



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:02 AM GMT

PDB ID : 2Z9O
Title : Crystal structure of the dimeric form of RepE in complex with the repE operator DNA
Authors : Nakamura, A.; Wada, C.; Miki, K.
Deposited on : 2007-09-21
Resolution : 3.14 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

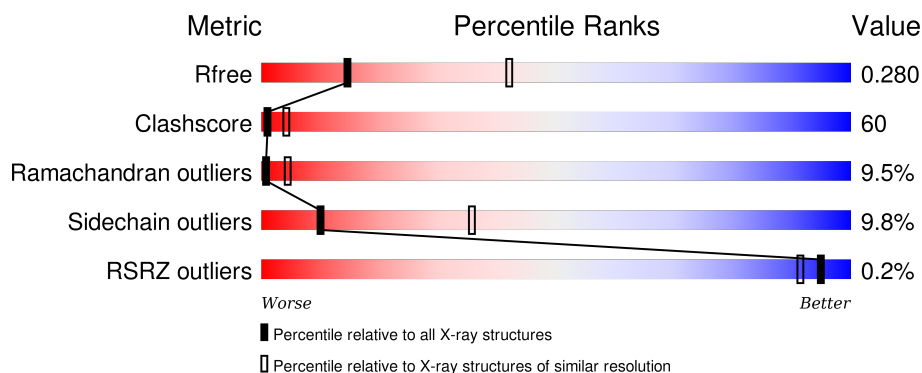
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

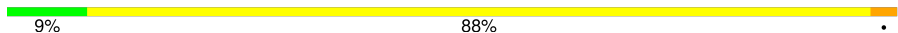


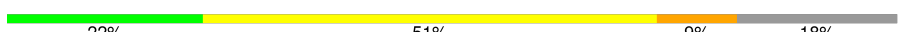
The reported resolution of this entry is 3.14 Å.

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}	91344	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)

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 $\leq 5\%$. 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	C	33	 9% 88%
2	D	33	 9% 91%
3	A	266	 20% 52% 11% 1% 17%
3	B	266	 22% 51% 9% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4926 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 DNA (33-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	33	Total	C	N	O	P	0	0	0
			669	323	118	196	32			

- Molecule 2 is a DNA chain called DNA (33-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	33	Total	C	N	O	P	0	0	0
			678	326	124	196	32			

- Molecule 3 is a protein called Replication initiation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	222	Total	C	N	O	S	0	0	0
			1796	1151	312	325	8			
3	B	218	Total	C	N	O	S	0	0	0
			1783	1142	310	324	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	EXPRESSION TAG	UNP P03856
A	-13	ARG	-	EXPRESSION TAG	UNP P03856
A	-12	GLY	-	EXPRESSION TAG	UNP P03856
A	-11	SER	-	EXPRESSION TAG	UNP P03856
A	-10	HIS	-	EXPRESSION TAG	UNP P03856
A	-9	HIS	-	EXPRESSION TAG	UNP P03856
A	-8	HIS	-	EXPRESSION TAG	UNP P03856
A	-7	HIS	-	EXPRESSION TAG	UNP P03856
A	-6	HIS	-	EXPRESSION TAG	UNP P03856
A	-5	HIS	-	EXPRESSION TAG	UNP P03856
A	-4	GLY	-	EXPRESSION TAG	UNP P03856
A	-3	SER	-	EXPRESSION TAG	UNP P03856

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ILE	-	EXPRESSION TAG	UNP P03856
A	-1	GLU	-	EXPRESSION TAG	UNP P03856
A	0	GLY	-	EXPRESSION TAG	UNP P03856
A	1	ARG	-	EXPRESSION TAG	UNP P03856
B	-14	MET	-	EXPRESSION TAG	UNP P03856
B	-13	ARG	-	EXPRESSION TAG	UNP P03856
B	-12	GLY	-	EXPRESSION TAG	UNP P03856
B	-11	SER	-	EXPRESSION TAG	UNP P03856
B	-10	HIS	-	EXPRESSION TAG	UNP P03856
B	-9	HIS	-	EXPRESSION TAG	UNP P03856
B	-8	HIS	-	EXPRESSION TAG	UNP P03856
B	-7	HIS	-	EXPRESSION TAG	UNP P03856
B	-6	HIS	-	EXPRESSION TAG	UNP P03856
B	-5	HIS	-	EXPRESSION TAG	UNP P03856
B	-4	GLY	-	EXPRESSION TAG	UNP P03856
B	-3	SER	-	EXPRESSION TAG	UNP P03856
B	-2	ILE	-	EXPRESSION TAG	UNP P03856
B	-1	GLU	-	EXPRESSION TAG	UNP P03856
B	0	GLY	-	EXPRESSION TAG	UNP P03856
B	1	ARG	-	EXPRESSION TAG	UNP P03856

D244	L183	R18	SER
I245	K184	A119	ASP
T246	I185	H120	GLY
MET	D186	S121	THR
	L188	P122	LEU
THR	I189	S123	GLN
THR	E190	R124	GLU
	R191	G125	HIS
GLY	Y192	L126	D57
	G193	Y127	G58
	L194	S128	I59
	P195	V129	C60
	Q196	H130	E61
	S197	I131	I62
	Y198	N132	H63
	I199	P133	V64
	R200	Y134	A65
	P201	L135	K66
	P202	I136	Y67
	D203	P137	A68
	F204	F138	E69
	R205	F139	I70
	R206		F71
	R207	L142	
	F208	R145	T74
	L209	F146	E77
	Q210	T147	A78
	V211	O148	S79
	C212	F149	K80
	V213	R150	D81
	N214	L151	I82
	E215	S152	R83
	T216	E153	Q84
		T154	A85
	R219	K155	
	T220	E156	F89
	P221		A90
	P222	N159	
	R223	P160	E93
	L224	Y161	
	S225	A162	R98
	T226	M163	P99
	E228	R164	E100
	K229	L165	E101
	K230	E167	D102
	K231	S168	A103
	G232	L169	
	K233	C170	E106
	Q234	Q171	K107
	T235	Y172	G108
	T236	R173	Y109
	H237	K174	E110
	T238	P175	S111
	F239		F112
	F240		P113
	S241	S178	W114
	F242	V181	F115
	P243	E182	I116
			K117

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.73 Å 99.32 Å 95.00 Å 90.00° 108.55° 90.00°	Depositor
Resolution (Å)	45.03 – 3.14 45.03 – 3.14	Depositor EDS
% Data completeness (in resolution range)	87.8 (45.03-3.14) 87.8 (45.03-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.12 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.266 , 0.313 0.247 , 0.280	Depositor DCC
R_{free} test set	850 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	1.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , -6.0	EDS
Estimated twinning fraction	0.088 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 16519 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4926	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	C	0.46	0/749	0.72	0/1153
2	D	0.43	0/761	0.69	0/1174
3	A	0.47	0/1839	0.71	0/2480
3	B	0.47	0/1826	0.68	0/2462
All	All	0.46	0/5175	0.70	0/7269

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1	DT	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	C	669	0	376	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	678	0	376	67	0
3	A	1796	0	1742	226	0
3	B	1783	0	1735	230	0
All	All	4926	0	4229	552	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 60.

All (552) 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:B:200:ARG:HG2	3:B:202:PRO:HD2	1.15	1.10
2:D:39:DG:H2"	2:D:40:DT:H5"	1.25	1.10
2:D:41:DG:H2"	2:D:42:DA:H5'	1.38	1.04
1:C:6:DG:C2'	1:C:7:DT:H5"	1.86	1.04
2:D:60:DA:H2"	2:D:61:DC:H5'	1.40	1.04
3:A:119:ALA:HB2	3:B:110:GLU:HA	1.42	0.99
2:D:39:DG:C2'	2:D:40:DT:H5"	1.93	0.99
1:C:6:DG:H2"	1:C:7:DT:H5"	1.43	0.98
3:B:164:ARG:HH11	3:B:164:ARG:HG2	1.25	0.98
1:C:24:DG:H2"	1:C:25:DT:H5'	1.45	0.98
3:B:63:HIS:HB2	3:B:66:LYS:HG2	1.45	0.97
3:A:42:PHE:HD1	3:A:131:ILE:HD11	1.30	0.96
3:A:244:ASP:OD2	3:A:246:THR:HG23	1.66	0.95
1:C:31:DT:H2"	1:C:32:DT:H5'	1.49	0.94
1:C:8:DG:H2"	1:C:9:DA:H5'	1.48	0.94
3:A:122:PRO:HG2	3:B:102:ASP:HA	1.49	0.93
2:D:60:DA:H62	3:B:200:ARG:HH12	1.12	0.92
3:B:223:ARG:HD3	3:B:245:ILE:HG13	1.51	0.92
1:C:1:DT:H2"	1:C:2:DT:H5'	1.54	0.89
1:C:21:DC:H2"	1:C:22:DT:H5"	1.54	0.89
3:B:206:ARG:O	3:B:207:ARG:HD3	1.73	0.88
2:D:50:DT:H2"	2:D:51:DT:H5'	1.55	0.88
3:A:132:ASN:HD22	3:A:132:ASN:C	1.77	0.88
3:A:116:ILE:HG12	3:B:116:ILE:HD12	1.56	0.88
1:C:6:DG:H2"	1:C:7:DT:C5'	2.03	0.87
3:B:98:ARG:HH11	3:B:98:ARG:HG2	1.40	0.86
3:B:37:ARG:HD2	3:B:71:PHE:CE2	2.10	0.86
1:C:22:DT:H2"	1:C:23:DT:H5'	1.56	0.85
3:A:42:PHE:O	3:A:46:ILE:HG12	1.75	0.85
3:A:132:ASN:HD22	3:A:133:PRO:N	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:160:PRO:O	3:A:164:ARG:HG3	1.76	0.84
1:C:4:DG:H5'	3:B:233:ARG:HB3	1.59	0.84
3:B:198:TYR:HE1	3:B:207:ARG:HB2	1.41	0.83
3:A:42:PHE:HD2	3:A:42:PHE:H	1.25	0.83
2:D:64:DT:H2''	2:D:65:DA:C8	2.14	0.83
1:C:29:DA:H2''	1:C:30:DC:H5''	1.60	0.83
2:D:52:DA:H1'	2:D:53:DG:H5''	1.60	0.82
1:C:7:DT:H4'	1:C:7:DT:OP1	1.79	0.82
3:A:164:ARG:HG2	3:A:164:ARG:HH11	1.45	0.80
3:A:145:ARG:HH11	3:A:145:ARG:HG2	1.46	0.80
3:A:42:PHE:CD1	3:A:131:ILE:HD11	2.15	0.80
3:A:99:PRO:HG2	3:A:100:GLU:H	1.45	0.80
3:B:160:PRO:HA	3:B:163:MET:HG2	1.64	0.79
3:A:37:ARG:HB3	3:A:71:PHE:CE1	2.17	0.79
3:A:213:VAL:HG13	3:A:224:LEU:HB3	1.63	0.79
3:B:116:ILE:HG12	3:B:132:ASN:HA	1.64	0.79
3:A:32:SER:OG	3:A:35:GLN:HG3	1.83	0.79
3:B:26:GLU:HB2	3:B:163:MET:SD	2.23	0.79
3:A:119:ALA:CB	3:B:110:GLU:HA	2.13	0.78
3:A:62:ILE:HG21	3:A:82:ILE:HD12	1.64	0.78
3:B:159:ASN:HD22	3:B:160:PRO:HD2	1.48	0.78
3:A:116:ILE:HD11	3:A:133:PRO:HD2	1.65	0.78
3:A:73:LEU:HD21	3:A:77:GLU:OE1	1.84	0.77
1:C:4:DG:C5'	3:B:233:ARG:HB3	2.14	0.77
3:B:187:TRP:CZ2	3:B:191:ARG:HG3	2.19	0.77
2:D:45:DA:H2''	2:D:46:DG:H5'	1.66	0.77
3:A:196:GLN:HG3	3:A:197:SER:N	1.99	0.77
2:D:41:DG:H2''	2:D:42:DA:C5'	2.15	0.76
3:A:31:LEU:HD22	3:A:35:GLN:NE2	2.00	0.76
3:A:73:LEU:HD22	3:A:77:GLU:HB2	1.67	0.76
3:B:154:THR:HG23	3:B:220:THR:HG22	1.66	0.75
3:B:173:ARG:O	3:B:174:LYS:HG3	1.86	0.75
2:D:60:DA:H2''	2:D:61:DC:C5'	2.16	0.75
2:D:60:DA:N6	3:B:200:ARG:HH12	1.84	0.75
3:A:116:ILE:HG13	3:A:132:ASN:HA	1.69	0.75
2:D:42:DA:H2''	2:D:43:DC:H5'	1.69	0.74
2:D:58:DT:H2''	2:D:59:DC:H5''	1.68	0.74
3:B:98:ARG:HB3	3:B:101:GLU:HB2	1.70	0.74
3:B:100:GLU:HG3	3:B:101:GLU:N	2.01	0.74
3:B:42:PHE:HE2	3:B:62:ILE:HD11	1.53	0.74
1:C:29:DA:C2'	1:C:30:DC:H5''	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:249:THR:O	3:A:249:THR:HG22	1.87	0.73
1:C:17:DA:H1'	1:C:18:DA:H5''	1.70	0.73
3:A:68:ALA:HB1	3:A:73:LEU:O	1.88	0.73
3:A:122:PRO:CG	3:B:102:ASP:HA	2.19	0.73
3:B:200:ARG:HG2	3:B:202:PRO:CD	2.08	0.73
1:C:1:DT:H3	2:D:66:DA:H2	1.37	0.73
3:B:164:ARG:NH1	3:B:164:ARG:HG2	2.02	0.72
3:B:172:TYR:HD1	3:B:181:VAL:HG21	1.54	0.72
3:B:61:GLU:OE1	3:B:126:LEU:HD11	1.90	0.72
3:A:34:ASP:HA	3:A:37:ARG:HG3	1.72	0.72
3:A:150:ARG:HH22	3:A:246:THR:HG21	1.53	0.72
3:B:36:LYS:HE2	3:B:154:THR:O	1.90	0.71
3:A:150:ARG:HH22	3:A:246:THR:CG2	2.02	0.71
3:A:223:ARG:HB3	3:A:243:ARG:NH1	2.06	0.71
1:C:12:DA:C2'	1:C:13:DT:H5''	2.21	0.71
3:A:228:GLU:HB3	3:A:235:THR:HG21	1.73	0.71
3:B:100:GLU:HG3	3:B:101:GLU:H	1.54	0.71
2:D:55:DT:H2''	2:D:56:DT:C5'	2.21	0.71
3:B:229:LYS:O	3:B:229:LYS:HG3	1.91	0.70
1:C:27:DA:H2''	1:C:28:DC:H5''	1.71	0.70
3:B:64:VAL:HG22	3:B:125:GLY:O	1.92	0.70
3:A:32:SER:HA	3:A:156:GLU:OE2	1.91	0.70
3:A:119:ALA:HB1	3:B:109:TYR:O	1.90	0.70
2:D:39:DG:H2''	2:D:40:DT:C5'	2.15	0.69
2:D:54:DA:H2''	2:D:55:DT:H5'	1.73	0.69
3:A:189:ILE:HD13	3:A:199:GLN:HG2	1.74	0.69
3:B:184:LYS:HD2	3:B:237:HIS:CD2	2.28	0.69
3:B:102:ASP:HB2	3:B:106:GLU:O	1.93	0.69
2:D:49:DT:H2''	2:D:50:DT:H5''	1.75	0.69
3:A:168:SER:O	3:A:171:GLN:HB3	1.93	0.69
3:B:227:ILE:HB	3:B:239:VAL:HB	1.74	0.69
3:A:100:GLU:HG2	3:A:101:GLU:N	2.07	0.69
3:B:200:ARG:CG	3:B:202:PRO:HD2	2.09	0.69
3:B:21:SER:O	3:B:22:ASN:HB3	1.93	0.69
3:A:178:SER:HA	3:A:243:ARG:HA	1.75	0.69
1:C:12:DA:H2''	1:C:13:DT:C5'	2.23	0.69
3:A:243:ARG:HG3	3:A:248:MET:SD	2.33	0.69
2:D:39:DG:C3'	2:D:40:DT:H5''	2.23	0.68
1:C:6:DG:H2'	1:C:7:DT:H5''	1.75	0.68
2:D:59:DC:H2''	2:D:60:DA:C8	2.27	0.68
1:C:31:DT:H2''	1:C:32:DT:C5'	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:145:ARG:CG	3:A:145:ARG:HH11	2.06	0.68
2:D:54:DA:H2"	2:D:55:DT:C5'	2.24	0.68
2:D:58:DT:C2'	2:D:59:DC:H5"	2.23	0.68
3:B:196:GLN:H	3:B:196:GLN:CD	1.97	0.68
1:C:12:DA:H2"	1:C:13:DT:H5"	1.76	0.68
3:B:160:PRO:HA	3:B:163:MET:CG	2.24	0.67
3:B:74:THR:HG23	3:B:77:GLU:CD	2.13	0.67
3:B:116:ILE:HD11	3:B:133:PRO:HD2	1.77	0.67
3:B:160:PRO:HB2	3:B:164:ARG:CZ	2.25	0.67
3:B:198:TYR:CE1	3:B:207:ARG:HB2	2.27	0.67
3:B:230:LYS:HA	3:B:235:THR:HA	1.76	0.67
3:B:98:ARG:NH1	3:B:98:ARG:HG2	2.07	0.67
3:A:102:ASP:HB3	3:A:108:GLY:H	1.59	0.67
3:A:172:TYR:CB	3:A:181:VAL:HG21	2.25	0.67
2:D:58:DT:H2"	2:D:59:DC:C5'	2.25	0.67
3:B:160:PRO:O	3:B:164:ARG:HG3	1.95	0.67
1:C:21:DC:H2"	1:C:22:DT:C5'	2.25	0.66
3:B:160:PRO:HB2	3:B:164:ARG:NH2	2.10	0.66
3:B:102:ASP:HB3	3:B:108:GLY:N	2.09	0.66
3:A:116:ILE:CD1	3:A:133:PRO:HD2	2.25	0.66
2:D:61:DC:H2"	2:D:62:DA:C8	2.30	0.66
3:B:110:GLU:HG2	3:B:112:PHE:CZ	2.31	0.66
3:A:245:ILE:HD13	3:A:245:ILE:O	1.96	0.66
3:B:164:ARG:HH11	3:B:164:ARG:CG	2.07	0.65
3:B:200:ARG:HE	3:B:202:PRO:HG2	1.62	0.65
2:D:57:DG:H1'	2:D:58:DT:H5"	1.79	0.65
3:B:133:PRO:HA	3:B:136:ILE:CD1	2.26	0.65
3:A:208:PHE:HD1	3:A:209:LEU:N	1.94	0.65
3:A:97:TYR:O	3:A:98:ARG:HD2	1.96	0.65
3:A:136:ILE:N	3:A:137:PRO:HD2	2.11	0.65
1:C:6:DG:H2"	1:C:7:DT:C4'	2.26	0.64
1:C:14:DC:H2"	1:C:15:DT:O5'	1.97	0.64
3:A:200:ARG:HH12	3:A:202:PRO:HB2	1.63	0.64
3:A:42:PHE:N	3:A:42:PHE:HD2	1.93	0.64
1:C:12:DA:H1'	1:C:13:DT:H5"	1.78	0.64
1:C:24:DG:H2"	1:C:25:DT:C5'	2.25	0.63
1:C:26:DC:H2"	1:C:27:DA:C8	2.32	0.63
2:D:55:DT:H2"	2:D:56:DT:H5'	1.78	0.63
3:A:174:LYS:O	3:A:176:ASP:N	2.31	0.63
3:A:122:PRO:HG2	3:B:102:ASP:CA	2.26	0.63
3:B:212:CYS:O	3:B:216:ILE:HG13	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:249:THR:O	3:A:249:THR:CG2	2.47	0.63
3:A:27:ALA:O	3:A:30:SER:HB3	1.99	0.63
3:A:200:ARG:NH1	3:A:202:PRO:HB2	2.14	0.62
2:D:38:DT:H2''	2:D:39:DG:OP2	1.98	0.62
3:B:170:CYS:O	3:B:173:ARG:HG3	1.98	0.62
2:D:60:DA:H62	3:B:200:ARG:NH1	1.91	0.62
3:A:150:ARG:NH2	3:A:246:THR:HG21	2.12	0.62
3:A:116:ILE:O	3:B:113:PRO:HD2	2.00	0.62
3:A:123:SER:HB3	3:B:101:GLU:O	2.00	0.62
3:A:169:LEU:HD13	3:A:224:LEU:HD11	1.81	0.62
3:A:172:TYR:CG	3:A:181:VAL:HG21	2.34	0.62
3:B:20:GLN:O	3:B:145:ARG:NH1	2.33	0.62
3:A:223:ARG:NE	3:A:245:ILE:HG13	2.13	0.62
3:B:66:LYS:O	3:B:70:ILE:HG12	1.99	0.62
3:A:93:GLU:OE2	3:B:118:ARG:NH2	2.33	0.62
3:A:116:ILE:HG12	3:B:116:ILE:CD1	2.29	0.62
3:A:165:LEU:CD2	3:A:169:LEU:HG	2.30	0.61
3:A:224:LEU:CD1	3:A:242:PHE:HB3	2.29	0.61
3:A:165:LEU:HA	3:A:192:TYR:CZ	2.35	0.61
3:B:42:PHE:CE2	3:B:62:ILE:HD11	2.34	0.61
1:C:25:DT:H2''	1:C:26:DC:H5''	1.81	0.61
3:A:194:LEU:HD21	3:A:208:PHE:CD2	2.34	0.61
3:A:224:LEU:HD12	3:A:242:PHE:HB3	1.81	0.61
3:A:208:PHE:CD1	3:A:209:LEU:N	2.68	0.61
3:B:128:SER:O	3:B:129:VAL:HG23	2.00	0.61
3:B:195:PRO:HD2	3:B:198:TYR:CD2	2.35	0.61
3:B:195:PRO:O	3:B:198:TYR:HB2	2.00	0.61
3:B:146:PHE:HD2	3:B:152:SER:HB2	1.65	0.61
3:B:172:TYR:HD1	3:B:181:VAL:CG2	2.13	0.61
2:D:44:DA:H2''	2:D:45:DA:H5'	1.83	0.61
3:B:59:ILE:HG22	3:B:60:CYS:N	2.13	0.61
3:B:24:LEU:O	3:B:24:LEU:HD23	2.01	0.60
3:A:184:LYS:HA	3:A:237:HIS:CD2	2.36	0.60
2:D:45:DA:H1'	2:D:46:DG:H5''	1.83	0.60
1:C:16:DA:H2''	1:C:17:DA:OP2	2.01	0.60
3:B:183:LEU:HD13	3:B:187:TRP:HZ3	1.64	0.60
3:B:146:PHE:HA	3:B:151:LEU:H	1.66	0.60
1:C:25:DT:C2'	1:C:26:DC:H5''	2.32	0.60
2:D:50:DT:C2'	2:D:51:DT:H5'	2.31	0.60
3:B:78:ALA:O	3:B:82:ILE:HG12	2.02	0.60
3:B:38:MET:CE	3:B:82:ILE:HG23	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:DG:OP1	3:B:234:GLN:HB2	2.01	0.59
3:A:140:ILE:O	3:A:143:GLN:HG2	2.01	0.59
3:A:123:SER:CB	3:B:101:GLU:O	2.51	0.59
3:A:196:GLN:HG3	3:A:197:SER:H	1.68	0.59
2:D:57:DG:H2''	2:D:58:DT:H5'	1.84	0.59
3:B:67:TYR:O	3:B:70:ILE:N	2.34	0.59
3:A:67:TYR:O	3:A:70:ILE:HG22	2.03	0.59
3:B:230:LYS:HG3	3:B:234:GLN:C	2.22	0.59
1:C:24:DG:H1'	1:C:25:DT:H5''	1.85	0.59
3:B:160:PRO:O	3:B:163:MET:HG2	2.03	0.59
3:A:132:ASN:ND2	3:A:132:ASN:C	2.51	0.59
3:B:209:LEU:O	3:B:210:GLN:C	2.41	0.58
3:B:192:TYR:HB2	3:B:194:LEU:HD13	1.84	0.58
3:A:164:ARG:HG2	3:A:164:ARG:NH1	2.14	0.58
3:B:126:LEU:C	3:B:126:LEU:HD23	2.23	0.58
3:B:22:ASN:O	3:B:25:THR:HB	2.02	0.58
3:B:63:HIS:HB2	3:B:66:LYS:CG	2.27	0.58
3:B:37:ARG:HD2	3:B:71:PHE:HE2	1.67	0.58
3:B:37:ARG:NH1	3:B:71:PHE:CD2	2.72	0.58
3:A:174:LYS:C	3:A:176:ASP:H	2.06	0.58
3:A:205:ARG:HG3	3:A:205:ARG:HH11	1.68	0.58
3:B:131:ILE:HD13	3:B:139:PHE:CZ	2.39	0.58
3:A:110:GLU:CD	3:B:117:LYS:HE3	2.23	0.58
2:D:35:DA:H1'	2:D:36:DA:H5''	1.85	0.58
1:C:11:DA:H2''	1:C:12:DA:H5'	1.85	0.57
2:D:45:DA:H2''	2:D:46:DG:C5'	2.33	0.57
3:B:223:ARG:HD3	3:B:245:ILE:CG1	2.30	0.57
3:A:62:ILE:CG2	3:A:82:ILE:HD12	2.34	0.57
3:A:200:ARG:HG2	3:A:202:PRO:HD2	1.87	0.57
1:C:25:DT:H2''	1:C:26:DC:C5'	2.35	0.57
3:A:113:PRO:HD2	3:B:116:ILE:O	2.05	0.57
1:C:12:DA:C1'	1:C:13:DT:H5''	2.35	0.57
3:A:97:TYR:HE2	3:A:107:LYS:HZ2	1.53	0.57
2:D:62:DA:H1'	2:D:63:DC:H5'	1.86	0.56
1:C:27:DA:C2'	1:C:28:DC:H5''	2.35	0.56
3:A:36:LYS:CE	3:A:151:LEU:HD11	2.35	0.56
1:C:18:DA:H5'	1:C:18:DA:H8	1.70	0.56
3:A:205:ARG:NH1	3:A:205:ARG:HG3	2.21	0.56
3:A:34:ASP:CA	3:A:37:ARG:HG3	2.35	0.56
3:A:47:ARG:HG2	3:A:47:ARG:HH11	1.71	0.56
1:C:17:DA:C2'	1:C:18:DA:H5''	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:DG:H5"	3:B:233:ARG:C	2.26	0.56
3:B:67:TYR:O	3:B:69:GLU:N	2.39	0.56
3:B:33:ARG:NH2	3:B:34:ASP:OD1	2.39	0.56
3:B:187:TRP:CE2	3:B:191:ARG:HG3	2.41	0.56
1:C:29:DA:C3'	1:C:30:DC:H5"	2.36	0.55
3:A:99:PRO:O	3:A:102:ASP:OD1	2.25	0.55
3:B:159:ASN:ND2	3:B:160:PRO:HD2	2.21	0.55
3:B:38:MET:HE1	3:B:82:ILE:HG23	1.89	0.55
3:A:184:LYS:HG3	3:A:237:HIS:CD2	2.42	0.55
3:A:100:GLU:HG2	3:A:101:GLU:H	1.72	0.55
3:A:223:ARG:O	3:A:242:PHE:HA	2.06	0.55
3:A:130:HIS:HD1	3:B:134:TYR:HH	1.53	0.55
3:B:160:PRO:HG2	3:B:161:TYR:H	1.72	0.55
3:A:177:GLY:O	3:A:244:ASP:N	2.40	0.55
3:A:122:PRO:HB2	3:B:103:ALA:HB3	1.89	0.55
3:B:32:SER:HA	3:B:156:GLU:OE2	2.06	0.55
1:C:4:DG:H2"	1:C:5:DT:OP2	2.07	0.54
3:A:117:LYS:HE3	3:B:112:PHE:CE2	2.42	0.54
3:A:100:GLU:CG	3:A:101:GLU:N	2.70	0.54
3:B:160:PRO:CA	3:B:163:MET:HG2	2.35	0.54
1:C:17:DA:C1'	1:C:18:DA:H5"	2.36	0.54
3:B:129:VAL:O	3:B:130:HIS:HD2	1.91	0.54
2:D:49:DT:C2'	2:D:50:DT:H5"	2.37	0.54
2:D:42:DA:C2'	2:D:43:DC:H5'	2.37	0.54
3:B:102:ASP:HB3	3:B:108:GLY:H	1.70	0.54
3:A:33:ARG:HD2	3:A:153:GLU:HA	1.90	0.54
3:A:174:LYS:HG2	3:A:178:SER:O	2.08	0.54
3:A:31:LEU:HD22	3:A:35:GLN:HE22	1.71	0.54
3:A:179:GLY:O	3:A:241:SER:HA	2.08	0.54
3:A:227:ILE:HG13	3:A:227:ILE:O	2.08	0.54
3:B:231:LYS:O	3:B:231:LYS:HG3	2.08	0.54
3:A:213:VAL:O	3:A:217:ASN:ND2	2.41	0.54
3:A:223:ARG:HB3	3:A:243:ARG:HH11	1.70	0.54
3:B:229:LYS:HG2	3:B:237:HIS:HB2	1.90	0.54
2:D:63:DC:C2'	2:D:64:DT:H72	2.37	0.53
3:B:167:GLU:O	3:B:171:GLN:HG2	2.08	0.53
2:D:63:DC:H2"	2:D:64:DT:H72	1.90	0.53
3:B:243:ARG:NH1	3:B:245:ILE:HD13	2.23	0.53
3:B:67:TYR:HD2	3:B:68:ALA:N	2.07	0.53
3:B:194:LEU:HD21	3:B:208:PHE:CD2	2.44	0.53
3:A:142:LEU:O	3:A:145:ARG:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:187:TRP:C	3:B:189:ILE:H	2.11	0.52
3:A:45:GLN:C	3:A:47:ARG:H	2.11	0.52
1:C:19:DA:H1'	1:C:20:DA:H5'	1.91	0.52
3:B:118:ARG:HG2	3:B:119:ALA:N	2.25	0.52
3:B:155:LYS:HD2	3:B:219:ARG:HD2	1.90	0.52
3:B:229:LYS:CG	3:B:237:HIS:HB2	2.40	0.52
2:D:57:DG:N7	3:B:207:ARG:NH1	2.56	0.52
3:A:37:ARG:O	3:A:38:MET:C	2.48	0.52
3:A:81:ASP:O	3:A:82:ILE:C	2.48	0.52
3:B:150:ARG:NH1	3:B:244:ASP:OD1	2.40	0.52
1:C:19:DA:H2''	1:C:20:DA:O5'	2.09	0.52
3:B:169:LEU:HB3	3:B:242:PHE:CD2	2.45	0.52
1:C:6:DG:H2''	1:C:7:DT:O4'	2.10	0.52
3:B:116:ILE:CG1	3:B:132:ASN:HA	2.36	0.52
3:A:142:LEU:O	3:A:145:ARG:HB2	2.10	0.52
3:B:164:ARG:O	3:B:166:TYR:N	2.43	0.52
3:A:190:GLU:C	3:A:192:TYR:H	2.12	0.52
3:A:165:LEU:HA	3:A:192:TYR:OH	2.10	0.52
3:B:183:LEU:HD13	3:B:187:TRP:CZ3	2.44	0.52
3:B:151:LEU:HA	3:B:154:THR:OG1	2.10	0.52
3:A:22:ASN:OD1	3:A:24:LEU:HB3	2.10	0.52
3:B:133:PRO:HA	3:B:136:ILE:HD12	1.90	0.51
3:A:100:GLU:CG	3:A:101:GLU:H	2.22	0.51
3:A:36:LYS:HE3	3:A:151:LEU:HD11	1.91	0.51
3:B:196:GLN:C	3:B:198:TYR:H	2.14	0.51
3:A:168:SER:HB2	3:A:192:TYR:OH	2.11	0.51
1:C:28:DC:H2'	1:C:29:DA:C8	2.46	0.51
3:A:184:LYS:HG3	3:A:237:HIS:NE2	2.25	0.51
2:D:55:DT:H2''	2:D:56:DT:H5''	1.91	0.51
3:B:198:TYR:HE1	3:B:207:ARG:CB	2.19	0.51
3:B:229:LYS:CD	3:B:237:HIS:HB2	2.40	0.51
1:C:29:DA:H2''	1:C:30:DC:O4'	2.11	0.51
3:A:129:VAL:HG23	3:A:129:VAL:O	2.11	0.51
3:B:110:GLU:HG2	3:B:112:PHE:HZ	1.73	0.51
3:A:32:SER:O	3:A:35:GLN:HB2	2.11	0.51
3:B:35:GLN:HG2	3:B:85:ALA:HB1	1.92	0.50
1:C:21:DC:C6	1:C:22:DT:H72	2.45	0.50
1:C:16:DA:C2	2:D:52:DA:C2	2.99	0.50
3:A:139:PHE:O	3:A:141:GLY:N	2.44	0.50
1:C:6:DG:C2'	1:C:7:DT:C5'	2.67	0.50
3:B:164:ARG:NH1	3:B:164:ARG:CG	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:149:PHE:CD1	3:B:149:PHE:N	2.79	0.50
3:A:90:ALA:O	3:A:92:LYS:N	2.44	0.50
3:A:42:PHE:N	3:A:42:PHE:CD2	2.65	0.50
2:D:43:DC:H2''	2:D:44:DA:C8	2.45	0.50
3:A:119:ALA:HA	3:B:109:TYR:CE1	2.47	0.50
3:A:102:ASP:HA	3:B:122:PRO:HG2	1.92	0.50
3:A:172:TYR:CD1	3:A:181:VAL:HG11	2.47	0.50
3:B:209:LEU:HD22	3:B:226:TYR:CD2	2.47	0.50
3:B:25:THR:C	3:B:27:ALA:H	2.13	0.50
1:C:25:DT:H1'	1:C:26:DC:H5''	1.94	0.50
3:B:195:PRO:HD2	3:B:198:TYR:HD2	1.77	0.49
2:D:60:DA:N6	3:B:200:ARG:HH22	2.10	0.49
3:B:203:ASP:O	3:B:206:ARG:N	2.45	0.49
3:A:184:LYS:O	3:A:187:TRP:HB3	2.12	0.49
3:A:236:THR:O	3:A:237:HIS:HD2	1.95	0.49
3:A:146:PHE:HD2	3:A:152:SER:HG	1.59	0.49
2:D:52:DA:C1'	2:D:53:DG:H5''	2.37	0.49
3:A:102:ASP:HB3	3:A:108:GLY:N	2.25	0.49
3:B:74:THR:HG23	3:B:77:GLU:OE2	2.12	0.49
3:A:120:HIS:ND1	3:A:127:TYR:CE1	2.81	0.49
3:B:196:GLN:O	3:B:199:GLN:HG2	2.11	0.49
3:B:32:SER:O	3:B:33:ARG:C	2.51	0.49
3:A:116:ILE:CG1	3:B:116:ILE:HD12	2.36	0.49
3:A:145:ARG:NH1	3:A:145:ARG:CG	2.69	0.49
3:A:37:ARG:HB3	3:A:71:PHE:HE1	1.73	0.49
3:B:59:ILE:CG2	3:B:60:CYS:N	2.75	0.49
3:A:133:PRO:O	3:A:134:TYR:C	2.51	0.49
3:B:59:ILE:HG23	3:B:130:HIS:CD2	2.48	0.48
3:B:196:GLN:N	3:B:196:GLN:CD	2.66	0.48
1:C:4:DG:H5''	3:B:233:ARG:HB3	1.94	0.48
3:B:243:ARG:HH11	3:B:245:ILE:HD13	1.78	0.48
3:B:151:LEU:HA	3:B:154:THR:HG1	1.78	0.48
3:A:229:LYS:O	3:A:236:THR:HG23	2.14	0.48
3:A:218:SER:O	3:A:219:ARG:HD3	2.13	0.48
3:A:228:GLU:HB3	3:A:235:THR:CG2	2.42	0.48
3:B:169:LEU:HB3	3:B:242:PHE:CE2	2.47	0.48
3:B:173:ARG:O	3:B:174:LYS:CG	2.58	0.48
1:C:13:DT:H2''	1:C:14:DC:O5'	2.12	0.48
3:B:168:SER:O	3:B:169:LEU:C	2.51	0.48
3:B:155:LYS:HB3	3:B:219:ARG:HB3	1.96	0.48
3:A:112:PHE:N	3:A:112:PHE:CD1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:213:VAL:HG21	3:B:226:TYR:HD2	1.79	0.48
3:B:229:LYS:HD2	3:B:237:HIS:HB2	1.96	0.48
3:B:206:ARG:HA	3:B:210:GLN:OE1	2.13	0.48
1:C:23:DT:H1'	1:C:24:DG:H5''	1.96	0.48
3:A:42:PHE:HE1	3:A:115:PHE:HE1	1.62	0.47
3:B:116:ILE:HG13	3:B:133:PRO:HD3	1.96	0.47
3:B:185:ILE:HA	3:B:188:ILE:HG12	1.96	0.47
3:A:25:THR:C	3:A:27:ALA:H	2.17	0.47
3:A:183:LEU:HD12	3:A:240:PHE:CE1	2.50	0.47
3:A:190:GLU:O	3:A:193:GLN:N	2.39	0.47
3:A:132:ASN:ND2	3:A:134:TYR:N	2.62	0.47
3:B:196:GLN:O	3:B:198:TYR:N	2.47	0.47
3:A:117:LYS:HB2	3:B:112:PHE:CD2	2.49	0.47
3:A:160:PRO:O	3:A:164:ARG:CG	2.57	0.47
3:A:32:SER:O	3:A:36:LYS:HG2	2.14	0.47
3:A:68:ALA:O	3:A:73:LEU:N	2.47	0.47
3:A:230:LYS:CB	3:A:235:THR:HA	2.45	0.47
3:B:162:ALA:HA	3:B:212:CYS:HB3	1.97	0.47
1:C:17:DA:H2''	1:C:18:DA:H5''	1.96	0.47
3:B:142:LEU:O	3:B:145:ARG:HB2	2.15	0.47
3:B:213:VAL:HG13	3:B:224:LEU:HD23	1.97	0.46
3:B:35:GLN:CG	3:B:85:ALA:HB1	2.45	0.46
2:D:63:DC:H2''	2:D:64:DT:C7	2.46	0.46
3:A:29:TYR:HA	3:A:36:LYS:NZ	2.31	0.46
3:A:185:ILE:HG12	3:A:236:THR:O	2.16	0.46
3:A:229:LYS:O	3:A:236:THR:CG2	2.63	0.46
3:B:203:ASP:O	3:B:204:PHE:C	2.53	0.46
3:A:207:ARG:HA	3:A:207:ARG:HD3	1.57	0.46
3:A:46:ILE:HG22	3:A:46:ILE:O	2.15	0.46
3:A:213:VAL:HG22	3:A:224:LEU:HD23	1.97	0.46
3:A:32:SER:OG	3:A:35:GLN:CG	2.60	0.46
3:A:236:THR:OG1	3:A:237:HIS:CD2	2.69	0.46
3:A:216:ILE:HA	3:A:220:THR:HG23	1.97	0.46
3:B:173:ARG:HH11	3:B:173:ARG:HB2	1.81	0.46
3:A:47:ARG:HG2	3:A:47:ARG:NH1	2.31	0.46
3:A:40:TYR:O	3:A:41:LEU:C	2.54	0.46
3:B:230:LYS:HD3	3:B:233:ARG:O	2.16	0.46
3:A:70:ILE:O	3:A:71:PHE:CD2	2.69	0.46
3:A:191:ARG:O	3:A:192:TYR:HD1	1.98	0.46
3:B:173:ARG:NH1	3:B:173:ARG:HB2	2.30	0.46
2:D:60:DA:C2'	2:D:61:DC:C5'	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:DA:H5'	1:C:18:DA:C8	2.51	0.46
3:B:37:ARG:CZ	3:B:71:PHE:CD2	2.99	0.46
3:A:120:HIS:CE1	3:A:127:TYR:CE1	3.04	0.46
3:A:183:LEU:HD12	3:A:240:PHE:HE1	1.81	0.46
3:B:196:GLN:C	3:B:198:TYR:N	2.68	0.45
3:B:120:HIS:CD2	3:B:122:PRO:HD3	2.51	0.45
3:B:146:PHE:O	3:B:150:ARG:HA	2.16	0.45
3:B:31:LEU:CD1	3:B:39:LEU:HD22	2.45	0.45
1:C:24:DG:C2'	1:C:25:DT:H5'	2.31	0.45
3:A:117:LYS:HE3	3:B:112:PHE:HE2	1.81	0.45
3:A:104:GLY:C	3:A:106:GLU:H	2.19	0.45
3:B:172:TYR:CD1	3:B:181:VAL:HG21	2.43	0.45
3:A:169:LEU:CD1	3:A:224:LEU:HD11	2.46	0.45
3:A:156:GLU:CD	3:A:156:GLU:H	2.20	0.45
3:B:184:LYS:HD2	3:B:237:HIS:HD2	1.77	0.45
3:B:203:ASP:O	3:B:205:ARG:N	2.49	0.45
1:C:5:DT:OP1	3:B:205:ARG:NH2	2.50	0.45
3:B:33:ARG:O	3:B:37:ARG:HG3	2.17	0.45
3:A:182:SER:HB2	3:A:239:VAL:HG22	1.99	0.45
3:B:213:VAL:HA	3:B:224:LEU:HD23	1.98	0.45
2:D:41:DG:O6	3:A:206:ARG:NH2	2.45	0.45
3:B:139:PHE:HA	3:B:142:LEU:HB3	1.99	0.45
3:A:102:ASP:HB2	3:A:106:GLU:O	2.16	0.45
3:A:190:GLU:O	3:A:192:TYR:N	2.49	0.45
3:B:78:ALA:O	3:B:81:ASP:N	2.50	0.45
3:B:155:LYS:HE3	3:B:155:LYS:HB2	1.84	0.45
3:A:84:GLN:CA	3:A:84:GLN:HE21	2.29	0.45
3:B:67:TYR:CD2	3:B:68:ALA:N	2.84	0.45
3:B:164:ARG:C	3:B:166:TYR:N	2.70	0.44
3:B:133:PRO:HA	3:B:136:ILE:HG13	1.98	0.44
3:B:136:ILE:HB	3:B:137:PRO:CD	2.47	0.44
3:A:176:ASP:N	3:A:176:ASP:OD1	2.49	0.44
3:B:189:ILE:HG22	3:B:190:GLU:N	2.31	0.44
3:A:109:TYR:HB2	3:A:110:GLU:H	1.55	0.44
3:A:117:LYS:HB2	3:B:112:PHE:CE2	2.52	0.44
3:A:139:PHE:O	3:A:140:ILE:C	2.56	0.44
3:A:212:CYS:O	3:A:213:VAL:C	2.55	0.44
3:A:25:THR:C	3:A:27:ALA:N	2.70	0.44
3:B:89:PHE:C	3:B:90:ALA:O	2.54	0.44
3:A:201:MET:O	3:A:204:PHE:HB3	2.18	0.44
1:C:22:DT:H2''	1:C:23:DT:C5'	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:198:TYR:CE1	3:B:207:ARG:CB	2.99	0.44
2:D:62:DA:N3	2:D:63:DC:O4'	2.51	0.44
1:C:28:DC:H6	1:C:28:DC:C5'	2.30	0.44
3:A:116:ILE:HG13	3:A:132:ASN:CA	2.45	0.44
3:A:170:CYS:O	3:A:172:TYR:N	2.51	0.44
3:A:41:LEU:O	3:A:44:ASP:N	2.50	0.44
3:B:164:ARG:O	3:B:167:GLU:N	2.50	0.44
3:A:165:LEU:HD23	3:A:169:LEU:HG	1.99	0.44
3:B:165:LEU:O	3:B:165:LEU:HG	2.18	0.44
3:A:99:PRO:HG2	3:A:100:GLU:N	2.23	0.44
3:A:120:HIS:ND1	3:A:127:TYR:CD1	2.85	0.44
3:A:83:ARG:HB2	3:A:127:TYR:OH	2.18	0.44
3:A:209:LEU:O	3:A:210:GLN:C	2.55	0.43
3:A:97:TYR:HE2	3:A:107:LYS:NZ	2.17	0.43
3:B:214:ASN:C	3:B:216:ILE:H	2.21	0.43
2:D:35:DA:H1'	2:D:36:DA:C5'	2.46	0.43
2:D:58:DT:H1'	2:D:59:DC:H5''	1.99	0.43
3:A:200:ARG:HD3	3:A:203:ASP:OD2	2.18	0.43
3:B:112:PHE:CE2	3:B:134:TYR:CD2	3.06	0.43
3:A:33:ARG:O	3:A:37:ARG:HG3	2.17	0.43
3:A:169:LEU:HB3	3:A:242:PHE:CE2	2.53	0.43
3:B:151:LEU:C	3:B:154:THR:HG1	2.20	0.43
2:D:54:DA:H2''	2:D:55:DT:H5''	1.98	0.43
2:D:55:DT:C2'	2:D:56:DT:H5''	2.47	0.43
3:B:83:ARG:HG3	3:B:84:GLN:N	2.33	0.43
2:D:62:DA:H1'	2:D:63:DC:C5'	2.49	0.43
3:A:185:ILE:HD11	3:A:238:ILE:HG12	2.00	0.43
3:B:195:PRO:HB2	3:B:198:TYR:CD2	2.54	0.43
3:B:145:ARG:HH21	3:B:167:GLU:CD	2.21	0.43
3:B:146:PHE:CE1	3:B:151:LEU:HD23	2.54	0.43
2:D:57:DG:H2''	2:D:58:DT:C5'	2.48	0.43
1:C:21:DC:C2'	1:C:22:DT:H5''	2.36	0.43
3:A:211:VAL:HG12	3:A:212:CYS:N	2.32	0.43
3:A:109:TYR:CD1	3:A:109:TYR:N	2.87	0.43
3:B:24:LEU:HD13	3:B:138:PHE:HB2	2.01	0.43
1:C:7:DT:H2''	1:C:8:DG:C8	2.54	0.43
3:A:203:ASP:O	3:A:204:PHE:C	2.56	0.43
3:B:100:GLU:CG	3:B:101:GLU:N	2.77	0.43
3:A:139:PHE:O	3:A:142:LEU:N	2.41	0.43
3:A:180:ILE:HG12	3:A:241:SER:OG	2.18	0.43
3:A:201:MET:HB3	3:A:202:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:146:PHE:CD2	3:B:152:SER:HB2	2.51	0.42
3:B:30:SER:OG	3:B:31:LEU:N	2.52	0.42
3:B:121:SER:O	3:B:123:SER:N	2.52	0.42
3:B:164:ARG:HB3	3:B:192:TYR:CD1	2.53	0.42
3:B:220:THR:HB	3:B:221:PRO:HD2	2.00	0.42
3:A:139:PHE:C	3:A:141:GLY:N	2.72	0.42
3:B:169:LEU:HD21	3:B:240:PHE:CD1	2.54	0.42
3:B:112:PHE:CD1	3:B:112:PHE:N	2.87	0.42
1:C:6:DG:O6	2:D:61:DC:N4	2.42	0.42
2:D:44:DA:H1'	2:D:45:DA:H5''	2.01	0.42
2:D:45:DA:C2'	2:D:46:DG:C5'	2.97	0.42
3:A:73:LEU:CD2	3:A:77:GLU:OE1	2.63	0.42
1:C:30:DC:C6	1:C:31:DT:H72	2.55	0.42
3:A:159:ASN:OD1	3:A:162:ALA:N	2.50	0.42
3:B:174:LYS:O	3:B:175:PRO:C	2.58	0.42
3:B:24:LEU:CD1	3:B:138:PHE:HB2	2.49	0.42
2:D:48:DT:H2''	2:D:49:DT:C6	2.55	0.42
3:A:172:TYR:CD1	3:A:181:VAL:HG21	2.54	0.42
3:A:209:LEU:HD13	3:A:226:TYR:CE1	2.55	0.42
3:B:93:GLU:HG2	3:B:113:PRO:HA	2.01	0.42
3:B:133:PRO:HA	3:B:136:ILE:CG1	2.49	0.42
3:B:178:SER:HA	3:B:243:ARG:HA	2.01	0.42
3:A:168:SER:CB	3:A:192:TYR:OH	2.68	0.42
3:A:188:ILE:C	3:A:190:GLU:N	2.73	0.42
3:B:174:LYS:HB3	3:B:174:LYS:NZ	2.35	0.42
3:B:165:LEU:HD11	3:B:240:PHE:CE1	2.55	0.42
3:A:159:ASN:O	3:A:161:TYR:N	2.53	0.41
3:A:223:ARG:HD2	3:A:223:ARG:HA	1.78	0.41
2:D:39:DG:O6	3:A:200:ARG:NH2	2.54	0.41
3:B:32:SER:OG	3:B:35:GLN:HG3	2.20	0.41
3:A:99:PRO:CG	3:A:100:GLU:H	2.21	0.41
3:A:223:ARG:HD3	3:A:245:ILE:HB	2.01	0.41
3:B:117:LYS:HD3	3:B:130:HIS:CE1	2.54	0.41
3:B:206:ARG:HE	3:B:206:ARG:HB3	1.70	0.41
3:A:145:ARG:O	3:A:146:PHE:C	2.58	0.41
1:C:11:DA:C6	1:C:12:DA:C6	3.08	0.41
3:A:100:GLU:O	3:A:102:ASP:N	2.54	0.41
3:B:151:LEU:CA	3:B:154:THR:HG1	2.32	0.41
3:A:198:TYR:CD2	3:A:198:TYR:N	2.89	0.41
3:B:187:TRP:O	3:B:191:ARG:HB2	2.20	0.41
1:C:1:DT:C2'	1:C:2:DT:H5'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:241:SER:O	3:A:243:ARG:NH2	2.53	0.41
3:B:25:THR:C	3:B:27:ALA:N	2.74	0.41
3:B:25:THR:CG2	3:B:145:ARG:NE	2.84	0.41
3:A:78:ALA:O	3:A:82:ILE:HG12	2.21	0.41
1:C:12:DA:H2''	1:C:13:DT:H5'	2.02	0.41
3:A:170:CYS:O	3:A:173:ARG:N	2.50	0.41
3:A:202:PRO:O	3:A:205:ARG:HB2	2.20	0.41
3:A:93:GLU:HA	3:A:113:PRO:HA	2.03	0.41
3:A:188:ILE:O	3:A:190:GLU:N	2.54	0.41
3:A:192:TYR:O	3:A:193:GLN:C	2.59	0.41
3:A:122:PRO:HG2	3:B:102:ASP:C	2.40	0.41
1:C:16:DA:H2	2:D:52:DA:C2	2.40	0.41
3:A:159:ASN:HA	3:A:160:PRO:HD2	1.80	0.41
3:A:169:LEU:HD11	3:A:224:LEU:HD21	2.03	0.41
3:A:190:GLU:C	3:A:192:TYR:N	2.75	0.41
1:C:11:DA:H2''	1:C:12:DA:OP2	2.21	0.41
3:B:115:PHE:CD2	3:B:129:VAL:HG13	2.55	0.41
3:B:136:ILE:O	3:B:137:PRO:C	2.59	0.40
3:A:43:VAL:O	3:A:47:ARG:HG3	2.21	0.40
3:A:84:GLN:C	3:A:84:GLN:HE21	2.25	0.40
3:B:30:SER:O	3:B:31:LEU:C	2.60	0.40
2:D:63:DC:H2''	2:D:64:DT:OP2	2.21	0.40
2:D:45:DA:H1'	2:D:46:DG:C5'	2.49	0.40
3:B:99:PRO:O	3:B:102:ASP:OD1	2.38	0.40
2:D:51:DT:H1'	2:D:52:DA:H5'	2.03	0.40
3:A:31:LEU:HB2	3:A:36:LYS:HD2	2.02	0.40
2:D:55:DT:H1'	2:D:56:DT:H5''	2.02	0.40
3:A:145:ARG:HA	3:A:149:PHE:HD1	1.86	0.40
3:B:173:ARG:HB3	3:B:173:ARG:CZ	2.51	0.40
2:D:45:DA:C1'	2:D:46:DG:H5''	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	218/266 (82%)	158 (72%)	40 (18%)	20 (9%)	1	4
3	B	214/266 (80%)	158 (74%)	35 (16%)	21 (10%)	1	4
All	All	432/532 (81%)	316 (73%)	75 (17%)	41 (10%)	1	4

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	91	GLY
3	A	99	PRO
3	B	68	ALA
3	B	147	THR
3	B	209	LEU
3	B	211	VAL
3	A	46	ILE
3	A	101	GLU
3	A	191	ARG
3	A	209	LEU
3	B	31	LEU
3	B	125	GLY
3	B	165	LEU
3	B	173	ARG
3	A	39	LEU
3	A	72	GLY
3	A	82	ILE
3	A	171	GLN
3	A	175	PRO
3	B	22	ASN
3	B	67	TYR
3	B	204	PHE
3	B	210	GLN
3	B	215	GLU
3	A	79	SER
3	A	81	ASP
3	A	201	MET
3	B	45	GLN
3	B	64	VAL
3	B	197	SER
3	B	202	PRO
3	B	246	THR
3	A	140	ILE

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Mol	Chain	Res	Type
3	A	152	SER
3	A	193	GLN
3	A	211	VAL
3	B	23	ASP
3	B	122	PRO
3	A	125	GLY
3	B	188	ILE
3	A	58	GLY

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	
3	A	188/238 (79%)	162 (86%)	26 (14%)	4	19
3	B	189/238 (79%)	178 (94%)	11 (6%)	25	61
All	All	377/476 (79%)	340 (90%)	37 (10%)	10	36

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	36	LYS
3	A	42	PHE
3	A	69	GLU
3	A	73	LEU
3	A	84	GLN
3	A	89	PHE
3	A	98	ARG
3	A	100	GLU
3	A	102	ASP
3	A	117	LYS
3	A	118	ARG
3	A	126	LEU
3	A	132	ASN
3	A	135	LEU
3	A	145	ARG

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Mol	Chain	Res	Type
3	A	152	SER
3	A	165	LEU
3	A	176	ASP
3	A	189	ILE
3	A	193	GLN
3	A	205	ARG
3	A	218	SER
3	A	220	THR
3	A	245	ILE
3	A	246	THR
3	A	247	SER
3	B	80	LYS
3	B	83	ARG
3	B	89	PHE
3	B	98	ARG
3	B	100	GLU
3	B	126	LEU
3	B	154	THR
3	B	191	ARG
3	B	215	GLU
3	B	223	ARG
3	B	226	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	35	GLN
3	A	84	GLN
3	A	132	ASN
3	A	148	GLN
3	A	171	GLN
3	A	196	GLN
3	A	237	HIS
3	B	84	GLN
3	B	130	HIS
3	B	148	GLN
3	B	159	ASN
3	B	237	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	33/33 (100%)	-0.88	0 100 100	22, 65, 95, 99	0
2	D	33/33 (100%)	-0.85	0 100 100	39, 59, 103, 109	0
3	A	222/266 (83%)	-0.29	0 100 100	3, 33, 66, 79	0
3	B	218/266 (81%)	-0.22	1 (0%) 91 84	5, 41, 69, 80	0
All	All	506/598 (84%)	-0.33	1 (0%) 95 91	3, 41, 75, 109	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	246	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.