



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:03 pm BST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

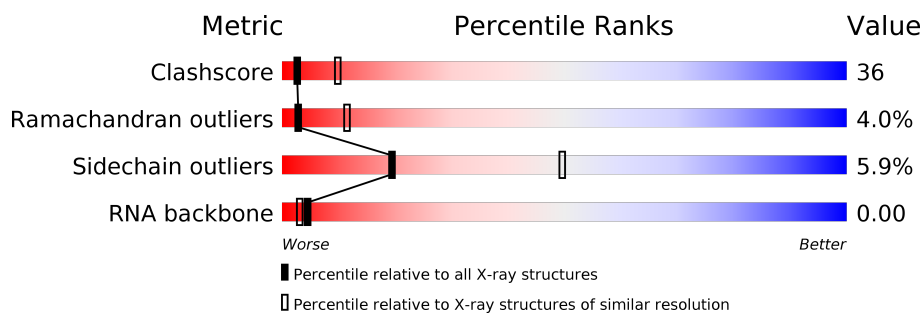
1 Overall quality at a glance

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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 



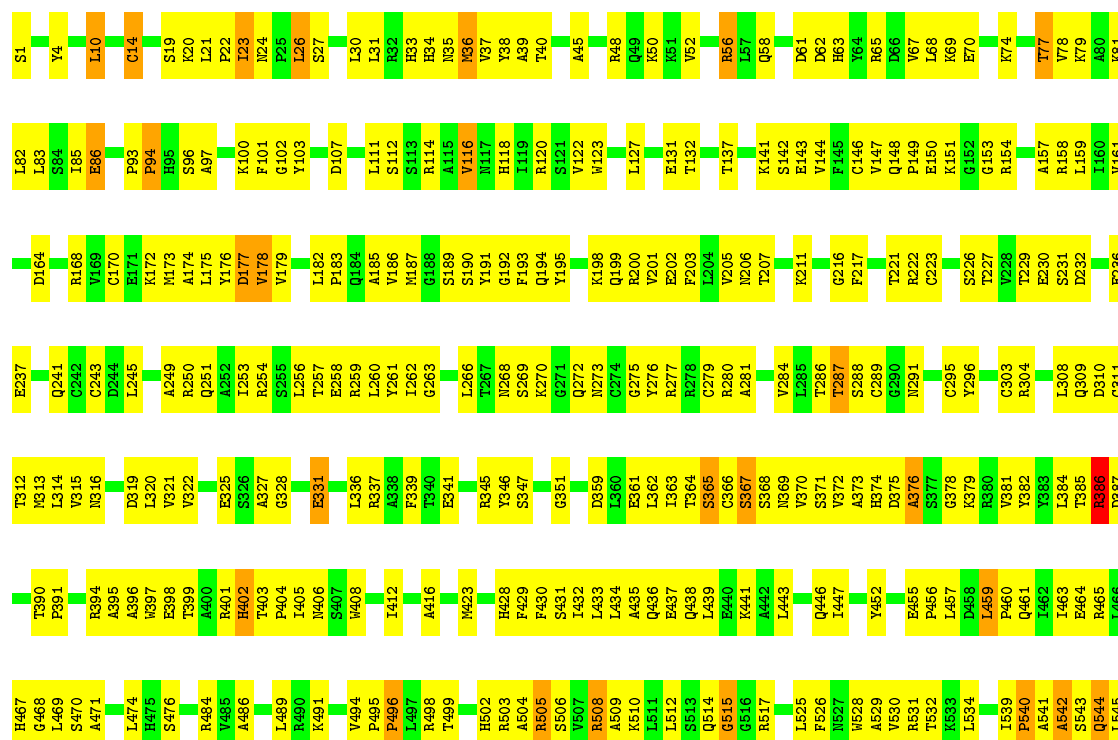
- Molecule 1: 5'-R(*UP*UP*UP*U)-3'

Chain F: 



- Molecule 2: polypeptide

Chain A: 



D546
L547
S548
G549
W550
F551
S556
G557
I560
Y561
H562
S563
L564
S565
R566
ALA
ARG
PRO
ARG

- Molecule 2: polyprotein

Chain B:  44% 50% 5%

K533	I462	P388	V315	T227	Q148	V78	S1
L534	I463	T389	N316	S231	P149	K79	M2
K535	E464	T390	G317	D232	E150	A90	S3
P540	R465	P391	D318	L233	K151	K81	Y4
	L466	L392	D319	T233	G152	L82	T5
A541	H467	A393	L320	R234	G153	L83	W6
A542	S476	R394	V321	V235	P156	E86	T7
S543		V322	E236				
Q544	E398	E325	E237	E238	A157	E87	L10
L545	P479	E401	S238	L239	R158	A88	I11
D546	G480	H402	T329	A249	C89	S89	T12
L547	E481	T403	Q330		L160	K90	L91
S548	L482	P404	E331	T253	V167	T32	C14
W550	N483	R484	D332	T257	R168	P93	L21
	V485	T405	A333	E258	V169	P94	
Y555	A486	N406	A334	S255	G170	H95	N24
	S407	A407	A335	L256	E171	S96	T23
S556	S487	N408	L336	T257	K172	A97	I24
G557	C488	L409	R337	R259	E176	K98	P25
D559	L489	Y415	A338	L260	D177	F101	L26
I560	R490	A416	F339	Y261	V178	S27	S27
Y561	V494	P417	T340	L262	V179	G104	N28
I564	P495	A421	Y346	G263	G104	A105	S29
	P496	R422	S347	G264	A105	K106	
S565	L497	N423	P350	T267	D107	V108	V37
ALA	R498	T424	G351	N268	R109	R38	Y38
ARG	T499	L425	P354	S269	N110	A39	S42
ARG	N500	L426	P354	K270	L111	S29	
PRO	R501	N426	Q355	G271	Y191	S112	S44
ARG	H502	T427	Q355	G271	G192	S112	A45
S506	R503	H428	P356	C274	Q194	S113	S46
	S506	L432	E357	G274	V195	R114	L57
V507	V507	L433	V368	G275	S196	A115	R48
R508	L434	L434	D359	Y276	P197	V116	Q49
A509	A435	A435	L360	R277	K198	M117	K50
C510	Q436	Q436	E361	R278	Q199	H118	V52
L511	P437	P437	L362	C279	R200	I119	D55
L512	L512	Q438	L363	R280	V201	V122	R56
S513	S513	L439	T364	A281	E202	V122	O58
Q514	Q514	E440	S365	S282	F203	L126	V59
G515	G515	R441	C366	G283	L204	L126	L60
R517	R517	A442	S367	V284	V205	T130	D61
A518	A518	L443	S368	V284	N206	T130	Y64
A519	A519	D444	N369	T287	K211	E131	R65
T520	T520	Q445	V370	S288	K212	L131	L68
C521	C521	Q446	S371	C289	K212	T132	K74
G522	G522	L447	V372	T292	M215	F133	A75
R523	R523	A450	A373	T292	G216	D135	S76
Y524	Y524	A450	H374	Y296	Y219	D135	T77
L525	L525	L454	G378	Y296	Y219	I138	R74
F526	F526	L454	G378	L308	D220	L138	
N527	N527	P456	Y382	Q309	T221	K141	A75
L528	L528	L457	Y383	D310	R222	S142	S76
A529	A529	D458	L384	C311	C223	E143	R74
V530	V530	L459	T385	T312	F224	V144	
R531	R531	P460	R386	T312	P224	F145	A75
E532	E532	O461	R383	N313	D225	C146	S76
S533	S533	T461	N383	L314	S226	V417	T77

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	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(°)	Ideal(°)
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 ⓘ

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
2:A:195:TYR:HB3	2:A:199:GLN:HB2	1.43	1.00
1:F:1:U:HO5'	1:F:1:U:H6	1.03	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:175:LEU:HD13	2:A:286:THR:CG2	2.18	0.73
2:A:179:VAL:HG13	2:A:289:CYS:HB2	1.70	0.73
2:A:33:HIS:CE1	2:B:212:LYS:HE2	2.24	0.73
2:B:388:PRO:HG2	2:B:488:CYS:SG	2.29	0.73
2:A:374:HIS:ND1	2:A:476:SER:HB2	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:HH11	2:B:158:ARG:HB3	1.54	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
2:A:328:GLY:HA3	2:A:331:GLU:HG2	1.73	0.71
2:A:439:LEU:HB3	2:A:457:LEU:HG	1.72	0.71
2:B:308:LEU:HB3	2:B:311:CYS:SG	2.30	0.71
2:B:82:LEU:H	2:B:82:LEU:HD12	1.55	0.71
1:E:3:U:C2'	1:E:4:U:OP2	2.37	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:E:1:U:H2'	1:E:2:U:H5	1.56	0.70
1:F:3:U:O2'	1:F:4:U:OP2	2.08	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:A:313:MET:HE2	2:A:322:VAL:HB	1.77	0.67
2:A:58:GLN:HB2	2:A:347:SER:HB3	1.77	0.67
2:B:390:THR:HB	2:B:391:PRO:HD3	1.75	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:263:GLY:HA2	2:A:277:ARG:NH1	2.12	0.65
2:A:386:ARG:NE	2:A:387:ASP:O	2.29	0.65
2:B:506:SER:O	2:B:510:LYS:HG3	1.97	0.65
2:A:172:LYS:HE3	2:A:560:ILE:HD13	1.77	0.65
2:B:86:GLU:CG	2:B:111:LEU:HD11	2.27	0.65
2:B:255:SER:O	2:B:259:ARG:HB2	1.96	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:A:36:MET:HE3	2:A:491:LYS:HG2	1.80	0.63
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:B:126:LEU:HA	2:B:259:ARG:NH2	2.14	0.63
2:B:93:PRO:HB3	2:B:561:TYR:HB2	1.80	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:224:PHE:CD2	2:B:318:ASP:HB3	2.33	0.62
2:B:126:LEU:HD21	2:B:256:LEU:CD2	2.26	0.62
2:A:457:LEU:CD1	2:A:517:ARG:HH21	2.12	0.62
2:B:4:TYR:CE2	2:B:52:VAL:HG22	2.35	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:254:ARG:HH22	2:B:258:GLU:HG2	1.64	0.62
2:B:526:PHE:O	2:B:528:TRP:N	2.31	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: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:182:LEU:HD11	2:B:239:ILE:HG22	1.82	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:256:LEU:HB3	2:A:261:TYR:CE2	2.36	0.60
2:A:328:GLY:HA3	2:A:331:GLU:CG	2.31	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:A:48:ARG:HG2	2:A:159:LEU:HG	1.85	0.59
2:B:81:LYS:HG2	2:B:177:ASP:OD2	2.01	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:A:254:ARG:NH2	2:A:258:GLU:HG2	2.17	0.59
2:B:108:VAL:C	2:B:110:ASN:H	2.04	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
2:B:101:PHE:CD1	2:B:118:HIS:CE1	2.91	0.59
1:E:3:U:H2'	1:E:4:U:OP2	2.02	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: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
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
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:249:ALA:O	2:B:253:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:THR:HB	2:B:404:PRO:HD2	1.86	0.58
2:A:38:TYR:O	2:A:144:VAL:HG23	2.03	0.58
1:F:4:U:H2'	2:B:282:SER:O	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:423:MET:HA	2:A:528:TRP:CH2	2.39	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: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: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:555:TYR:HB2	2:B:560:ILE:HG13	1.86	0.57
2:B:148:GLN:HG2	2:B:152:GLY:O	2.04	0.57
2:B:74:LYS:O	2:B:77:THR:HG22	2.04	0.56
1:F:2:U:OP1	1:F:2:U:C6	2.58	0.56
2:A:211:LYS:HA	2:A:325:GLU:OE2	2.06	0.56
2:A:195:TYR:CB	2:A:199:GLN:HB2	2.29	0.56
2:B:416:ALA:HB3	2:B:417:PRO:HD3	1.87	0.56
2:B:547:LEU:HD12	2:B:547:LEU:H	1.70	0.56
2:A:310:ASP:OD2	2:A:325:GLU:HG3	2.05	0.56
2:B:234:ARG:NH2	2:B:262:ILE:CD1	2.68	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:A:465:ARG:HD3	2:A:543:SER:HA	1.87	0.56
2:B:116:VAL:CG2	2:B:117:ASN:N	2.69	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:217:PHE:CD1	2:A:336:LEU:HD11	2.42	0.55
2:A:399:THR:OG1	2:A:428:HIS:CE1	2.58	0.55
2:A:506:SER:O	2:A:509:ALA:N	2.38	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:A:45:ALA:O	2:A:48:ARG:HB3	2.07	0.55
2:B:423:MET:HA	2:B:528:TRP:CH2	2.42	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:189:SER:HB2	2:A:203:PHE:CE1	2.42	0.54
2:A:237:GLU:HG3	2:A:257:THR:OG1	2.07	0.54
2:B:372:VAL:HG12	2:B:373:ALA:H	1.72	0.54
2:A:26:LEU:HD21	2:A:432:ILE:HD11	1.89	0.54
2:B:236:GLU:O	2:B:239:ILE:HB	2.07	0.54
2:B:296:TYR:HB2	2:B:315:VAL:HG21	1.89	0.54
2:B:3:SER:HB3	2:B:56:ARG:HE	1.72	0.54
2:A:118:HIS:O	2:A:122:VAL:HG23	2.08	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
2:B:86:GLU:HA	2:B:111:LEU:HD21	1.88	0.54
2:A:23:ILE:HG13	2:A:23:ILE:O	2.08	0.54
1:E:4:U:H6	2:A:556:SER:OG	1.91	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:101:PHE:CD1	2:A:101:PHE:N	2.77	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: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
1:F:4:U:H4'	2:B:141:LYS:HZ1	1.69	0.53
2:A:123:TRP:CH2	2:A:174:ALA:HB2	2.43	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: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:303:CYS:SG	2:A:339:PHE:HE2	2.31	0.53
2:A:432:ILE:HG23	2:A:436:GLN:HE22	1.72	0.53
2:B:372:VAL:HG12	2:B:373:ALA:N	2.24	0.53
2:A:137:THR:O	2:A:161:VAL:HA	2.09	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:B:508:ARG:CZ	2:B:530:VAL:HG11	2.39	0.53
2:B:310:ASP:HB2	2:B:325:GLU:HG2	1.90	0.52
2:A:430:PHE:O	2:A:434:LEU:HB3	2.09	0.52
2:B:365:SER:O	2:B:366:CYS:HB2	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
2:A:564:LEU:O	2:A:566:ARG:N	2.43	0.52
1:E:3:U:O2'	1:E:4:U:OP2	2.28	0.52
2:A:464:GLU:O	2:A:468:GLY:N	2.41	0.52
2:A:506:SER:O	2:A:510:LYS:HG3	2.10	0.52
2:A:142:SER:O	2:A:143:GLU:HG2	2.10	0.52
2:A:245:LEU:CD1	2:A:253:ILE:HD12	2.37	0.52
2:A:375:ASP:OD1	2:A:379:LYS:N	2.43	0.52
2:B:132:THR:O	2:B:259:ARG:HD2	2.09	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:56:ARG:HD2	2:A:226:SER:O	2.10	0.51
2:A:254:ARG:HH11	2:A:254:ARG:CA	2.22	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:B:101:PHE:HD2	2:B:101:PHE:N	2.08	0.51
2:B:254:ARG:HA	2:B:254:ARG:HH11	1.75	0.51
2:A:21:LEU:HD11	2:A:397:TRP:HA	1.92	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:452:TYR:CE2	2:A:562:HIS:HB2	2.45	0.51
2:B:11:ILE:HD13	2:B:159:LEU:HD22	1.92	0.51
2:A:164:ASP:O	2:A:168:ARG:HG3	2.11	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:148:GLN:C	2:A:150:GLU:H	2.14	0.51
2:A:508:ARG:NH1	2:A:530:VAL:HG11	2.25	0.51
2:B:88:ALA:HA	2:B:91:LEU:HD12	1.92	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
1:F:1:U:H5'	2:B:14:CYS:SG	2.50	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:A:548:SER:OG	2:A:549:GLY:N	2.43	0.51
2:B:501:ARG:NH1	2:B:528:TRP:HE3	2.09	0.51
2:A:148:GLN:CD	2:A:150:GLU:HG2	2.31	0.50
2:A:21:LEU:CD1	2:A:397:TRP:HA	2.41	0.50
2:A:504:ALA:O	2:A:505:ARG:C	2.50	0.50
2:A:539:ILE:HG23	2:A:540:PRO:HD2	1.94	0.50
2:A:395:ALA:HB1	2:A:429:PHE:HZ	1.75	0.50
2:B:130:THR:O	2:B:130:THR:CG2	2.59	0.50
2:B:446:GLN:HB2	2:B:450:ALA:O	2.11	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:39:ALA:HA	2:B:143:GLU:O	2.12	0.50
2:B:440:GLU:HG2	2:B:457:LEU:HD12	1.94	0.50
2:A:505:ARG:HG2	2:A:529:ALA:O	2.11	0.50
2:B:101:PHE:N	2:B:101:PHE:CD2	2.78	0.50
2:B:211:LYS:NZ	2:B:312:THR:OG1	2.45	0.50
2:B:534:LEU:HD12	2:B:535:LYS:N	2.27	0.50
2:B:547:LEU:CD1	2:B:547:LEU:H	2.20	0.50
2:A:432:ILE:HG22	2:A:436:GLN:NE2	2.27	0.50
2:A:439:LEU:CD2	2:A:439:LEU:H	2.20	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: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:330:GLN:O	2:B:333:ALA:HB3	2.12	0.50
2:B:454:ILE:HG21	2:B:462:ILE:CD1	2.41	0.50
2:B:10:LEU:HD22	2:B:10:LEU:N	2.27	0.49
2:B:147:VAL:HB	2:B:152:GLY:HA2	1.94	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:148:GLN:HG2	2:A:150:GLU:N	2.25	0.49
2:A:403:THR:OG1	2:A:404:PRO:HD2	2.12	0.49
2:A:459:LEU:N	2:A:460:PRO:CD	2.75	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:154:ARG:HG3	2:A:154:ARG:HH11	1.77	0.49
2:A:78:VAL:HG12	2:A:79:LYS:N	2.26	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:A:455:GLU:HG3	2:A:566:ARG:O	2.12	0.49
2:B:5:THR:O	2:B:275:GLY:CA	2.60	0.49
2:A:284:VAL:HG23	2:A:287:THR:N	2.27	0.49
2:B:7:THR:HG23	2:B:274:CYS:C	2.33	0.49
2:B:361:GLU:HG2	2:B:370:VAL:O	2.13	0.49
2:B:366:CYS:C	2:B:368:SER:H	2.14	0.49
2:B:461:GLN:OE1	2:B:461:GLN:N	2.39	0.49
1:F:1:U:H5	2:B:98:LYS:HZ3	1.57	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:A:207:THR:HG23	2:A:312:THR:HG21	1.95	0.48
2:A:328:GLY:CA	2:A:331:GLU:HG2	2.41	0.48
2:A:144:VAL:CG1	2:A:394:ARG:HG2	2.42	0.48
2:B:390:THR:HG22	2:B:394:ARG:HD2	1.94	0.48
2:B:434:LEU:HD13	2:B:511:LEU:CD2	2.43	0.48
2:A:36:MET:CE	2:A:491:LYS:HG2	2.44	0.48
2:B:507:VAL:O	2:B:508:ARG:C	2.50	0.48
2:B:518:ALA:O	2:B:521:CYS:HB2	2.13	0.48
2:A:216:GLY:CA	2:A:363:ILE:HD11	2.42	0.48
2:B:526:PHE:C	2:B:528:TRP:N	2.67	0.48
2:A:260:LEU:O	2:A:277:ARG:NH2	2.44	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:38:TYR:O	2:A:144:VAL:HA	2.14	0.48
2:A:280:ARG:HD2	2:A:291:ASN:OD1	2.13	0.48
2:A:79:LYS:HE2	2:A:81:LYS:CE	2.42	0.48
2:A:463:ILE:HD12	2:A:525:LEU:HD21	1.96	0.48
2:B:267:THR:HG23	2:B:271:GLY:O	2.13	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
2:A:175:LEU:HA	2:A:178:VAL:HG23	1.96	0.47
2:B:461:GLN:HB3	2:B:542:ALA:CA	2.44	0.47
2:B:501:ARG:HH11	2:B:501:ARG:HG3	1.79	0.47
1:E:2:U:OP1	1:E:2:U:C6	2.67	0.47
2:A:447:ILE:CD1	2:A:550:TRP:CZ3	2.98	0.47
2:B:38:TYR:HE1	2:B:147:VAL:HA	1.79	0.47
2:B:93:PRO:CB	2:B:561:TYR:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:106:LYS:HB2	2:B:106:LYS:HZ3	1.76	0.47
2:B:119:ILE:HD13	2:B:169:VAL:HG11	1.96	0.47
2:B:96:SER:HB3	2:B:168:ARG:NH2	2.30	0.47
1:E:1:U:C2'	1:E:2:U:H5	2.23	0.47
1:F:1:U:C5	2:B:98:LYS:HG2	2.49	0.47
2:B:115:ALA:O	2:B:119:ILE:HG13	2.15	0.47
2:B:461:GLN:CB	2:B:542:ALA:HB2	2.45	0.47
2:A:148:GLN:HB3	2:A:153:GLY:O	2.15	0.47
2:A:385:THR:HG23	2:A:386:ARG:N	2.28	0.47
2:B:201:VAL:HG21	2:B:383:TYR:HA	1.96	0.47
2:B:490:ARG:HA	2:B:490:ARG:NE	2.30	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
1:F:2:U:C2	2:B:95:HIS:O	2.68	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:A:438:GLN:O	2:A:441:LYS:HB3	2.14	0.46
2:B:336:LEU:HD23	2:B:354:PRO:HB2	1.96	0.46
2:B:463:ILE:HG23	2:B:467:HIS:CD2	2.50	0.46
2:B:52:VAL:HG23	2:B:226:SER:HG	1.78	0.46
2:A:175:LEU:HD13	2:A:286:THR:HG23	1.94	0.46
2:A:486:ALA:O	2:A:489:LEU:HB2	2.16	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:A:227:THR:HB	2:A:347:SER:O	2.16	0.46
2:A:245:LEU:HD13	2:A:253:ILE:CD1	2.43	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:123:TRP:HH2	2:A:174:ALA:HB2	1.80	0.46
2:A:281:ALA:O	2:A:284:VAL:HG22	2.15	0.46
2:A:40:THR:HB	2:A:157:ALA:HA	1.97	0.46
1:E:4:U:C6	2:A:556:SER:HB3	2.51	0.46
2:B:114:ARG:O	2:B:115:ALA:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ILE:HD13	2:B:261:TYR:O	2.15	0.46
2:B:134:ILE:HG13	2:B:259:ARG:HB3	1.97	0.46
2:B:372:VAL:HG22	2:B:382:TYR:CD1	2.51	0.46
2:B:374:HIS:HB2	2:B:476:SER:HB3	1.96	0.46
2:B:141:LYS:NZ	2:B:158:ARG:HH22	2.14	0.46
2:B:346:TYR:O	2:B:347:SER:HB3	2.16	0.46
2:B:361:GLU:HG2	2:B:371:SER:HA	1.98	0.46
2:B:385:THR:OG1	2:B:386:ARG:N	2.49	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:B:48:ARG:O	2:B:52:VAL:HG12	2.16	0.46
2:A:100:LYS:HE3	2:A:100:LYS:HB2	1.85	0.45
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:540:PRO:HG2	2:A:541:ALA:H	1.80	0.45
2:B:388:PRO:O	2:B:392:LEU:HG	2.16	0.45
2:A:175:LEU:O	2:A:176:TYR:C	2.55	0.45
2:B:331:GLU:H	2:B:331:GLU:CD	2.17	0.45
2:B:4:TYR:CE2	2:B:52:VAL:CG2	2.99	0.45
2:B:540:PRO:O	2:B:541:ALA:C	2.54	0.45
1:F:2:U:O2'	1:F:3:U:P	2.74	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:A:175:LEU:HD23	2:A:178:VAL:HG21	1.98	0.45
2:A:385:THR:OG1	2:A:386:ARG:N	2.47	0.45
2:A:93:PRO:HA	2:A:94:PRO:HD3	1.86	0.45
2:B:256:LEU:O	2:B:260:LEU:N	2.49	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
1:E:4:U:H6	2:A:556:SER:CB	2.29	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:177:ASP:O	2:A:178:VAL:C	2.54	0.45
2:A:52:VAL:HG13	2:A:226:SER:OG	2.16	0.45
2:A:50:LYS:HD3	2:A:50:LYS:HA	1.82	0.45
2:A:65:ARG:O	2:A:69:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:24:ASN:HD21	2:A:399:THR:HG22	1.82	0.45
2:A:365:SER:O	2:A:366:CYS:HB2	2.17	0.45
2:B:138:ILE:HG23	2:B:138:ILE:O	2.17	0.45
2:B:192:GLY:HA2	2:B:314:LEU:HD11	1.98	0.45
2:B:428:HIS:O	2:B:432:ILE:HG12	2.17	0.45
2:B:374:HIS:HB2	2:B:476:SER:HB2	1.99	0.45
2:B:555:TYR:O	2:B:556:SER:O	2.34	0.45
2:A:284:VAL:HG23	2:A:287:THR:H	1.82	0.45
2:A:313:MET:HB3	2:A:322:VAL:HB	1.99	0.45
2:B:144:VAL:HG21	2:B:394:ARG:HA	1.97	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:A:127:LEU:HD23	2:A:251:GLN:HG2	1.99	0.44
2:A:287:THR:CG2	2:A:288:SER:H	2.30	0.44
2:A:313:MET:HE2	2:A:313:MET:HB3	1.53	0.44
2:B:168:ARG:O	2:B:171:GLU:HB2	2.16	0.44
2:B:93:PRO:CD	2:B:559:ASP:HB3	2.46	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:CZ	2:A:345:ARG:HB2	2.47	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:B:112:SER:O	2:B:113:SER:C	2.56	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
2:A:78:VAL:CG1	2:A:79:LYS:N	2.80	0.44
2:A:67:VAL:O	2:A:70:GLU:HB2	2.18	0.44
1:E:1:U:C3'	1:E:2:U:H5	2.31	0.44
2:B:216:GLY:O	2:B:357:GLU:N	2.47	0.44
2:A:102:GLY:O	2:A:103:TYR:HB3	2.18	0.44
2:B:106:LYS:CB	2:B:106:LYS:NZ	2.78	0.44
2:B:141:LYS:HZ2	2:B:158:ARG:HH22	1.64	0.43
2:B:187:MET:SD	2:B:292:THR:HG22	2.57	0.43
2:B:215:MET:HA	2:B:357:GLU:O	2.17	0.43
2:B:93:PRO:CA	2:B:561:TYR:HB2	2.48	0.43
2:A:194:GLN:HA	2:A:551:PHE:O	2.18	0.43
2:B:104:GLY:O	2:B:105:ALA:C	2.56	0.43
2:B:315:VAL:HG12	2:B:316:ASN:N	2.32	0.43
2:A:314:LEU:HB3	2:A:321:VAL:HG13	1.99	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:B:508:ARG:NE	2:B:530:VAL:CG1	2.81	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
2:B:202:GLU:O	2:B:206:ASN:OD1	2.36	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:485:VAL:O	2:B:488:CYS:HB3	2.17	0.43
2:B:56:ARG:C	2:B:57:LEU:HD22	2.39	0.43
1:F:4:U:C6	2:B:556:SER:HB2	2.52	0.43
2:A:254:ARG:NH2	2:A:258:GLU:CG	2.81	0.43
2:A:398:GLU:OE2	2:A:403:THR:HG21	2.18	0.43
2:A:441:LYS:HE2	2:A:443:LEU:CD2	2.49	0.43
2:B:263:GLY:HA2	2:B:277:ARG:CZ	2.48	0.43
2:B:94:PRO:O	2:B:95:HIS:ND1	2.49	0.43
2:B:454:ILE:HG23	2:B:565:SER:O	2.19	0.43
2:B:458:ASP:O	2:B:462:ILE:HG13	2.18	0.43
2:A:103:TYR:CD1	2:A:103:TYR:C	2.92	0.43
2:A:148:GLN:NE2	2:A:150:GLU:HG2	2.34	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:A:401:ARG:O	2:A:402:HIS:C	2.57	0.43
2:A:435:ALA:HB3	2:A:436:GLN:OE1	2.18	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:B:457:LEU:CD1	2:B:517:ARG:HH12	2.31	0.43
1:F:2:U:HO2'	1:F:3:U:P	2.42	0.43
2:A:376:ALA:C	2:A:378:GLY:H	2.21	0.43
2:A:514:GLN:HB3	2:A:514:GLN:HE21	1.68	0.43
2:B:94:PRO:C	2:B:95:HIS:ND1	2.72	0.43
2:A:70:GLU:OE2	2:A:304:ARG:NH2	2.48	0.43
2:A:86:GLU:N	2:A:86:GLU:OE1	2.51	0.43
2:B:257:THR:HA	2:B:261:TYR:HB2	2.00	0.43
1:F:3:U:O2'	1:F:4:U:P	2.76	0.43
2:B:45:ALA:C	2:B:49:GLN:HG3	2.40	0.42
2:A:310:ASP:HB2	2:A:325:GLU:HG2	2.01	0.42
2:A:489:LEU:HD23	2:A:489:LEU:HA	1.72	0.42
2:A:531:ARG:NH2	2:B:198:LYS:HZ2	2.16	0.42
2:B:446:GLN:O	2:B:447:ILE:HD12	2.17	0.42
2:B:459:LEU:O	2:B:463:ILE:HG13	2.19	0.42
2:B:523:ARG:O	2:B:527:ASN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:LEU:HD13	2:B:64:TYR:CE1	2.54	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: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:B:36:MET:O	2:B:146:CYS:HA	2.19	0.42
2:A:236:GLU:CD	2:A:280:ARG:HH22	2.18	0.42
2:A:368:SER:HB2	2:A:384:LEU:CD1	2.50	0.42
2:B:172:LYS:HE2	2:B:559:ASP:O	2.19	0.42
2:B:45:ALA:O	2:B:46:SER:C	2.58	0.42
2:B:530:VAL:HG23	2:B:533:LYS:HD3	2.02	0.42
2:B:83:LEU:HD12	2:B:83:LEU:N	2.33	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:B:86:GLU:OE2	2:B:90:LYS:NZ	2.50	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: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:A:504:ALA:C	2:A:506:SER:N	2.73	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
2:A:48:ARG:CG	2:A:159:LEU:HG	2.49	0.42
2:A:405:ILE:O	2:A:405:ILE:HG23	2.20	0.42
2:A:433:LEU:HA	2:A:433:LEU:HD12	1.75	0.42
1:F:4:U:H2'	1:F:4:U:O2	2.19	0.42
2:A:254:ARG:NH1	2:A:254:ARG:O	2.53	0.42
2:A:456:PRO:HA	2:A:459:LEU:CD2	2.50	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:372:VAL:HG22	2:A:382:TYR:CE1	2.55	0.41
2:A:541:ALA:O	2:A:544:GLN:N	2.53	0.41
2:B:10:LEU:CD2	2:B:10:LEU:N	2.82	0.41
2:A:408:TRP:O	2:A:412:ILE:HG13	2.20	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
1:F:4:U:C6	2:B:556:SER:CB	3.03	0.41
2:B:434:LEU:HD12	2:B:439:LEU:HD21	2.02	0.41
2:B:4:TYR:HE2	2:B:52:VAL:HG22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:280:ARG:HG3	2:A:281:ALA:N	2.35	0.41
2:A:498:ARG:HD3	2:B:206:ASN:HD21	1.85	0.41
2:B:494:VAL:HA	2:B:495:PRO:HD2	1.84	0.41
2:A:368:SER:CB	2:A:385:THR:O	2.67	0.41
2:B:401:ARG:HH11	2:B:401:ARG:HG2	1.84	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
1:F:3:U:O3'	2:B:556:SER:O	2.39	0.41
2:A:241:GLN:OE1	2:A:250:ARG:HG3	2.20	0.41
2:A:365:SER:O	2:A:366:CYS:CB	2.68	0.41
2:B:423:MET:HG2	2:B:528:TRP:CZ3	2.56	0.41
2:A:321:VAL:O	2:A:321:VAL:CG1	2.67	0.41
2:A:336:LEU:O	2:A:339:PHE:HB3	2.21	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:B:366:CYS:O	2:B:367:SER:HB2	2.21	0.41
2:B:58:GLN:HB2	2:B:347:SER:HB2	2.02	0.41
2:B:75:ALA:C	2:B:77:THR:N	2.74	0.41
2:A:222:ARG:O	2:A:223:CYS:C	2.59	0.41
2:A:201:VAL:HG23	2:A:370:VAL:HG22	2.03	0.41
2:B:329:THR:HG22	2:B:330:GLN:N	2.35	0.41
2:B:200:ARG:O	2:B:204:LEU:HG	2.20	0.41
2:B:456:PRO:O	2:B:459:LEU:HB2	2.21	0.41
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:B:374:HIS:N	2:B:476:SER:HB3	2.35	0.40
1:E:1:U:H2'	1:E:2:U:C4	2.54	0.40
2:A:148:GLN:O	2:A:150:GLU:N	2.54	0.40
2:A:182:LEU:O	2:A:185:ALA:HB3	2.20	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:167:VAL:O	2:B:171:GLU:HG3	2.21	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:78:VAL:HG12	2:B:79:LYS:N	2.36	0.40
2:A:85:ILE:HG12	2:A:173:MET:SD	2.62	0.40
2:A:254:ARG:O	2:A:257:THR:HB	2.21	0.40
2:A:268:ASN:C	2:A:270:LYS:H	2.25	0.40
2:A:36:MET:O	2:A:146:CYS:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:77:THR:HG22	2:A:78:VAL:N	2.36	0.40
2:B:268:ASN:OD1	2:B:270:LYS:N	2.50	0.40
1:F:4:U:O2'	2:B:282:SER:HB2	2.21	0.40
2:B:368:SER:HA	2:B:386:ARG:HB3	2.03	0.40
1:F:3:U:O2'	2:B:446:GLN:OE1	2.36	0.40
2:A:198:LYS:C	2:A:201:VAL:HG12	2.42	0.40
2:A:530:VAL:C	2:A:532:THR:H	2.25	0.40
2:B:110:ASN:O	2:B:111:LEU:C	2.59	0.40
1:F:3:U:C2'	1:F:3:U:O2	2.68	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%)	2	10
2	B	563/570 (99%)	466 (83%)	76 (14%)	21 (4%)	3	13
All	All	1127/1140 (99%)	932 (83%)	150 (13%)	45 (4%)	3	11

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%)	22	54
2	B	474/485 (98%)	443 (94%)	31 (6%)	17	45
All	All	949/970 (98%)	893 (94%)	56 (6%)	19	49

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 ⓘ

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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 [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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.