0.41
2:B:75:ALA:C	2:B:77:THR:N	2.74	0.41
2:B:58:GLN:HB2	2:B:347:SER:HB2	2.02	0.41
2:B:456:PRO:O	2:B:459:LEU:HB2	2.21	0.41
2:B:200:ARG:O	2:B:204:LEU:HG	2.20	0.41
1:E:1:U:H2'	1:E:2:U:C4	2.54	0.40
2:B:374:HIS:N	2:B:476:SER:HB3	2.35	0.40
2:A:35:ASN:C	2:A:37:VAL:H	2.24	0.40
2:A:406:ASN:HB3	2:A:408:TRP:CD1	2.56	0.40
2:A:182:LEU:O	2:A:185:ALA:HB3	2.20	0.40
2:A:148:GLN:O	2:A:150:GLU:N	2.54	0.40
2:A:200:ARG:HH21	2:A:316:ASN:ND2	2.19	0.40
2:A:62:ASP:O	2:A:63:HIS:C	2.59	0.40
2:A:361:GLU:HA	2:A:370:VAL:O	2.22	0.40
2:B:319:ASP:OD2	2:B:366:CYS:HA	2.22	0.40
2:B:458:ASP:HA	2:B:461:GLN:HE22	1.86	0.40
2:B:167:VAL:O	2:B:171:GLU:HG3	2.21	0.40
2:B:78:VAL:HG12	2:B:79:LYS:N	2.36	0.40
1:F:4:U:O2'	2:B:282:SER:HB2	2.21	0.40
1:F:3:U:O2'	2:B:446:GLN:OE1	2.36	0.40
2:A:268:ASN:C	2:A:270:LYS:H	2.25	0.40
2:A:77:THR:HG22	2:A:78:VAL:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:254:ARG:O	2:A:257:THR:HB	2.21	0.40
2:A:36:MET:O	2:A:146:CYS:HA	2.21	0.40
2:B:368:SER:HA	2:B:386:ARG:HB3	2.03	0.40
2:B:268:ASN:OD1	2:B:270:LYS:N	2.50	0.40
2:A:85:ILE:HG12	2:A:173:MET:SD	2.62	0.40
1:F:3:U:C2'	1:F:3:U:O2	2.68	0.40
2:B:110:ASN:O	2:B:111:LEU:C	2.59	0.40
2:A:530:VAL:C	2:A:532:THR:H	2.25	0.40
2:A:198:LYS:C	2:A:201:VAL:HG12	2.42	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	564/570 (99%)	466 (83%)	74 (13%)	24 (4%)	3	13
2	B	563/570 (99%)	466 (83%)	76 (14%)	21 (4%)	4	17
All	All	1127/1140 (99%)	932 (83%)	150 (13%)	45 (4%)	4	15

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	23	ILE
2	A	505	ARG
2	A	565	SER
2	B	109	ARG
2	B	113	SER
2	B	151	LYS
2	B	556	SER
2	A	14	CYS
2	A	515	GLY

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Mol	Chain	Res	Type
2	A	545	LEU
2	B	495	PRO
2	B	527	ASN
2	B	544	GLN
2	A	151	LYS
2	A	542	ALA
2	A	544	GLN
2	B	43	ARG
2	B	513	SER
2	B	548	SER
2	A	19	SER
2	A	193	PHE
2	A	367	SER
2	A	437	GLU
2	A	540	PRO
2	B	564	LEU
2	A	36	MET
2	A	269	SER
2	A	376	ALA
2	A	402	HIS
2	B	94	PRO
2	B	339	PHE
2	A	386	ARG
2	B	25	PRO
2	B	149	PRO
2	B	406	ASN
2	B	514	GLN
2	A	178	VAL
2	A	149	PRO
2	B	558	GLY
2	A	416	ALA
2	A	496	PRO
2	B	197	PRO
2	B	479	PRO
2	A	183	PRO
2	B	23	ILE

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
2	A	475/485 (98%)	450 (95%)	25 (5%)	28 63
2	B	474/485 (98%)	443 (94%)	31 (6%)	21 52
All	All	949/970 (98%)	893 (94%)	56 (6%)	24 58

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	10	LEU
2	A	26	LEU
2	A	56	ARG
2	A	68	LEU
2	A	77	THR
2	A	83	LEU
2	A	86	GLU
2	A	94	PRO
2	A	116	VAL
2	A	131	GLU
2	A	177	ASP
2	A	221	THR
2	A	273	ASN
2	A	276	TYR
2	A	287	THR
2	A	309	GLN
2	A	331	GLU
2	A	364	THR
2	A	365	SER
2	A	386	ARG
2	A	431	SER
2	A	459	LEU
2	A	469	LEU
2	A	508	ARG
2	A	534	LEU
2	B	29	SER
2	B	55	ASP
2	B	56	ARG
2	B	68	LEU
2	B	82	LEU
2	B	94	PRO
2	B	98	LYS
2	B	101	PHE

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Mol	Chain	Res	Type
2	B	106	LYS
2	B	112	SER
2	B	113	SER
2	B	126	LEU
2	B	135	ASP
2	B	144	VAL
2	B	179	VAL
2	B	231	SER
2	B	269	SER
2	B	308	LEU
2	B	355	GLN
2	B	364	THR
2	B	384	LEU
2	B	407	SER
2	B	425	LEU
2	B	439	LEU
2	B	459	LEU
2	B	490	ARG
2	B	513	SER
2	B	517	ARG
2	B	531	ARG
2	B	547	LEU
2	B	550	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	24	ASN
2	A	35	ASN
2	A	49	GLN
2	A	117	ASN
2	A	194	GLN
2	A	206	ASN
2	A	272	GLN
2	A	273	ASN
2	A	309	GLN
2	A	428	HIS
2	A	446	GLN
2	A	483	ASN
2	A	502	HIS
2	A	514	GLN
2	B	24	ASN

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Mol	Chain	Res	Type
2	B	35	ASN
2	B	49	GLN
2	B	148	GLN
2	B	206	ASN
2	B	273	ASN
2	B	316	ASN
2	B	355	GLN
2	B	374	HIS
2	B	483	ASN
2	B	502	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	4/4 (100%)	3 (75%)	3 (75%)
1	F	4/4 (100%)	3 (75%)	3 (75%)
All	All	8/8 (100%)	6 (75%)	6 (75%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	2	U
1	E	3	U
1	E	4	U
1	F	2	U
1	F	3	U
1	F	4	U

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	1	U
1	E	2	U
1	E	3	U
1	F	1	U
1	F	2	U
1	F	3	U

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.