Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 07:36 AM EDT

PDB ID	:	2NTZ
Title	:	Structure of a ParB-DNA complex reveals a double B-box interaction
Authors	:	Schumacher, M.A.; Mansoor, A.; Funnell, B.E.
Deposited on	:	2006-11-08
Resolution	:	3.35 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 (1)) were used in the production of this report:

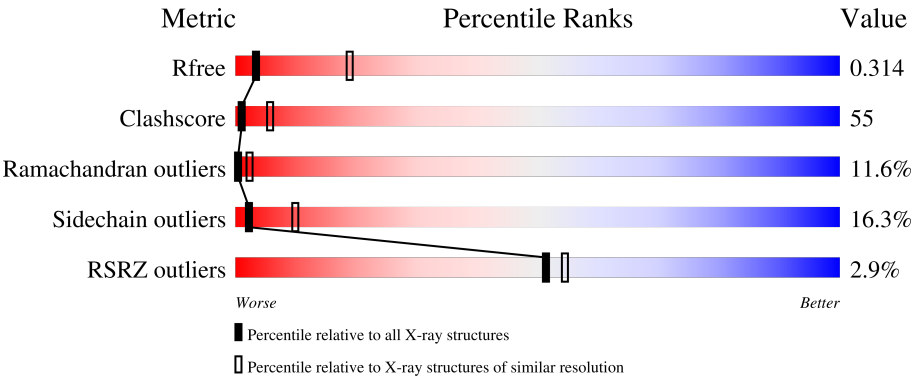
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	E	16	38% 56% 6%
1	Y	16	6% 69% 25%
2	U	16	62% 38%
2	W	16	25% 50% 25%
3	A	192	3% 18% 54% 22% • 5%

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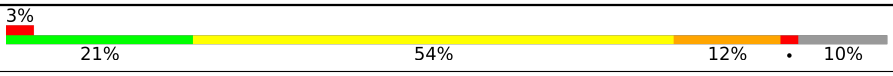
Mol	Chain	Length	Quality of chain
3	B	192	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4144 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 DNA chain called 5'-D(*CP*GP*TP*GP*AP*AP*AP*TP*CP*GP*CP*CP*AP*CP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Y	16	Total	C	N	O	P	0	0	0
			325	155	64	91	15			
1	E	16	Total	C	N	O	P	0	0	0
			325	155	64	91	15			

- Molecule 2 is a DNA chain called 5'-D(*TP*CP*GP*TP*GP*GP*CP*GP*AP*TP*TP*TP*CP*AP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	16	Total	C	N	O	P	0	0	0
			325	156	57	97	15			
2	U	16	Total	C	N	O	P	0	0	0
			325	156	57	97	15			

- Molecule 3 is a protein called ParB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	183	Total	C	N	O	S	Se	0	0	0
			1465	920	257	281	1	6			
3	B	172	Total	C	N	O	S	Se	0	0	0
			1379	864	241	267	1	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	MSE	MET	modified residue	UNP Q38420
A	161	MSE	MET	modified residue	UNP Q38420
A	166	MSE	MET	modified residue	UNP Q38420
A	220	MSE	MET	modified residue	UNP Q38420
A	247	MSE	MET	modified residue	UNP Q38420
A	318	MSE	MET	modified residue	UNP Q38420

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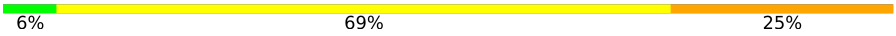
Chain	Residue	Modelled	Actual	Comment	Reference
B	159	MSE	MET	modified residue	UNP Q38420
B	161	MSE	MET	modified residue	UNP Q38420
B	166	MSE	MET	modified residue	UNP Q38420
B	220	MSE	MET	modified residue	UNP Q38420
B	247	MSE	MET	modified residue	UNP Q38420
B	318	MSE	MET	modified residue	UNP Q38420

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.

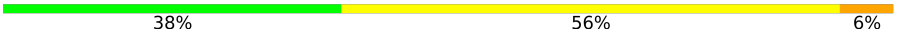
• Molecule 1: 5'-D(*CP*GP*TP*GP*AP*AP*AP*TP*CP*GP*CP*CP*AP*CP*GP*A)-3'

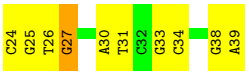
Chain Y:



• Molecule 1: 5'-D(*CP*GP*TP*GP*AP*AP*AP*TP*CP*GP*CP*CP*AP*CP*GP*A)-3'

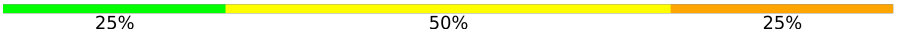
Chain E:

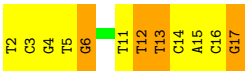




• Molecule 2: 5'-D(*TP*CP*GP*TP*GP*GP*CP*GP*AP*TP*TP*TP*CP*AP*CP*G)-3'

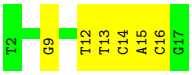
Chain W:





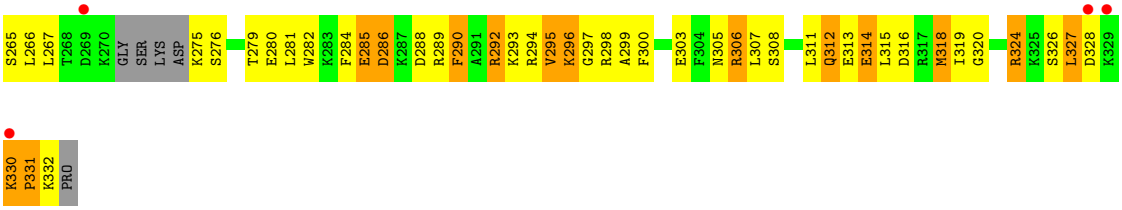
• Molecule 2: 5'-D(*TP*CP*GP*TP*GP*GP*CP*GP*AP*TP*TP*TP*CP*AP*CP*G)-3'

Chain U:

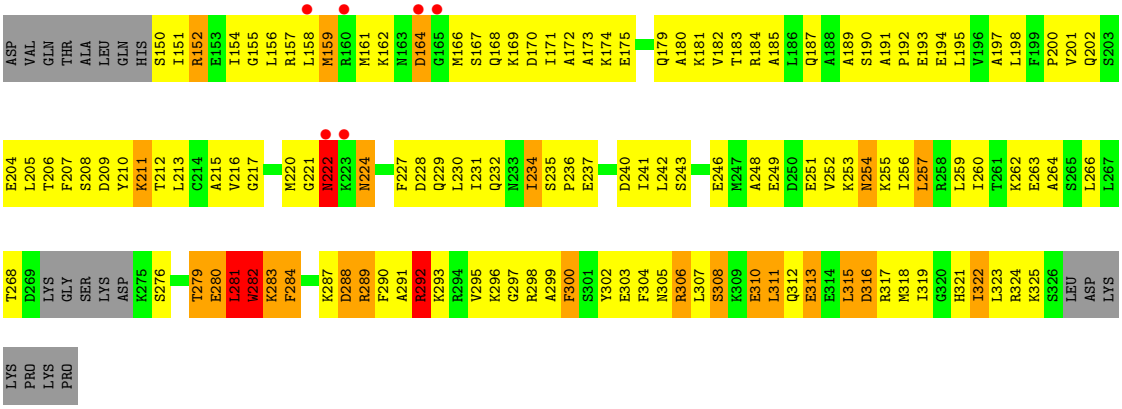


• Molecule 3: ParB

Chain A:



• Molecule 3: ParB



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.42Å 144.42Å 78.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.72 – 3.35 66.72 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.8 (66.72-3.35) 97.9 (66.72-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.288 , 0.336 0.276 , 0.314	Depositor DCC
R_{free} test set	692 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å^2)	121.6	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 110.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4144	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.45	0/365	0.66	0/561
1	Y	0.97	0/365	1.12	2/561 (0.4%)
2	U	0.44	0/363	0.70	0/559
2	W	0.92	0/363	0.95	1/559 (0.2%)
3	A	0.65	1/1473 (0.1%)	1.05	9/1957 (0.5%)
3	B	0.65	1/1386 (0.1%)	0.77	1/1842 (0.1%)
All	All	0.68	2/4315 (0.0%)	0.91	13/6039 (0.2%)

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
1	Y	0	2
2	W	0	3
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	282	TRP	CB-CG	-6.96	1.37	1.50
3	A	318	MSE	CG-SE	-5.10	1.78	1.95

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	330	LYS	C-N-CD	-15.46	86.59	120.60
3	A	150	SER	N-CA-C	-10.38	82.97	111.00
3	A	330	LYS	C-N-CA	8.02	155.70	122.00
3	B	292	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	Y	31	DT	C5'-C4'-O4'	-6.65	96.67	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	327	LEU	CA-CB-CG	6.37	129.95	115.30
1	Y	30	DA	OP1-P-O3'	6.04	118.49	105.20
3	A	147	LEU	CA-CB-CG	-5.88	101.77	115.30
3	A	327	LEU	N-CA-C	5.46	125.73	111.00
3	A	327	LEU	CB-CG-CD1	-5.40	101.82	111.00
3	A	328	ASP	CB-CG-OD2	5.20	122.98	118.30
2	W	12	DT	OP1-P-O3'	5.06	116.32	105.20
3	A	295	VAL	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	27	DG	Sidechain
2	W	13	DT	Sidechain
2	W	17	DG	Sidechain
2	W	6	DG	Sidechain
1	Y	32	DC	Sidechain
1	Y	36	DA	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	325	0	180	15	0
1	Y	325	0	180	29	0
2	U	325	0	183	8	0
2	W	325	0	183	21	0
3	A	1465	0	1507	212	0
3	B	1379	0	1413	164	0
All	All	4144	0	3646	424	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 55.

All (424) 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)
3:A:275:LYS:HD3	3:A:276:SER:N	1.65	1.11
1:E:25:DG:H2"	1:E:26:DT:H5'	1.32	1.11
1:Y:30:DA:H2"	1:Y:31:DT:C5'	1.83	1.09
1:Y:25:DG:H2"	1:Y:26:DT:H5'	1.11	1.08
3:B:283:LYS:HA	3:B:283:LYS:HZ3	1.12	1.07
1:Y:30:DA:H2"	1:Y:31:DT:H5'	1.33	1.06
3:A:195:LEU:HD13	3:A:260:ILE:HD11	1.36	1.05
3:A:218:ASP:HA	3:A:222:ASN:HB2	1.32	1.05
3:A:307:LEU:HB3	3:A:311:LEU:HD12	1.39	1.04
3:B:311:LEU:CD2	3:B:315:LEU:HD12	1.93	0.98
3:A:149:HIS:O	3:A:149:HIS:ND1	1.99	0.95
3:A:235:SER:O	3:A:238:ILE:HG22	1.66	0.94
3:B:183:THR:O	3:B:187:GLN:HG3	1.68	0.94
3:B:311:LEU:HD22	3:B:315:LEU:HD12	1.49	0.93
3:A:152:ARG:HD2	3:A:210:TYR:HE1	1.34	0.92
3:A:161:MSE:HB3	3:A:166:MSE:HE2	1.50	0.92
3:B:221:GLY:O	3:B:222:ASN:HB2	1.72	0.90
3:A:295:VAL:O	3:A:297:GLY:N	2.05	0.90
3:A:218:ASP:O	3:A:220:MSE:N	2.05	0.89
1:Y:25:DG:C2'	1:Y:26:DT:H5'	2.00	0.89
3:A:314:GLU:O	3:A:318:MSE:HG2	1.73	0.89
1:Y:38:DG:H2"	1:Y:39:DA:N7	1.90	0.87
3:A:256:ILE:O	3:A:260:ILE:HG22	1.74	0.87
3:A:305:ASN:OD1	3:B:299:ALA:HB2	1.76	0.85
3:B:234:ILE:HA	3:B:237:GLU:OE1	1.76	0.85
3:A:155:GLY:HA3	3:A:189:ALA:HB2	1.56	0.85
3:A:211:LYS:O	3:A:213:LEU:N	2.10	0.84
3:A:192:PRO:O	3:A:196:VAL:HG23	1.78	0.84
2:W:12:DT:H2"	2:W:13:DT:C5'	2.09	0.82
3:B:279:THR:O	3:B:281:LEU:N	2.11	0.82
3:B:220:MSE:HE1	3:B:230:LEU:HD12	1.61	0.81
3:A:152:ARG:HD2	3:A:210:TYR:CE1	2.16	0.81
3:B:283:LYS:NZ	3:B:284:PHE:H	1.79	0.80
3:B:283:LYS:HA	3:B:283:LYS:NZ	1.96	0.79
3:A:307:LEU:HB3	3:A:311:LEU:CD1	2.13	0.79
1:Y:25:DG:H2"	1:Y:26:DT:C5'	2.04	0.78
3:A:197:ALA:O	3:A:199:PHE:N	2.17	0.78
3:B:170:ASP:O	3:B:174:LYS:HG2	1.83	0.78
1:Y:30:DA:H2"	1:Y:31:DT:H5"	1.65	0.78
3:B:283:LYS:HZ2	3:B:284:PHE:H	1.29	0.78
3:A:209:ASP:HA	3:A:212:THR:CG2	2.14	0.77
3:B:321:HIS:HE1	3:B:325:LYS:HD2	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:245:GLU:CD	3:A:245:GLU:H	1.86	0.77
3:A:252:VAL:HG13	3:A:253:LYS:N	2.00	0.76
3:A:230:LEU:HD13	3:A:263:GLU:O	1.85	0.76
3:A:201:VAL:HB	3:A:249:GLU:OE2	1.85	0.76
3:B:317:ARG:HG3	3:B:317:ARG:HH11	1.50	0.76
3:A:299:ALA:HB2	3:B:305:ASN:HD22	1.51	0.76
3:A:257:LEU:O	3:A:259:LEU:N	2.18	0.76
3:B:248:ALA:O	3:B:252:VAL:HG23	1.85	0.75
2:W:12:DT:H2"	2:W:13:DT:H5"	1.67	0.75
3:B:179:GLN:O	3:B:182:VAL:HB	1.87	0.75
1:Y:39:DA:O5'	1:Y:39:DA:H8	1.70	0.74
3:A:220:MSE:HE3	3:A:226:GLU:HB3	1.69	0.74
3:B:166:MSE:SE	3:B:171:ILE:HG12	2.37	0.74
3:B:263:GLU:HA	3:B:266:LEU:HD21	1.70	0.73
3:A:227:PHE:O	3:A:231:ILE:HG13	1.89	0.73
1:E:30:DA:H1'	1:E:31:DT:H5"	1.69	0.73
3:B:161:MSE:HA	3:B:164:ASP:HB2	1.71	0.73
1:Y:30:DA:C2'	1:Y:31:DT:H5"	2.18	0.73
1:Y:38:DG:H2"	1:Y:39:DA:C8	2.24	0.72
3:A:193:GLU:O	3:A:196:VAL:HB	1.90	0.72
3:B:206:THR:HG22	3:B:208:SER:H	1.53	0.72
3:B:216:VAL:HG11	3:B:260:ILE:HG22	1.72	0.71
3:B:322:ILE:HD13	3:B:322:ILE:N	2.04	0.71
3:A:252:VAL:HG13	3:A:253:LYS:H	1.55	0.71
3:A:218:ASP:C	3:A:220:MSE:H	1.91	0.71
3:B:158:LEU:HA	3:B:161:MSE:HE3	1.72	0.71
3:A:290:PHE:CZ	3:A:305:ASN:HB2	2.24	0.70
3:B:288:ASP:O	3:B:289:ARG:HB2	1.90	0.70
3:A:211:LYS:C	3:A:213:LEU:H	1.93	0.70
1:Y:30:DA:C2'	1:Y:31:DT:C5'	2.65	0.70
2:W:13:DT:H2"	2:W:14:DC:O5'	1.90	0.70
3:A:324:ARG:HG2	3:A:324:ARG:HH11	1.56	0.70
3:B:263:GLU:HA	3:B:266:LEU:CD2	2.21	0.70
3:A:237:GLU:HA	3:A:240:ASP:HB3	1.73	0.70
3:A:154:ILE:HG22	3:A:158:LEU:HD11	1.72	0.69
3:A:237:GLU:O	3:A:241:ILE:HG13	1.92	0.69
3:B:156:LEU:H	3:B:156:LEU:HD22	1.57	0.69
3:A:261:THR:OG1	3:A:262:LYS:N	2.24	0.69
3:A:295:VAL:O	3:A:295:VAL:HG12	1.91	0.69
3:A:172:ALA:HB1	3:A:177:LEU:O	1.92	0.69
3:A:293:LYS:HE3	3:B:316:ASP:OD1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:5:DT:H2"	2:W:6:DG:OP2	1.93	0.68
3:A:312:GLN:HG2	3:B:300:PHE:CE2	2.28	0.68
3:B:194:GLU:HB3	3:B:231:ILE:HD11	1.74	0.68
3:A:201:VAL:HB	3:A:249:GLU:HG3	1.74	0.68
1:Y:32:DC:H2"	1:Y:33:DG:H5'	1.76	0.67
3:A:198:LEU:HD21	3:A:231:ILE:HG23	1.74	0.67
3:A:206:THR:HB	3:A:209:ASP:OD2	1.94	0.67
3:A:245:GLU:N	3:A:245:GLU:OE1	2.27	0.67
3:A:167:SER:HB3	3:A:170:ASP:OD2	1.95	0.67
3:B:318:MSE:SE	3:B:322:ILE:HD11	2.45	0.66
1:Y:24:DC:H2"	1:Y:25:DG:OP2	1.96	0.66
2:W:16:DC:H2"	2:W:17:DG:C8	2.31	0.66
3:A:311:LEU:O	3:A:315:LEU:HG	1.96	0.66
3:A:318:MSE:HB3	3:B:318:MSE:HE2	1.77	0.65
3:B:152:ARG:O	3:B:156:LEU:HD22	1.96	0.65
3:A:252:VAL:CG1	3:A:253:LYS:H	2.10	0.64
1:E:26:DT:H2"	1:E:27:DG:OP2	1.96	0.64
1:Y:35:DC:H6	1:Y:35:DC:OP2	1.80	0.64
2:W:12:DT:H2"	2:W:13:DT:H5'	1.78	0.64
3:A:212:THR:O	3:A:216:VAL:HG23	1.97	0.64
3:B:157:ARG:O	3:B:161:MSE:HE2	1.98	0.64
3:B:321:HIS:O	3:B:324:ARG:N	2.30	0.64
2:W:2:DT:H2"	2:W:3:DC:C6	2.34	0.63
3:A:275:LYS:HD3	3:A:275:LYS:C	2.18	0.63
3:A:161:MSE:HE2	3:A:166:MSE:HE1	1.80	0.63
3:B:195:LEU:HA	3:B:198:LEU:HG	1.79	0.63
1:Y:25:DG:H1	2:W:16:DC:H42	1.47	0.63
3:B:151:ILE:HA	3:B:154:ILE:HD12	1.81	0.63
3:A:275:LYS:HD3	3:A:276:SER:H	1.62	0.62
3:B:283:LYS:HZ3	3:B:283:LYS:CA	1.99	0.62
3:B:306:ARG:HH11	3:B:306:ARG:HG2	1.63	0.62
3:B:235:SER:HB3	3:B:236:PRO:HD3	1.82	0.62
3:B:200:PRO:HG2	3:B:242:LEU:HD21	1.81	0.62
3:B:209:ASP:O	3:B:213:LEU:HG	1.99	0.62
3:A:238:ILE:CG2	3:A:239:ASN:N	2.62	0.61
3:B:283:LYS:NZ	3:B:284:PHE:N	2.48	0.61
3:B:291:ALA:C	3:B:292:ARG:HG2	2.19	0.61
3:A:257:LEU:C	3:A:259:LEU:H	2.04	0.61
3:A:275:LYS:HE3	3:A:276:SER:HB2	1.83	0.60
3:B:284:PHE:HD1	3:B:289:ARG:NH2	1.99	0.60
3:A:308:SER:HB3	3:A:311:LEU:HG	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:159:MSE:O	3:B:162:LYS:HB2	2.01	0.60
3:B:234:ILE:HD13	3:B:234:ILE:H	1.66	0.60
3:B:237:GLU:HA	3:B:240:ASP:HB3	1.84	0.60
3:A:201:VAL:C	3:A:203:SER:H	2.05	0.60
3:B:152:ARG:HD2	3:B:210:TYR:CE1	2.36	0.60
3:A:252:VAL:CG1	3:A:253:LYS:N	2.64	0.60
3:B:161:MSE:O	3:B:166:MSE:HB3	2.01	0.59
3:A:252:VAL:O	3:A:256:ILE:HG12	2.01	0.59
3:A:306:ARG:HA	3:B:298:ARG:HG3	1.84	0.59
3:A:192:PRO:HG2	3:A:217:GLY:CA	2.33	0.59
3:A:300:PHE:CZ	3:B:312:GLN:HG3	2.38	0.59
3:B:255:LYS:O	3:B:259:LEU:HG	2.03	0.59
3:A:229:GLN:O	3:A:232:GLN:HB2	2.02	0.59
3:A:180:ALA:HB1	3:A:184:ARG:NH1	2.18	0.59
3:A:208:SER:O	3:A:212:THR:HG22	2.02	0.59
3:A:230:LEU:O	3:A:234:ILE:HG12	2.02	0.59
3:B:208:SER:O	3:B:212:THR:HG23	2.03	0.59
3:B:281:LEU:HD11	3:B:292:ARG:CA	2.33	0.59
3:B:257:LEU:O	3:B:260:ILE:N	2.36	0.58
3:B:284:PHE:N	3:B:284:PHE:CD2	2.70	0.58
3:A:218:ASP:HA	3:A:222:ASN:CB	2.20	0.58
3:B:322:ILE:HD13	3:B:322:ILE:H	1.67	0.58
3:B:216:VAL:HG13	3:B:264:ALA:HB2	1.86	0.58
3:B:227:PHE:O	3:B:230:LEU:N	2.35	0.58
1:Y:36:DA:N6	2:W:4:DG:N1	2.51	0.58
3:A:201:VAL:CB	3:A:249:GLU:HG3	2.34	0.58
3:A:181:LYS:HA	3:A:184:ARG:HB2	1.84	0.57
3:A:326:SER:O	3:A:327:LEU:HB2	2.04	0.57
3:A:209:ASP:O	3:A:212:THR:HG23	2.04	0.57
3:A:239:ASN:C	3:A:241:ILE:H	2.05	0.57
3:A:154:ILE:HG22	3:A:158:LEU:CD1	2.33	0.57
3:A:211:LYS:C	3:A:213:LEU:N	2.56	0.57
3:A:290:PHE:CE2	3:A:305:ASN:HB2	2.39	0.57
3:A:315:LEU:O	3:A:319:ILE:HG12	2.05	0.57
3:B:150:SER:O	3:B:154:ILE:HG13	2.04	0.57
2:U:12:DT:C2	2:U:13:DT:C5	2.93	0.56
3:A:149:HIS:O	3:A:150:SER:C	2.42	0.56
3:A:232:GLN:O	3:A:234:ILE:N	2.39	0.56
3:B:311:LEU:O	3:B:315:LEU:HB2	2.05	0.56
3:A:245:GLU:OE1	3:A:245:GLU:CA	2.51	0.56
3:B:201:VAL:HG12	3:B:201:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:37:DC:H2"	1:Y:38:DG:C8	2.41	0.56
3:B:264:ALA:O	3:B:268:THR:HG23	2.06	0.56
1:Y:39:DA:O5'	1:Y:39:DA:C8	2.57	0.56
3:A:169:LYS:HG3	3:A:179:GLN:NE2	2.21	0.55
1:Y:31:DT:H73	3:B:287:LYS:HD2	1.88	0.55
3:A:145:THR:O	3:A:146:ALA:HB2	2.07	0.55
3:A:207:PHE:O	3:A:209:ASP:N	2.39	0.55
3:A:300:PHE:CE2	3:B:312:GLN:HG3	2.42	0.55
3:A:201:VAL:HG12	3:A:201:VAL:O	2.05	0.55
3:A:149:HIS:ND1	3:A:149:HIS:C	2.60	0.55
3:B:170:ASP:C	3:B:174:LYS:HG2	2.27	0.55
1:E:24:DC:C2	1:E:25:DG:N7	2.75	0.55
3:A:299:ALA:HB2	3:B:305:ASN:ND2	2.19	0.55
1:Y:30:DA:C2	1:Y:31:DT:C2	2.94	0.55
3:A:194:GLU:O	3:A:197:ALA:HB3	2.06	0.55
3:A:229:GLN:OE1	3:A:267:LEU:HD11	2.06	0.55
3:A:243:SER:O	3:A:244:ILE:C	2.44	0.54
3:A:230:LEU:HD21	3:A:264:ALA:HB2	1.89	0.54
3:A:156:LEU:HD13	3:A:156:LEU:C	2.28	0.54
1:E:24:DC:H2"	1:E:25:DG:OP2	2.06	0.54
3:A:195:LEU:CD1	3:A:260:ILE:HD11	2.24	0.54
3:B:321:HIS:ND1	3:B:322:ILE:HD13	2.23	0.54
1:Y:31:DT:H2"	1:Y:32:DC:O5'	2.08	0.54
3:B:253:LYS:HG3	3:B:254:ASN:N	2.23	0.54
3:B:281:LEU:HD11	3:B:292:ARG:N	2.22	0.54
3:B:284:PHE:HD1	3:B:289:ARG:HH21	1.54	0.54
3:B:184:ARG:HG3	3:B:184:ARG:HH11	1.73	0.53
3:A:275:LYS:CE	3:A:276:SER:HB2	2.37	0.53
3:B:256:ILE:O	3:B:259:LEU:HB2	2.09	0.53
3:A:238:ILE:CD1	3:A:256:ILE:HD12	2.39	0.53
3:A:171:ILE:O	3:A:173:ALA:N	2.42	0.53
3:B:281:LEU:O	3:B:282:TRP:HD1	1.91	0.53
3:B:283:LYS:HD3	3:B:283:LYS:C	2.28	0.53
2:W:12:DT:C2'	2:W:13:DT:H5"	2.37	0.53
3:B:201:VAL:HG21	3:B:249:GLU:HG2	1.89	0.53
3:A:209:ASP:HA	3:A:212:THR:HG22	1.91	0.53
1:E:33:DG:C2	2:U:9:DG:N2	2.77	0.53
3:A:149:HIS:O	3:A:151:ILE:N	2.42	0.53
3:A:195:LEU:HD22	3:A:260:ILE:CD1	2.38	0.53
3:B:154:ILE:O	3:B:158:LEU:HG	2.09	0.52
2:U:13:DT:H2"	2:U:14:DC:O5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:VAL:HB	3:A:249:GLU:CG	2.40	0.52
3:B:293:LYS:HE2	3:B:295:VAL:CG2	2.40	0.52
3:B:152:ARG:HG3	3:B:156:LEU:HD21	1.90	0.52
3:A:159:MSE:HE3	3:A:162:LYS:HD3	1.91	0.52
3:A:201:VAL:C	3:A:203:SER:N	2.63	0.52
3:A:306:ARG:HE	3:B:298:ARG:HG2	1.75	0.52
3:A:173:ALA:O	3:A:174:LYS:C	2.48	0.52
3:B:184:ARG:HG3	3:B:184:ARG:NH1	2.24	0.52
3:A:235:SER:C	3:A:238:ILE:HG22	2.30	0.52
3:A:238:ILE:HG23	3:A:239:ASN:N	2.24	0.52
3:B:230:LEU:O	3:B:234:ILE:CD1	2.58	0.52
3:B:259:LEU:O	3:B:262:LYS:HB3	2.09	0.52
3:A:215:ALA:O	3:A:219:GLU:HG2	2.09	0.52
3:B:204:GLU:HA	3:B:204:GLU:OE2	2.10	0.52
3:B:180:ALA:CB	3:B:184:ARG:HH12	2.23	0.51
3:B:321:HIS:ND1	3:B:321:HIS:C	2.63	0.51
3:A:257:LEU:C	3:A:259:LEU:N	2.62	0.51
3:B:230:LEU:O	3:B:234:ILE:HD12	2.10	0.51
3:B:156:LEU:HD13	3:B:189:ALA:HB1	1.91	0.51
1:Y:25:DG:H1	2:W:16:DC:N4	2.09	0.51
1:E:25:DG:OP2	1:E:25:DG:C8	2.63	0.51
2:U:15:DA:H2”	2:U:16:DC:H5”	1.92	0.51
3:A:172:ALA:HB2	3:A:182:VAL:HG21	1.93	0.51
3:A:195:LEU:HD22	3:A:260:ILE:HD12	1.92	0.51
3:A:218:ASP:OD2	3:A:219:GLU:N	2.44	0.51
3:A:257:LEU:HA	3:A:260:ILE:CG2	2.41	0.51
2:W:15:DA:H1’	2:W:16:DC:H5”	1.93	0.51
3:A:290:PHE:C	3:A:290:PHE:CD2	2.84	0.51
3:B:168:GLN:HB3	3:B:182:VAL:HG11	1.93	0.51
3:B:205:LEU:HD12	3:B:210:TYR:OH	2.11	0.51
3:A:300:PHE:CE1	3:B:312:GLN:HG3	2.47	0.50
3:B:170:ASP:O	3:B:174:LYS:N	2.44	0.50
3:A:293:LYS:HE3	3:B:316:ASP:CG	2.31	0.50
3:B:234:ILE:CA	3:B:237:GLU:OE1	2.55	0.50
3:B:311:LEU:HD22	3:B:315:LEU:CD1	2.34	0.50
3:B:311:LEU:HD21	3:B:315:LEU:HD12	1.88	0.50
3:B:304:PHE:HB3	3:B:307:LEU:HD11	1.94	0.50
3:A:306:ARG:O	3:A:307:LEU:HD23	2.12	0.49
3:A:230:LEU:CD2	3:A:264:ALA:HB2	2.42	0.49
3:B:172:ALA:HB2	3:B:182:VAL:HG21	1.94	0.49
3:B:234:ILE:HD13	3:B:234:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:153:GLU:O	3:A:154:ILE:C	2.50	0.49
3:A:296:LYS:O	3:A:296:LYS:HG3	2.11	0.49
3:B:291:ALA:O	3:B:292:ARG:HG2	2.11	0.49
2:W:15:DA:H2"	2:W:16:DC:H5"	1.95	0.49
3:B:201:VAL:HG21	3:B:249:GLU:CD	2.33	0.49
3:A:174:LYS:HG2	3:A:175:GLU:OE2	2.13	0.49
3:A:239:ASN:C	3:A:241:ILE:N	2.66	0.49
3:A:281:LEU:HD23	3:A:292:ARG:HA	1.95	0.49
1:E:33:DG:H2"	1:E:34:DC:C5'	2.42	0.49
3:A:197:ALA:C	3:A:199:PHE:N	2.64	0.49
3:A:234:ILE:HA	3:A:237:GLU:OE1	2.13	0.49
2:U:12:DT:O2	2:U:13:DT:C6	2.66	0.48
3:A:192:PRO:HG2	3:A:217:GLY:HA3	1.94	0.48
3:A:242:LEU:O	3:A:242:LEU:HD23	2.13	0.48
3:A:207:PHE:O	3:A:208:SER:C	2.51	0.48
3:B:224:ASN:O	3:B:227:PHE:N	2.46	0.48
3:B:251:GLU:O	3:B:255:LYS:HG2	2.13	0.48
3:A:289:ARG:HD2	3:A:307:LEU:HD23	1.94	0.48
3:B:290:PHE:CD2	3:B:290:PHE:C	2.86	0.48
1:E:38:DG:C6	1:E:39:DA:N6	2.82	0.48
3:A:206:THR:HG22	3:A:208:SER:HB3	1.95	0.48
1:Y:36:DA:N6	2:W:4:DG:C6	2.81	0.48
3:A:192:PRO:HG2	3:A:217:GLY:HA2	1.96	0.48
1:E:30:DA:H2"	1:E:31:DT:OP2	2.14	0.48
3:A:192:PRO:C	3:A:196:VAL:HG23	2.33	0.48
3:B:321:HIS:O	3:B:323:LEU:N	2.46	0.48
3:A:182:VAL:O	3:A:186:LEU:HD12	2.13	0.48
3:B:281:LEU:O	3:B:282:TRP:CD1	2.66	0.48
3:A:206:THR:CG2	3:A:208:SER:HB3	2.44	0.47
1:Y:30:DA:H1'	1:Y:31:DT:H5"	1.95	0.47
3:A:235:SER:HB3	3:A:236:PRO:HD3	1.96	0.47
3:B:287:LYS:HG3	3:B:288:ASP:H	1.79	0.47
3:B:296:LYS:O	3:B:297:GLY:C	2.52	0.47
1:Y:38:DG:C2'	1:Y:39:DA:N7	2.71	0.47
2:W:15:DA:C2'	2:W:16:DC:H5"	2.45	0.47
3:B:201:VAL:HG21	3:B:249:GLU:CG	2.43	0.47
3:A:285:GLU:OE1	3:A:286:ASP:N	2.48	0.47
3:B:304:PHE:HB3	3:B:307:LEU:CD1	2.45	0.47
3:B:315:LEU:O	3:B:319:ILE:HG13	2.15	0.47
3:A:192:PRO:HD3	3:A:214:CYS:HA	1.97	0.47
3:A:331:PRO:C	3:A:332:LYS:HG3	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:185:ALA:O	3:A:186:LEU:C	2.53	0.46
3:A:284:PHE:CD2	3:A:289:ARG:HG2	2.49	0.46
3:B:220:MSE:HE3	3:B:264:ALA:HA	1.96	0.46
3:B:318:MSE:O	3:B:321:HIS:N	2.47	0.46
3:A:290:PHE:CD1	3:A:292:ARG:NH2	2.84	0.46
3:B:263:GLU:O	3:B:266:LEU:HD23	2.15	0.46
1:Y:27:DG:H1	2:W:14:DC:H42	1.62	0.46
3:A:275:LYS:HD3	3:A:276:SER:CA	2.42	0.46
3:B:241:ILE:C	3:B:243:SER:H	2.19	0.46
3:B:306:ARG:HG2	3:B:306:ARG:NH1	2.30	0.46
3:A:204:GLU:HG3	3:A:249:GLU:O	2.15	0.46
3:A:220:MSE:HG2	3:A:220:MSE:O	2.16	0.46
3:A:275:LYS:CD	3:A:276:SER:N	2.57	0.46
1:Y:28:DA:H2"	1:Y:29:DA:OP2	2.16	0.46
3:A:154:ILE:O	3:A:158:LEU:HG	2.16	0.46
3:A:279:THR:HG22	3:A:280:GLU:N	2.31	0.46
2:W:15:DA:H2"	2:W:16:DC:C5'	2.45	0.46
3:B:252:VAL:HG12	3:B:256:ILE:CD1	2.46	0.45
3:B:321:HIS:ND1	3:B:322:ILE:N	2.63	0.45
3:A:183:THR:HG22	3:A:184:ARG:N	2.32	0.45
3:A:207:PHE:O	3:A:210:TYR:N	2.50	0.45
3:A:320:GLY:O	3:A:324:ARG:HB2	2.15	0.45
3:A:201:VAL:O	3:A:203:SER:N	2.50	0.45
3:A:205:LEU:HD23	3:A:205:LEU:HA	1.57	0.45
3:A:238:ILE:HG22	3:A:239:ASN:H	1.82	0.45
3:A:315:LEU:O	3:A:316:ASP:C	2.54	0.45
3:A:209:ASP:O	3:A:212:THR:CG2	2.64	0.45
3:B:206:THR:O	3:B:209:ASP:N	2.50	0.45
3:B:308:SER:OG	3:B:310:GLU:HG3	2.16	0.45
3:A:290:PHE:C	3:A:290:PHE:HD2	2.20	0.45
3:A:240:ASP:OD1	3:A:240:ASP:O	2.34	0.45
3:A:284:PHE:HD2	3:A:289:ARG:O	2.00	0.45
3:A:171:ILE:C	3:A:173:ALA:H	2.20	0.45
3:A:178:SER:O	3:A:179:GLN:C	2.56	0.45
3:A:204:GLU:OE2	3:A:204:GLU:HA	2.17	0.44
3:A:234:ILE:O	3:A:235:SER:C	2.56	0.44
3:A:246:GLU:O	3:A:247:MSE:HB3	2.17	0.44
3:B:173:ALA:C	3:B:175:GLU:H	2.20	0.44
3:A:197:ALA:O	3:A:198:LEU:C	2.56	0.44
3:A:308:SER:O	3:A:311:LEU:N	2.49	0.44
3:A:312:GLN:O	3:A:313:GLU:C	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:157:ARG:O	3:B:161:MSE:CE	2.63	0.44
3:A:235:SER:HA	3:A:238:ILE:CG2	2.48	0.44
2:W:6:DG:N7	3:A:298:ARG:NH2	2.66	0.44
3:B:236:PRO:HB2	3:B:237:GLU:OE2	2.17	0.44
3:B:281:LEU:CD1	3:B:292:ARG:HA	2.47	0.44
1:Y:26:DT:H2"	1:Y:27:DG:C8	2.53	0.44
1:E:33:DG:H5'	1:E:33:DG:H8	1.83	0.44
3:A:311:LEU:O	3:A:314:GLU:HB2	2.17	0.44
3:B:195:LEU:HD22	3:B:260:ILE:HD13	1.99	0.44
3:A:260:ILE:O	3:A:264:ALA:HB2	2.18	0.44
3:B:280:GLU:OE2	3:B:292:ARG:HD3	2.18	0.44
1:E:24:DC:H1'	1:E:25:DG:C8	2.53	0.44
3:B:181:LYS:HA	3:B:184:ARG:HH11	1.82	0.44
3:B:262:LYS:HE2	3:B:266:LEU:HD22	2.00	0.44
3:B:224:ASN:O	3:B:227:PHE:HB2	2.17	0.44
3:A:171:ILE:C	3:A:173:ALA:N	2.71	0.43
3:A:181:LYS:O	3:A:182:VAL:C	2.56	0.43
3:A:192:PRO:CD	3:A:214:CYS:HA	2.48	0.43
3:A:201:VAL:HB	3:A:249:GLU:CD	2.38	0.43
3:A:265:SER:C	3:A:267:LEU:H	2.21	0.43
3:B:197:ALA:O	3:B:198:LEU:C	2.56	0.43
1:Y:30:DA:C1'	1:Y:31:DT:H5"	2.49	0.43
3:A:214:CYS:O	3:A:215:ALA:C	2.57	0.43
3:B:281:LEU:CD1	3:B:292:ARG:CA	2.95	0.43
3:A:197:ALA:C	3:A:199:PHE:H	2.21	0.43
3:A:213:LEU:O	3:A:217:GLY:N	2.51	0.43
3:B:156:LEU:HD22	3:B:156:LEU:N	2.30	0.43
3:A:201:VAL:CB	3:A:249:GLU:OE2	2.63	0.43
3:A:289:ARG:HG3	3:A:305:ASN:O	2.18	0.43
3:B:171:ILE:C	3:B:173:ALA:N	2.71	0.43
2:U:15:DA:C2'	2:U:16:DC:H5"	2.49	0.43
3:A:260:ILE:O	3:A:264:ALA:CB	2.67	0.43
3:A:232:GLN:O	3:A:233:ASN:C	2.57	0.43
3:B:284:PHE:H	3:B:284:PHE:HD2	1.66	0.43
2:W:5:DT:OP1	3:B:308:SER:HA	2.19	0.42
3:B:162:LYS:HD3	3:B:162:LYS:HA	1.89	0.42
3:B:198:LEU:O	3:B:200:PRO:HD3	2.18	0.42
3:B:304:PHE:CD2	3:B:304:PHE:N	2.87	0.42
1:E:24:DC:O2	1:E:25:DG:N7	2.52	0.42
3:A:188:ALA:C	3:A:190:SER:N	2.71	0.42
3:A:239:ASN:O	3:A:241:ILE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:324:ARG:HG2	3:A:324:ARG:NH1	2.28	0.42
3:A:331:PRO:HG2	3:A:332:LYS:HG3	2.01	0.42
3:B:318:MSE:O	3:B:321:HIS:HB3	2.19	0.42
2:W:12:DT:N3	2:W:13:DT:C4	2.87	0.42
3:A:185:ALA:O	3:A:188:ALA:N	2.50	0.42
3:B:167:SER:O	3:B:168:GLN:C	2.58	0.42
3:B:281:LEU:HD12	3:B:291:ALA:O	2.17	0.42
3:B:207:PHE:HE1	3:B:211:LYS:HE3	1.84	0.42
3:A:300:PHE:CD2	3:B:312:GLN:HG3	2.54	0.42
3:B:191:ALA:HA	3:B:192:PRO:HD3	1.86	0.42
3:B:281:LEU:CD1	3:B:291:ALA:C	2.88	0.42
2:W:11:DT:C2	2:W:12:DT:C5	3.08	0.42
3:A:178:SER:O	3:A:180:ALA:N	2.53	0.42
3:A:193:GLU:H	3:A:193:GLU:HG2	1.61	0.42
3:A:312:GLN:HG2	3:B:300:PHE:CZ	2.53	0.42
3:A:312:GLN:O	3:A:315:LEU:N	2.53	0.42
3:B:298:ARG:HD2	3:B:298:ARG:HA	1.89	0.42
1:E:33:DG:C2	2:U:9:DG:C2	3.07	0.42
2:U:14:DC:H2"	2:U:15:DA:OP2	2.20	0.42
3:A:184:ARG:O	3:A:185:ALA:O	2.38	0.42
3:A:228:ASP:O	3:A:232:GLN:HG2	2.19	0.42
3:B:151:ILE:HD11	3:B:185:ALA:CA	2.50	0.41
3:B:302:TYR:CD2	3:B:302:TYR:N	2.88	0.41
3:A:157:ARG:O	3:A:160:ARG:HB3	2.19	0.41
3:A:205:LEU:HB3	3:A:210:TYR:CE2	2.55	0.41
3:A:234:ILE:O	3:A:236:PRO:N	2.53	0.41
3:B:281:LEU:CD1	3:B:292:ARG:N	2.82	0.41
3:A:249:GLU:HA	3:A:252:VAL:CG1	2.51	0.41
3:B:215:ALA:C	3:B:217:GLY:N	2.74	0.41
3:A:286:ASP:HB2	3:A:289:ARG:HB3	2.03	0.41
3:B:232:GLN:HA	3:B:235:SER:HB2	2.01	0.41
3:A:231:ILE:O	3:A:235:SER:HB2	2.20	0.41
3:A:238:ILE:CG2	3:A:239:ASN:H	2.31	0.41
3:B:287:LYS:HG3	3:B:288:ASP:N	2.35	0.41
3:A:159:MSE:CE	3:A:162:LYS:HD3	2.50	0.41
3:A:262:LYS:O	3:A:266:LEU:HG	2.20	0.41
3:B:152:ARG:O	3:B:155:GLY:N	2.52	0.41
3:B:162:LYS:NZ	3:B:168:GLN:HG3	2.35	0.41
3:B:184:ARG:O	3:B:207:PHE:HE2	2.03	0.41
3:B:224:ASN:H	3:B:224:ASN:ND2	2.18	0.41
3:B:321:HIS:C	3:B:323:LEU:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:197:ALA:O	3:A:199:PHE:O	2.38	0.41
3:A:204:GLU:CD	3:A:204:GLU:O	2.60	0.41
3:B:262:LYS:HG3	3:B:263:GLU:N	2.35	0.41
3:A:245:GLU:HB2	3:A:246:GLU:H	1.73	0.40
3:B:205:LEU:HD12	3:B:210:TYR:CZ	2.56	0.40
3:B:252:VAL:HG12	3:B:256:ILE:HD11	2.03	0.40
3:A:155:GLY:O	3:A:156:LEU:C	2.60	0.40
1:E:25:DG:N2	1:E:26:DT:C2	2.89	0.40
3:A:230:LEU:C	3:A:232:GLN:N	2.72	0.40
3:A:238:ILE:HD11	3:A:256:ILE:HD12	2.02	0.40
3:A:324:ARG:HH11	3:A:324:ARG:CG	2.27	0.40
3:A:172:ALA:O	3:A:177:LEU:O	2.39	0.40
3:A:318:MSE:CB	3:B:318:MSE:HE2	2.48	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
3	A	177/192 (92%)	101 (57%)	46 (26%)	30 (17%)	0 1
3	B	168/192 (88%)	120 (71%)	38 (23%)	10 (6%)	1 11
All	All	345/384 (90%)	221 (64%)	84 (24%)	40 (12%)	0 2

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	149	HIS
3	A	185	ALA
3	A	198	LEU
3	A	212	THR
3	A	219	GLU

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Mol	Chain	Res	Type
3	A	244	ILE
3	A	247	MSE
3	A	258	ARG
3	A	296	LYS
3	A	331	PRO
3	B	222	ASN
3	B	224	ASN
3	B	280	GLU
3	B	289	ARG
3	A	200	PRO
3	A	208	SER
3	A	233	ASN
3	A	243	SER
3	A	245	GLU
3	A	286	ASP
3	A	312	GLN
3	B	281	LEU
3	B	322	ILE
3	A	211	LYS
3	A	236	PRO
3	A	254	ASN
3	B	169	LYS
3	B	246	GLU
3	B	313	GLU
3	A	147	LEU
3	A	172	ALA
3	A	179	GLN
3	A	180	ALA
3	A	240	ASP
3	A	306	ARG
3	B	202	GLN
3	A	186	LEU
3	A	202	GLN
3	A	330	LYS
3	A	235	SER

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
3	A	161/164 (98%)	139 (86%)	22 (14%)	3 15
3	B	152/164 (93%)	123 (81%)	29 (19%)	1 5
All	All	313/328 (95%)	262 (84%)	51 (16%)	2 10

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	147	LEU
3	A	149	HIS
3	A	159	MSE
3	A	178	SER
3	A	183	THR
3	A	193	GLU
3	A	202	GLN
3	A	204	GLU
3	A	206	THR
3	A	222	ASN
3	A	229	GLN
3	A	238	ILE
3	A	245	GLU
3	A	282	TRP
3	A	285	GLU
3	A	288	ASP
3	A	290	PHE
3	A	292	ARG
3	A	294	ARG
3	A	303	GLU
3	A	314	GLU
3	A	324	ARG
3	B	152	ARG
3	B	159	MSE
3	B	164	ASP
3	B	190	SER
3	B	193	GLU
3	B	211	LYS
3	B	222	ASN
3	B	228	ASP
3	B	229	GLN
3	B	234	ILE
3	B	254	ASN
3	B	257	LEU

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Mol	Chain	Res	Type
3	B	276	SER
3	B	279	THR
3	B	281	LEU
3	B	282	TRP
3	B	283	LYS
3	B	284	PHE
3	B	288	ASP
3	B	292	ARG
3	B	300	PHE
3	B	303	GLU
3	B	306	ARG
3	B	308	SER
3	B	310	GLU
3	B	311	LEU
3	B	313	GLU
3	B	315	LEU
3	B	316	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	179	GLN
3	A	187	GLN
3	A	222	ASN
3	A	233	ASN
3	B	168	GLN
3	B	202	GLN
3	B	224	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	E	16/16 (100%)	-0.57	0 100 100	137, 190, 200, 200	0
1	Y	16/16 (100%)	-0.80	0 100 100	43, 92, 118, 127	0
2	U	16/16 (100%)	-0.69	0 100 100	133, 184, 200, 200	0
2	W	16/16 (100%)	-0.60	0 100 100	60, 88, 139, 144	0
3	A	177/192 (92%)	-0.23	6 (3%) 45 47	45, 140, 200, 200	0
3	B	166/192 (86%)	-0.23	6 (3%) 42 45	39, 180, 200, 200	0
All	All	407/448 (90%)	-0.30	12 (2%) 51 54	39, 152, 200, 200	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	329	LYS	7.2
3	B	164	ASP	4.2
3	A	330	LYS	3.8
3	B	222	ASN	3.7
3	A	328	ASP	3.4
3	A	269	ASP	3.4
3	A	222	ASN	2.7
3	B	165	GLY	2.5
3	B	160	ARG	2.4
3	B	158	LEU	2.3
3	B	223	LYS	2.1
3	A	246	GLU	2.0

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

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

6.3 Carbohydrates (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.