



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:46 AM GMT

PDB ID : 2O61
Title : Crystal Structure of NFkB, IRF7, IRF3 bound to the interferon-b enhancer
Authors : Panne, D.
Deposited on : 2006-12-06
Resolution : 2.80 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

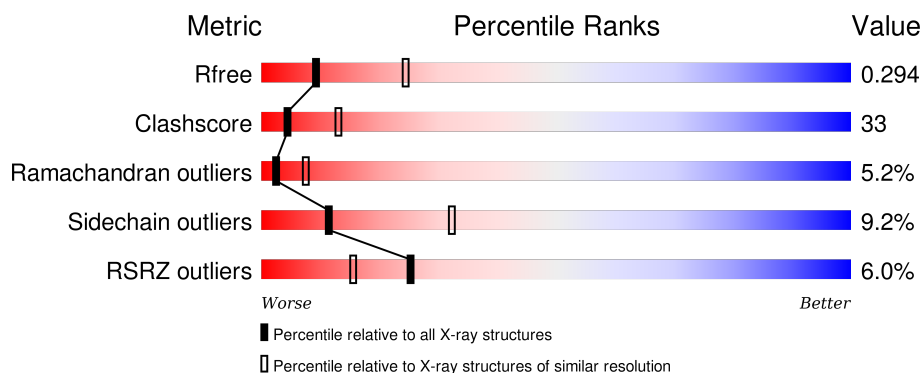
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	E	36	<div> <div>8%</div> <div>14%</div> <div>83%</div> <div>.</div> </div>
2	F	34	<div> <div>3%</div> <div>29%</div> <div>71%</div> </div>
3	A	540	<div> <div>6%</div> <div>49%</div> <div>36%</div> <div>6%</div> <div>.</div> <div>8%</div> </div>
4	B	314	<div> <div>5%</div> <div>52%</div> <div>39%</div> <div>8%</div> <div>.</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7912 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 36-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	36	Total	C	N	O	P	0	0	0
			750	357	147	211	35			

- Molecule 2 is a DNA chain called 34-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	34	Total	C	N	O	P	0	0	0
			678	328	110	207	33			

- Molecule 3 is a protein called Transcription factor p65/Interferon regulatory factor 7/Interferon regulatory factor 3 fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	498	Total	C	N	O	S	0	0	0
			3988	2505	745	722	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	INITIATING METHIONINE	UNP Q04206
A	19	GLY	-	CLONING ARTIFACT	UNP Q04206
A	292	GLY	-	LINKER	UNP Q04206
A	293	SER	-	LINKER	UNP Q04206
A	294	LEU	-	LINKER	UNP Q04206
A	295	SER	-	LINKER	UNP Q04206
A	296	SER	-	LINKER	UNP Q04206
A	297	GLY	-	LINKER	UNP Q04206
A	298	SER	-	LINKER	UNP Q04206
A	299	SER	-	LINKER	UNP Q04206
A	300	LEU	-	LINKER	UNP Q04206
A	301	SER	-	LINKER	UNP Q04206
A	302	SER	-	LINKER	UNP Q04206

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Chain	Residue	Modelled	Actual	Comment	Reference
A	303	PRO	-	LINKER	UNP Q04206
A	304	SER	-	LINKER	UNP Q04206
A	305	ALA	-	LINKER	UNP Q04206
A	306	GLY	-	LINKER	UNP Q04206
A	1118	GLN	PRO	ENGINEERED	UNP Q92985
A	1126	GLY	-	LINKER	UNP Q92985
A	1127	SER	-	LINKER	UNP Q92985
A	1128	LEU	-	LINKER	UNP Q92985
A	1129	SER	-	LINKER	UNP Q92985
A	1130	SER	-	LINKER	UNP Q92985
A	1131	ASP	-	LINKER	UNP Q92985
A	1132	SER	-	LINKER	UNP Q92985
A	1133	SER	-	LINKER	UNP Q92985
A	1134	LEU	-	LINKER	UNP Q92985
A	1135	SER	-	LINKER	UNP Q92985
A	1136	SER	-	LINKER	UNP Q92985
A	1137	PRO	-	LINKER	UNP Q92985
A	1138	SER	-	LINKER	UNP Q92985
A	1139	ALA	-	LINKER	UNP Q92985
A	1140	LEU	-	LINKER	UNP Q92985
A	1141	SER	-	LINKER	UNP Q92985
A	1142	PRO	-	LINKER	UNP Q92985
A	1143	LYS	-	LINKER	UNP Q92985
A	1144	PRO	-	LINKER	UNP Q92985
A	1145	ARG	-	LINKER	UNP Q92985
A	1146	ILE	-	LINKER	UNP Q92985
A	2112	GLY	-	EXPRESSION TAG	UNP Q14653
A	2113	LEU	-	EXPRESSION TAG	UNP Q14653
A	2114	GLU	-	EXPRESSION TAG	UNP Q14653
A	2115	HIS	-	EXPRESSION TAG	UNP Q14653
A	2116	HIS	-	EXPRESSION TAG	UNP Q14653
A	2117	HIS	-	EXPRESSION TAG	UNP Q14653
A	2118	HIS	-	EXPRESSION TAG	UNP Q14653
A	2119	HIS	-	EXPRESSION TAG	UNP Q14653
A	2120	HIS	-	EXPRESSION TAG	UNP Q14653

- Molecule 4 is a protein called Nuclear factor NF-kappa-B p105 subunit.

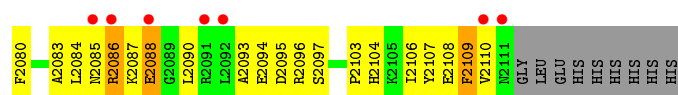
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	314	Total	C	N	O	S	0	0	0
			2471	1566	430	462	13			

There is a discrepancy between the modelled and reference sequences:

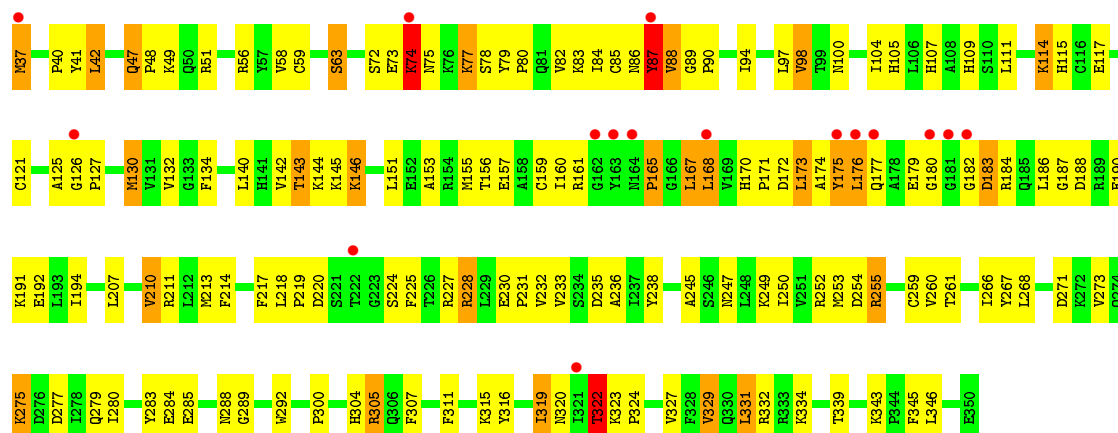
Chain	Residue	Modelled	Actual	Comment	Reference
B	37	MET	-	INITIATING METHIONINE	UNP P19838

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0
5	B	5	Total O 5 5	0	0
5	E	6	Total O 6 6	0	0
5	F	4	Total O 4 4	0	0



• Molecule 4: Nuclear factor NF-kappa-B p105 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.22Å 116.37Å 134.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.65 – 2.80 40.50 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.65-2.80) 99.0 (40.50-2.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.278 0.253 , 0.294	Depositor DCC
R_{free} test set	1863 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 38100 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7912	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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

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	0.47	0/845	0.82	2/1306 (0.2%)
2	F	0.42	0/755	0.79	0/1160
3	A	0.41	0/4094	0.67	2/5547 (0.0%)
4	B	0.41	0/2524	0.68	0/3407
All	All	0.42	0/8218	0.71	4/11420 (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	1	0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	35	DG	N9-C1'-C2'	6.43	124.82	112.60
1	E	35	DG	O4'-C1'-N9	5.13	111.59	108.00
3	A	1099	LEU	CA-CB-CG	5.10	127.03	115.30
3	A	175	LEU	CA-CB-CG	5.02	126.84	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	35	DG	C1'

There are no planarity outliers.

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	750	0	407	48	0
2	F	678	0	388	60	0
3	A	3988	0	3878	224	0
4	B	2471	0	2468	177	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
5	E	6	0	0	0	0
5	F	4	0	0	0	0
All	All	7912	0	7141	490	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 33.

All (490) 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)
4:B:47:GLN:HG3	4:B:48:PRO:HD2	1.29	1.10
3:A:2009:LEU:HG	3:A:2087:LYS:HE3	1.32	1.09
2:F:30:DC:H2''	2:F:31:DT:H5''	1.33	1.08
3:A:2086:ARG:CG	3:A:2086:ARG:HH11	1.67	1.07
3:A:2029:LYS:HD3	3:A:2029:LYS:H	1.20	1.06
1:E:11:DG:O6	3:A:2086:ARG:NH2	1.88	1.06
2:F:3:DA:H2''	2:F:4:DG:H5'	1.41	1.02
4:B:88:VAL:HB	4:B:218:LEU:HD22	1.44	0.99
4:B:77:LYS:HD3	4:B:77:LYS:H	1.29	0.95
3:A:41:ARG:HG2	3:A:42:SER:H	1.30	0.94
2:F:34:DC:H2''	2:F:35:DA:H5'	1.46	0.93
1:E:34:DT:H2''	1:E:35:DG:H1'	1.51	0.92
4:B:74:LYS:HG2	4:B:75:ASN:H	1.34	0.91
4:B:42:LEU:HD21	4:B:82:VAL:HB	1.51	0.91
4:B:146:LYS:HE3	4:B:146:LYS:HA	1.53	0.91
3:A:2073:LEU:HD22	3:A:2073:LEU:H	1.35	0.90
3:A:2086:ARG:HH11	3:A:2086:ARG:HG2	1.36	0.90
2:F:22:DA:H2''	2:F:23:DC:H5''	1.51	0.88
4:B:58:VAL:HG12	4:B:140:LEU:HD11	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:168:LEU:HD12	4:B:168:LEU:H	1.38	0.88
1:E:21:DT:H2''	1:E:22:DG:H5'	1.55	0.87
4:B:332:ARG:HG3	4:B:339:THR:HG22	1.57	0.87
4:B:211:ARG:HH11	4:B:233:VAL:HG11	1.41	0.84
3:A:2028:ASN:HB2	3:A:2033:ARG:HB3	1.60	0.84
3:A:2086:ARG:HH11	3:A:2086:ARG:HG3	1.42	0.84
3:A:41:ARG:HG2	3:A:42:SER:N	1.93	0.82
2:F:17:DC:H2'	2:F:18:DT:H72	1.61	0.82
4:B:153:ALA:O	4:B:157:GLU:HG3	1.81	0.81
3:A:2086:ARG:CG	3:A:2086:ARG:NH1	2.39	0.80
4:B:88:VAL:HG11	4:B:218:LEU:HD13	1.61	0.80
4:B:211:ARG:NH1	4:B:233:VAL:HG11	1.97	0.79
3:A:41:ARG:CG	3:A:42:SER:H	1.95	0.79
4:B:151:LEU:O	4:B:155:MET:HG2	1.82	0.79
4:B:284:GLU:HB3	4:B:327:VAL:HG12	1.65	0.78
3:A:224:ILE:HD13	3:A:225:GLU:N	1.99	0.78
3:A:50:ARG:HB2	3:A:50:ARG:HH21	1.49	0.78
4:B:88:VAL:HG21	4:B:218:LEU:CD1	2.14	0.78
4:B:109:HIS:HD2	4:B:142:VAL:HG12	1.49	0.78
3:A:2028:ASN:CB	3:A:2033:ARG:HB3	2.13	0.77
3:A:2040:HIS:O	3:A:2043:ARG:HG3	1.85	0.77
2:F:26:DC:H6	2:F:26:DC:H5'	1.47	0.77
4:B:88:VAL:HG21	4:B:218:LEU:HD13	1.67	0.76
3:A:1128:LEU:O	3:A:1128:LEU:HD12	1.86	0.75
1:E:33:DC:H2'	1:E:34:DT:H72	1.68	0.75
4:B:182:GLY:O	4:B:183:ASP:HB2	1.87	0.75
1:E:27:DA:H2''	1:E:28:DT:H5'	1.69	0.75
4:B:322:THR:HG23	4:B:323:LYS:H	1.52	0.75
1:E:35:DG:H2''	1:E:36:DT:OP2	1.87	0.74
3:A:274:ARG:HD2	3:A:277:ASP:OD1	1.86	0.74
4:B:104:ILE:HD13	4:B:233:VAL:HG21	1.68	0.74
4:B:41:TYR:CE1	4:B:85:CYS:HB2	2.23	0.73
3:A:1082:GLU:C	3:A:1084:GLU:H	1.92	0.73
3:A:1102:THR:HG22	3:A:1104:ARG:H	1.53	0.73
3:A:89:GLU:HB2	3:A:98:GLY:HA2	1.70	0.73
1:E:34:DT:H2''	1:E:35:DG:C1'	2.18	0.73
3:A:2029:LYS:N	3:A:2029:LYS:HD3	2.01	0.72
2:F:30:DC:H2''	2:F:31:DT:C5'	2.15	0.72
2:F:30:DC:H2'	2:F:31:DT:H72	1.73	0.71
4:B:254:ASP:HB3	4:B:255:ARG:HD2	1.73	0.70
4:B:254:ASP:HB2	4:B:267:TYR:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:DC:H2'	2:F:27:DT:H71	1.73	0.70
3:A:253:ARG:HD2	3:A:253:ARG:N	2.06	0.70
4:B:109:HIS:CD2	4:B:142:VAL:HG12	2.26	0.70
3:A:2090:LEU:HD12	3:A:2108:GLU:O	1.93	0.69
3:A:81:PRO:HB2	3:A:82:PRO:HD3	1.75	0.69
3:A:104:LEU:HD22	3:A:111:HIS:CE1	2.28	0.69
2:F:30:DC:H2'	2:F:31:DT:C7	2.23	0.68
4:B:220:ASP:N	4:B:224:SER:O	2.26	0.68
2:F:31:DT:H2''	2:F:32:DT:C5'	2.24	0.68
3:A:2032:THR:O	3:A:2108:GLU:HA	1.94	0.68
2:F:18:DT:OP1	3:A:1069:ARG:NH2	2.27	0.68
3:A:30:ARG:HH11	3:A:30:ARG:HG3	1.59	0.67
4:B:84:ILE:HB	4:B:130:MET:HG3	1.77	0.67
3:A:2073:LEU:HD22	3:A:2073:LEU:N	2.09	0.67
3:A:246:ARG:HH11	3:A:246:ARG:HG3	1.60	0.67
2:F:17:DC:H2'	2:F:18:DT:C7	2.24	0.67
2:F:3:DA:H3'	3:A:42:SER:CB	2.25	0.67
2:F:26:DC:C6	2:F:26:DC:H5'	2.29	0.67
4:B:47:GLN:HG3	4:B:48:PRO:CD	2.17	0.66
3:A:2083:ALA:O	3:A:2087:LYS:HD2	1.94	0.66
3:A:76:LEU:HD13	3:A:90:LEU:HD22	1.77	0.66
4:B:107:HIS:CD2	4:B:210:VAL:HG23	2.31	0.66
3:A:70:GLY:HA3	3:A:104:LEU:HD12	1.76	0.66
3:A:175:LEU:HD23	3:A:175:LEU:H	1.60	0.66
1:E:34:DT:C2'	1:E:35:DG:H1'	2.25	0.66
2:F:31:DT:H2''	2:F:32:DT:H5'	1.78	0.66
3:A:76:LEU:HD13	3:A:90:LEU:CD2	2.26	0.66
4:B:160:ILE:HD11	4:B:186:LEU:HB2	1.78	0.66
2:F:33:DT:H2''	2:F:34:DC:H5'	1.77	0.66
2:F:22:DA:C2'	2:F:23:DC:H5''	2.25	0.66
4:B:275:LYS:HG3	4:B:300:PRO:HB2	1.78	0.65
4:B:126:GLY:HA2	4:B:130:MET:SD	2.37	0.65
2:F:3:DA:C2'	2:F:4:DG:H5'	2.23	0.65
3:A:1102:THR:CG2	3:A:1104:ARG:H	2.10	0.65
3:A:24:ILE:HD11	3:A:62:LYS:HB3	1.78	0.65
4:B:146:LYS:HE3	4:B:146:LYS:CA	2.26	0.65
3:A:24:ILE:HD11	3:A:62:LYS:CB	2.26	0.65
3:A:185:ASP:O	3:A:191:THR:HG23	1.97	0.65
3:A:1070:TRP:CZ3	3:A:1087:GLU:HG3	2.32	0.65
2:F:3:DA:H3'	3:A:42:SER:HB3	1.79	0.64
4:B:220:ASP:HB2	4:B:224:SER:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:279:GLN:HE22	4:B:332:ARG:HH21	1.45	0.64
3:A:20:TYR:HA	3:A:175:LEU:HD12	1.79	0.64
3:A:2053:ILE:O	3:A:2053:ILE:HD13	1.98	0.64
3:A:72:VAL:HG22	3:A:163:VAL:HG22	1.78	0.64
2:F:17:DC:H2''	2:F:18:DT:H5'	1.79	0.64
2:F:18:DT:P	3:A:1069:ARG:NH2	2.70	0.64
4:B:176:LEU:HD22	4:B:184:ARG:HG2	1.80	0.64
4:B:168:LEU:HD12	4:B:168:LEU:N	2.12	0.63
3:A:2086:ARG:HG3	3:A:2086:ARG:NH1	2.06	0.63
4:B:305:ARG:HG3	4:B:305:ARG:HH11	1.64	0.63
1:E:21:DT:OP2	4:B:63:SER:HB3	1.99	0.63
3:A:86:HIS:CD2	3:A:157:VAL:HG12	2.34	0.63
3:A:1022:ILE:HA	3:A:1030:LEU:HD13	1.80	0.63
4:B:74:LYS:HD3	4:B:74:LYS:N	2.14	0.62
4:B:88:VAL:CB	4:B:218:LEU:HD22	2.26	0.62
2:F:17:DC:H2''	2:F:18:DT:C5'	2.30	0.62
4:B:86:ASN:O	4:B:87:TYR:O	2.19	0.61
4:B:179:GLU:HG3	4:B:180:GLY:H	1.66	0.61
3:A:2032:THR:HG1	3:A:2109:PHE:HD1	1.48	0.61
3:A:2096:ARG:HH11	3:A:2096:ARG:HG2	1.64	0.61
3:A:145:ILE:HA	3:A:148:GLN:HE21	1.65	0.61
3:A:127:GLU:O	3:A:130:ILE:HG22	2.00	0.61
2:F:33:DT:H2''	2:F:34:DC:C5'	2.31	0.61
4:B:167:LEU:HB2	4:B:168:LEU:HD12	1.82	0.61
3:A:2068:ARG:HG2	3:A:2068:ARG:HH11	1.66	0.60
3:A:186:ASN:ND2	3:A:193:GLU:H	1.99	0.60
3:A:165:VAL:HG23	3:A:166:ARG:N	2.16	0.60
3:A:81:PRO:O	3:A:83:HIS:N	2.33	0.60
1:E:2:DT:H6	1:E:2:DT:H5''	1.66	0.60
3:A:2009:LEU:HB2	3:A:2010:PRO:HD3	1.84	0.60
3:A:190:ASN:HD22	3:A:190:ASN:C	2.03	0.60
3:A:2011:TRP:O	3:A:2015:GLN:HG2	2.02	0.60
2:F:7:DG:H1'	2:F:8:DA:H5''	1.82	0.60
3:A:46:ILE:HG13	3:A:116:LEU:O	2.02	0.59
4:B:217:PHE:CE2	4:B:228:ARG:HB2	2.37	0.59
4:B:143:THR:CG2	4:B:145:LYS:HG2	2.31	0.59
4:B:165:PRO:HD3	4:B:177:GLN:OE1	2.01	0.59
1:E:22:DG:H1'	1:E:23:DG:H5''	1.85	0.59
3:A:2026:TRP:CZ3	3:A:2031:ARG:HA	2.38	0.59
3:A:252:PHE:C	3:A:253:ARG:HD2	2.23	0.59
3:A:163:VAL:O	3:A:175:LEU:HD23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2073:LEU:CD2	3:A:2073:LEU:H	2.10	0.59
2:F:26:DC:H2'	2:F:27:DT:C7	2.33	0.59
2:F:7:DG:O6	3:A:33:ARG:NH2	2.35	0.59
1:E:32:DT:H2''	1:E:33:DC:C6	2.37	0.59
3:A:1044:TRP:CE2	3:A:1120:LYS:HE3	2.38	0.59
3:A:214:LEU:C	3:A:214:LEU:HD23	2.22	0.59
3:A:1089:ALA:O	3:A:1093:THR:HG23	2.02	0.59
4:B:211:ARG:HD2	4:B:233:VAL:CG1	2.33	0.59
3:A:273:ARG:O	3:A:275:PRO:HD3	2.04	0.58
3:A:80:ASP:HB3	3:A:81:PRO:HD2	1.85	0.58
2:F:18:DT:P	3:A:1069:ARG:HH21	2.27	0.58
2:F:27:DT:H1'	2:F:28:DC:C5'	2.33	0.58
3:A:206:CYS:HB3	3:A:262:LEU:HD22	1.85	0.58
4:B:126:GLY:N	4:B:127:PRO:HD2	2.18	0.58
3:A:2086:ARG:NH1	3:A:2086:ARG:HG2	2.13	0.58
4:B:168:LEU:CD1	4:B:168:LEU:H	2.13	0.58
4:B:157:GLU:O	4:B:161:ARG:HG3	2.03	0.57
3:A:72:VAL:CG2	3:A:104:LEU:HD21	2.34	0.57
4:B:259:CYS:SG	4:B:261:THR:HB	2.44	0.57
4:B:40:PRO:HA	4:B:86:ASN:HB2	1.87	0.57
3:A:166:ARG:HH11	3:A:166:ARG:HG3	1.70	0.57
2:F:10:DT:H2''	2:F:11:DT:H5'	1.87	0.57
4:B:165:PRO:HG2	4:B:167:LEU:CD1	2.34	0.57
3:A:85:PRO:CB	3:A:133:ARG:HG2	2.35	0.57
3:A:84:ARG:HD3	3:A:147:GLU:O	2.05	0.57
3:A:2032:THR:O	3:A:2108:GLU:HG2	2.05	0.56
3:A:2084:LEU:HD22	3:A:2090:LEU:CD2	2.36	0.56
4:B:329:VAL:HG22	4:B:345:PHE:HB2	1.87	0.56
3:A:2026:TRP:HZ3	3:A:2032:THR:H	1.53	0.56
1:E:22:DG:C2'	1:E:23:DG:H5''	2.35	0.56
4:B:165:PRO:HB3	4:B:177:GLN:NE2	2.20	0.56
2:F:27:DT:H1'	2:F:28:DC:H5''	1.87	0.56
1:E:27:DA:H2''	1:E:28:DT:C5'	2.36	0.56
3:A:2047:GLN:HG2	3:A:2048:GLN:N	2.21	0.56
4:B:87:TYR:CD2	4:B:87:TYR:C	2.79	0.56
2:F:3:DA:H3'	3:A:42:SER:OG	2.06	0.55
1:E:21:DT:H2''	1:E:22:DG:C5'	2.30	0.55
3:A:82:PRO:O	3:A:84:ARG:HG3	2.06	0.55
3:A:239:PHE:HB2	3:A:243:ASP:HB2	1.89	0.55
4:B:88:VAL:HG21	4:B:218:LEU:HD11	1.88	0.55
4:B:56:ARG:O	4:B:140:LEU:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:176:LEU:HD13	4:B:184:ARG:HG2	1.88	0.55
1:E:2:DT:H4'	1:E:3:DG:OP1	2.07	0.55
4:B:249:LYS:HE2	4:B:271:ASP:OD1	2.07	0.55
3:A:1054:GLU:HG3	3:A:1055:ALA:N	2.21	0.55
4:B:172:ASP:O	4:B:174:ALA:N	2.40	0.54
3:A:188:ALA:HB3	3:A:191:THR:HG22	1.89	0.54
4:B:109:HIS:CD2	4:B:142:VAL:H	2.25	0.54
3:A:126:LEU:O	3:A:126:LEU:HD23	2.07	0.54
1:E:29:DT:H2''	1:E:30:DC:C5'	2.37	0.54
3:A:2051:PHE:HA	3:A:2054:PHE:HD2	1.71	0.54
4:B:100:ASN:HA	4:B:211:ARG:HH21	1.73	0.54
3:A:200:ASN:HB2	3:A:213:PHE:HB2	1.90	0.54
3:A:2031:ARG:N	3:A:2031:ARG:HD2	2.22	0.54
4:B:250:ILE:HG21	4:B:253:MET:HE3	1.90	0.54
1:E:33:DC:H2'	1:E:34:DT:C7	2.38	0.53
3:A:50:ARG:NH2	3:A:50:ARG:HB2	2.20	0.53
4:B:176:LEU:HD22	4:B:184:ARG:NE	2.23	0.53
3:A:262:LEU:HB2	3:A:290:PRO:HA	1.91	0.53
4:B:250:ILE:HG21	4:B:253:MET:CE	2.38	0.53
4:B:279:GLN:HE21	4:B:332:ARG:HE	1.54	0.53
3:A:1054:GLU:HG3	3:A:1055:ALA:H	1.73	0.53
3:A:1032:TRP:CE2	3:A:1037:ARG:HG2	2.44	0.53
4:B:323:LYS:HB3	4:B:324:PRO:HD2	1.90	0.53
3:A:1111:ASN:C	3:A:1113:GLY:H	2.11	0.53
3:A:50:ARG:CB	3:A:50:ARG:HH21	2.19	0.53
1:E:15:DT:H2''	1:E:16:DG:C8	2.44	0.53
2:F:18:DT:H2''	2:F:19:DT:H5'	1.90	0.53
3:A:131:SER:O	3:A:134:ILE:HG12	2.09	0.53
3:A:233:TRP:CZ2	3:A:235:ALA:HB2	2.44	0.53
1:E:6:DA:H2''	1:E:7:DG:H5'	1.90	0.53
3:A:1082:GLU:C	3:A:1084:GLU:N	2.62	0.52
4:B:288:ASN:N	4:B:288:ASN:HD22	2.06	0.52
3:A:2014:SER:O	3:A:2018:LEU:HG	2.08	0.52
4:B:261:THR:O	4:B:315:LYS:HE2	2.09	0.52
3:A:1011:ARG:NH2	3:A:1013:LEU:HD23	2.24	0.52
3:A:2084:LEU:HD22	3:A:2090:LEU:HD21	1.90	0.52
3:A:85:PRO:HB2	3:A:133:ARG:HG2	1.91	0.52
4:B:97:LEU:HG	4:B:111:LEU:HG	1.91	0.52
2:F:30:DC:C2'	2:F:31:DT:H5''	2.22	0.52
4:B:165:PRO:HA	4:B:177:GLN:HE22	1.73	0.52
3:A:190:ASN:O	3:A:191:THR:HB	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:140:PRO:HG3	3:A:162:GLN:NE2	2.25	0.52
3:A:39:GLU:OE2	3:A:187:ARG:NH2	2.41	0.52
3:A:85:PRO:HG3	3:A:139:ASN:HA	1.92	0.52
4:B:114:LYS:HD2	4:B:115:HIS:CD2	2.45	0.52
4:B:77:LYS:CD	4:B:77:LYS:H	2.10	0.52
3:A:206:CYS:CB	3:A:262:LEU:HD13	2.39	0.51
3:A:200:ASN:HB2	3:A:213:PHE:H	1.76	0.51
4:B:74:LYS:CG	4:B:75:ASN:H	2.12	0.51
1:E:7:DG:OP1	3:A:2077:LYS:NZ	2.37	0.51
4:B:219:PRO:HG3	4:B:225:PHE:CE1	2.45	0.51
3:A:1032:TRP:CD2	3:A:1037:ARG:HG2	2.45	0.51
1:E:17:DA:C8	1:E:17:DA:H5'	2.46	0.51
3:A:1063:TRP:CH2	3:A:1067:ARG:HD3	2.45	0.51
2:F:32:DT:H2''	2:F:33:DT:O5'	2.11	0.51
3:A:2103:PRO:O	3:A:2104:HIS:HB3	2.10	0.51
3:A:1041:ARG:HH22	3:A:1119:HIS:CE1	2.28	0.51
3:A:2043:ARG:NH1	3:A:2103:PRO:HG2	2.26	0.51
1:E:14:DG:H2''	1:E:15:DT:H5'	1.92	0.51
4:B:87:TYR:CE1	4:B:89:GLY:N	2.71	0.50
3:A:132:GLN:OE1	3:A:133:ARG:NH2	2.44	0.50
4:B:170:HIS:ND1	4:B:172:ASP:OD1	2.42	0.50
3:A:190:ASN:ND2	3:A:190:ASN:C	2.65	0.50
3:A:1054:GLU:CG	3:A:1055:ALA:N	2.75	0.50
4:B:279:GLN:NE2	4:B:332:ARG:HH21	2.10	0.50
4:B:280:ILE:HD13	4:B:311:PHE:CE2	2.47	0.50
4:B:73:GLU:CB	4:B:74:LYS:HD3	2.42	0.50
3:A:1018:LEU:HD22	3:A:1022:ILE:HD11	1.94	0.50
4:B:170:HIS:ND1	4:B:171:PRO:HD2	2.26	0.50
3:A:155:ASN:HB3	3:A:191:THR:HG21	1.93	0.50
1:E:7:DG:H2''	1:E:8:DG:H5'	1.94	0.50
4:B:159:CYS:SG	4:B:194:ILE:HD11	2.52	0.50
4:B:329:VAL:HG23	4:B:343:LYS:O	2.12	0.50
1:E:4:DA:H1'	1:E:5:DA:H5''	1.93	0.50
3:A:1012:VAL:O	3:A:1012:VAL:HG23	2.12	0.50
4:B:79:TYR:HB3	4:B:80:PRO:HD2	1.94	0.50
4:B:73:GLU:HB3	4:B:74:LYS:HD3	1.94	0.50
2:F:27:DT:H2''	2:F:28:DC:H5'	1.94	0.50
3:A:144:PRO:O	3:A:146:GLU:N	2.45	0.50
4:B:87:TYR:CG	4:B:88:VAL:N	2.80	0.49
4:B:126:GLY:O	4:B:127:PRO:C	2.49	0.49
4:B:305:ARG:NH1	4:B:305:ARG:HG3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:73:ARG:HA	3:A:100:TYR:O	2.12	0.49
4:B:211:ARG:HH11	4:B:233:VAL:CG1	2.21	0.49
3:A:225:GLU:HG3	3:A:273:ARG:HB3	1.94	0.49
4:B:323:LYS:HB3	4:B:324:PRO:CD	2.42	0.49
4:B:304:HIS:NE2	4:B:305:ARG:HD3	2.28	0.49
3:A:72:VAL:HG23	3:A:104:LEU:HD21	1.93	0.49
3:A:1109:ARG:HG2	3:A:2068:ARG:NH2	2.28	0.49
4:B:228:ARG:HG3	4:B:228:ARG:HH11	1.77	0.49
1:E:33:DC:H2''	1:E:34:DT:C6	2.47	0.49
4:B:161:ARG:HH11	4:B:161:ARG:HG2	1.78	0.49
4:B:288:ASN:N	4:B:288:ASN:ND2	2.60	0.49
3:A:1027:TYR:CD2	3:A:1058:ARG:HG2	2.48	0.49
2:F:4:DG:H1'	2:F:5:DA:N7	2.28	0.49
3:A:2016:LEU:HB3	3:A:2026:TRP:CZ2	2.48	0.49
2:F:27:DT:H2''	2:F:28:DC:OP2	2.13	0.49
1:E:4:DA:H2''	1:E:5:DA:H5''	1.95	0.49
4:B:37:MET:N	4:B:37:MET:SD	2.86	0.49
2:F:12:DT:H2''	2:F:13:DC:H5'	1.94	0.48
1:E:22:DG:H2''	1:E:23:DG:H5''	1.94	0.48
3:A:2012:LEU:O	3:A:2016:LEU:HG	2.13	0.48
1:E:29:DT:H1'	1:E:30:DC:H5''	1.95	0.48
3:A:85:PRO:HB3	3:A:133:ARG:HG2	1.95	0.48
2:F:23:DC:C6	2:F:24:DT:H72	2.48	0.48
3:A:2026:TRP:CH2	3:A:2031:ARG:HA	2.49	0.48
4:B:176:LEU:HD22	4:B:184:ARG:CD	2.44	0.48
3:A:257:TYR:CD2	3:A:258:ALA:N	2.80	0.48
4:B:167:LEU:N	4:B:167:LEU:CD1	2.77	0.48
3:A:24:ILE:HD11	3:A:62:LYS:HB2	1.96	0.48
3:A:171:ARG:H	3:A:171:ARG:CD	2.26	0.48
2:F:30:DC:OP1	2:F:30:DC:H4'	2.14	0.48
4:B:88:VAL:CG1	4:B:218:LEU:HD13	2.37	0.48
3:A:226:VAL:HG11	3:A:252:PHE:CZ	2.49	0.48
4:B:114:LYS:HD2	4:B:115:HIS:NE2	2.29	0.48
4:B:165:PRO:HG2	4:B:167:LEU:HD13	1.96	0.48
3:A:224:ILE:HD13	3:A:225:GLU:H	1.73	0.48
3:A:2053:ILE:HD12	3:A:2080:PHE:CE2	2.48	0.48
4:B:173:LEU:HD13	4:B:175:TYR:H	1.79	0.48
1:E:27:DA:H1'	1:E:28:DT:H5''	1.96	0.48
3:A:86:HIS:ND1	3:A:87:PRO:HD2	2.28	0.48
1:E:4:DA:C2'	1:E:5:DA:H5''	2.44	0.48
4:B:146:LYS:CE	4:B:146:LYS:HA	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:271:ASP:O	4:B:273:VAL:HG13	2.14	0.47
3:A:246:ARG:NH1	3:A:246:ARG:HG3	2.29	0.47
4:B:176:LEU:HD22	4:B:184:ARG:CG	2.44	0.47
3:A:142:GLN:HG3	3:A:142:GLN:O	2.14	0.47
4:B:214:PHE:HB2	4:B:232:VAL:HG22	1.96	0.47
2:F:11:DT:OP1	4:B:144:LYS:HG3	2.14	0.47
4:B:90:PRO:O	4:B:219:PRO:HD3	2.15	0.47
3:A:2031:ARG:O	3:A:2032:THR:HB	2.15	0.47
3:A:2033:ARG:HA	3:A:2108:GLU:HG2	1.96	0.47
3:A:251:VAL:HB	4:B:252:ARG:NH1	2.29	0.47
1:E:22:DG:H2''	1:E:23:DG:C5'	2.45	0.47
4:B:211:ARG:HG3	4:B:236:ALA:HA	1.95	0.47
4:B:275:LYS:HG3	4:B:300:PRO:CB	2.44	0.47
3:A:164:THR:HG23	3:A:174:ARG:HG2	1.96	0.47
4:B:238:TYR:HB3	4:B:245:ALA:HB1	1.97	0.47
4:B:94:ILE:HA	4:B:121:CYS:O	2.14	0.47
4:B:109:HIS:HE1	4:B:207:LEU:O	1.97	0.47
4:B:186:LEU:HG	4:B:191:LYS:HG2	1.97	0.47
2:F:26:DC:C2'	2:F:27:DT:H71	2.43	0.47
3:A:197:CYS:O	3:A:198:ARG:HG3	2.15	0.47
3:A:2096:ARG:HG2	3:A:2096:ARG:NH1	2.28	0.47
4:B:329:VAL:CG2	4:B:345:PHE:HB2	2.45	0.47
2:F:18:DT:H1'	2:F:19:DT:H5''	1.97	0.47
4:B:255:ARG:HG2	4:B:266:ILE:HD12	1.96	0.47
3:A:35:ARG:HG3	3:A:43:ALA:HB1	1.97	0.47
1:E:22:DG:C1'	1:E:23:DG:H5''	2.45	0.46
4:B:187:GLY:CA	4:B:190:GLU:HG2	2.45	0.46
2:F:31:DT:H2''	2:F:32:DT:H5''	1.96	0.46
2:F:10:DT:H1'	2:F:11:DT:H5''	1.97	0.46
3:A:158:ARG:CZ	3:A:182:PRO:HD3	2.45	0.46
3:A:158:ARG:NH1	3:A:182:PRO:HD3	2.31	0.46
2:F:32:DT:C6	2:F:33:DT:H72	2.50	0.46
1:E:20:DG:H2''	1:E:21:DT:H5'	1.97	0.46
4:B:228:ARG:HG3	4:B:228:ARG:NH1	2.30	0.46
3:A:1113:GLY:O	3:A:1114:ASP:C	2.54	0.46
3:A:171:ARG:H	3:A:171:ARG:HD3	1.80	0.46
2:F:34:DC:H6	2:F:34:DC:H5'	1.80	0.46
3:A:2034:PHE:CE1	3:A:2107:TYR:HB2	2.50	0.46
2:F:10:DT:H2''	2:F:11:DT:C5'	2.46	0.46
2:F:23:DC:H2'	2:F:24:DT:C7	2.45	0.46
2:F:12:DT:H2'	4:B:59:CYS:SG	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2029:LYS:H	3:A:2029:LYS:CD	2.04	0.46
4:B:104:ILE:CD1	4:B:233:VAL:HG21	2.43	0.46
1:E:17:DA:H1'	1:E:18:DA:H5'	1.98	0.46
3:A:2068:ARG:O	3:A:2069:ASP:CG	2.54	0.46
3:A:66:TYR:CE2	3:A:165:VAL:HB	2.50	0.46
2:F:7:DG:H2''	2:F:8:DA:H5'	1.97	0.46
3:A:202:ASN:O	3:A:286:PHE:HA	2.16	0.46
3:A:1085:THR:HG22	3:A:1085:THR:O	2.16	0.46
2:F:7:DG:H2''	2:F:8:DA:C5'	2.46	0.46
3:A:1114:ASP:HA	3:A:1115:PRO:HD2	1.65	0.46
3:A:1049:ARG:HH11	3:A:1051:ASP:CG	2.18	0.46
3:A:2009:LEU:O	3:A:2013:VAL:HG23	2.16	0.45
3:A:216:CYS:O	4:B:304:HIS:HE1	1.98	0.45
3:A:171:ARG:HD3	3:A:171:ARG:N	2.30	0.45
4:B:88:VAL:CG2	4:B:218:LEU:HD13	2.41	0.45
4:B:83:LYS:HE2	4:B:85:CYS:SG	2.56	0.45
4:B:170:HIS:CG	4:B:171:PRO:HD2	2.51	0.45
4:B:126:GLY:N	4:B:127:PRO:CD	2.80	0.45
3:A:246:ARG:HG2	4:B:307:PHE:CE1	2.50	0.45
1:E:17:DA:H2''	1:E:18:DA:O5'	2.15	0.45
3:A:2068:ARG:HG2	3:A:2068:ARG:NH1	2.30	0.45
3:A:166:ARG:HG3	3:A:166:ARG:NH1	2.31	0.45
3:A:271:GLN:NE2	3:A:281:SER:O	2.50	0.45
2:F:4:DG:H1'	2:F:5:DA:C8	2.52	0.45
4:B:211:ARG:HD2	4:B:233:VAL:HG12	1.97	0.45
3:A:84:ARG:CD	3:A:148:GLN:HA	2.47	0.45
3:A:1018:LEU:O	3:A:1022:ILE:HG13	2.17	0.45
3:A:1036:ALA:O	3:A:1037:ARG:HB2	2.17	0.45
1:E:5:DA:H2''	1:E:6:DA:H8	1.82	0.45
3:A:190:ASN:ND2	3:A:190:ASN:O	2.50	0.45
4:B:182:GLY:O	4:B:183:ASP:CB	2.61	0.44
3:A:1102:THR:HG23	3:A:1104:ARG:CB	2.47	0.44
4:B:346:LEU:HD13	4:B:346:LEU:C	2.36	0.44
4:B:98:VAL:HG11	4:B:213:MET:CE	2.47	0.44
4:B:87:TYR:C	4:B:88:VAL:HG23	2.38	0.44
1:E:29:DT:H2''	1:E:30:DC:H5'	1.98	0.44
1:E:29:DT:C2'	1:E:30:DC:H5''	2.48	0.44
3:A:196:ILE:CG1	3:A:272:LEU:HD22	2.47	0.44
1:E:20:DG:H2''	1:E:21:DT:C5'	2.48	0.44
3:A:219:VAL:O	3:A:247:GLN:HG2	2.17	0.44
4:B:74:LYS:HG2	4:B:75:ASN:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:82:PRO:O	3:A:84:ARG:N	2.49	0.44
3:A:185:ASP:O	3:A:191:THR:CG2	2.66	0.44
4:B:74:LYS:N	4:B:74:LYS:CD	2.79	0.44
2:F:23:DC:H2'	2:F:24:DT:H72	2.00	0.44
3:A:175:LEU:HD23	3:A:175:LEU:N	2.31	0.44
4:B:156:THR:HA	4:B:194:ILE:HD13	2.00	0.44
4:B:228:ARG:HD3	4:B:228:ARG:O	2.17	0.44
4:B:260:VAL:HG21	4:B:319:ILE:O	2.18	0.44
3:A:188:ALA:HB3	3:A:191:THR:CG2	2.48	0.44
2:F:27:DT:H1'	2:F:28:DC:H5'	1.98	0.44
3:A:84:ARG:HD2	3:A:148:GLN:HA	1.99	0.44
3:A:246:ARG:HG2	4:B:307:PHE:CD1	2.53	0.44
3:A:71:THR:CG2	3:A:72:VAL:N	2.80	0.43
3:A:226:VAL:HG11	3:A:252:PHE:CE1	2.53	0.43
1:E:5:DA:H2''	1:E:6:DA:C8	2.53	0.43
4:B:288:ASN:O	4:B:289:GLY:C	2.57	0.43
3:A:141:PHE:CD1	3:A:141:PHE:N	2.86	0.43
4:B:114:LYS:NZ	4:B:115:HIS:NE2	2.60	0.43
4:B:283:TYR:HA	4:B:292:TRP:O	2.19	0.43
4:B:87:TYR:O	4:B:88:VAL:CG2	2.67	0.43
3:A:1011:ARG:NH2	3:A:1013:LEU:CD2	2.81	0.43
4:B:126:GLY:H	4:B:127:PRO:HD2	1.83	0.43
4:B:98:VAL:HA	4:B:105:HIS:O	2.18	0.43
4:B:268:LEU:C	4:B:268:LEU:HD23	2.38	0.43
4:B:156:THR:O	4:B:160:ILE:HG12	2.18	0.43
3:A:139:ASN:C	3:A:139:ASN:HD22	2.22	0.43
4:B:230:GLU:HA	4:B:231:PRO:HD3	1.91	0.43
4:B:266:ILE:HG22	4:B:267:TYR:N	2.32	0.43
4:B:47:GLN:HB2	4:B:47:GLN:HE21	1.58	0.42
3:A:2028:ASN:ND2	3:A:2030:SER:OG	2.52	0.42
3:A:66:TYR:CZ	3:A:165:VAL:HB	2.54	0.42
3:A:142:GLN:CG	3:A:142:GLN:O	2.67	0.42
4:B:143:THR:HG21	4:B:145:LYS:HG2	2.00	0.42
3:A:198:ARG:HB3	4:B:267:TYR:OH	2.19	0.42
3:A:171:ARG:HA	3:A:172:PRO:HD3	1.86	0.42
3:A:2031:ARG:HG2	3:A:2031:ARG:HH11	1.85	0.42
4:B:188:ASP:HA	4:B:191:LYS:HE3	2.01	0.42
4:B:261:THR:O	4:B:315:LYS:HG2	2.19	0.42
3:A:196:ILE:HG12	3:A:272:LEU:HD22	2.01	0.42
1:E:9:DG:H2''	1:E:10:DA:H5'	2.00	0.42
4:B:143:THR:HG22	4:B:146:LYS:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:218:LEU:O	4:B:227:ARG:HB2	2.18	0.42
4:B:107:HIS:CG	4:B:210:VAL:HG23	2.55	0.42
4:B:73:GLU:HB3	4:B:74:LYS:CD	2.49	0.42
2:F:26:DC:H2"	2:F:27:DT:C6	2.54	0.42
3:A:2009:LEU:N	3:A:2010:PRO:CD	2.83	0.42
3:A:2087:LYS:O	3:A:2088:GLU:C	2.58	0.42
3:A:65:GLY:O	3:A:66:TYR:HB2	2.19	0.42
3:A:100:TYR:CD1	3:A:100:TYR:C	2.93	0.42
4:B:260:VAL:HB	4:B:316:TYR:HB3	2.01	0.42
3:A:96:ARG:HD2	3:A:97:ASP:OD2	2.20	0.42
4:B:88:VAL:HG11	4:B:218:LEU:HB3	2.01	0.42
3:A:200:ASN:CB	3:A:213:PHE:H	2.32	0.42
3:A:167:ASP:O	3:A:168:PRO:C	2.58	0.42
1:E:23:DG:H2"	1:E:24:DG:C8	2.55	0.41
3:A:1012:VAL:HG23	3:A:1067:ARG:HH11	1.84	0.41
2:F:17:DC:H2"	2:F:18:DT:H5"	2.03	0.41
3:A:1038:THR:OG1	3:A:1128:LEU:HD21	2.20	0.41
3:A:163:VAL:HB	3:A:175:LEU:HD21	2.02	0.41
4:B:277:ASP:OD2	4:B:334:LYS:HB2	2.19	0.41
4:B:82:VAL:HG22	4:B:134:PHE:HE2	1.85	0.41
4:B:187:GLY:O	4:B:191:LYS:HG3	2.21	0.41
3:A:86:HIS:CG	3:A:87:PRO:HD2	2.56	0.41
3:A:2011:TRP:CE3	3:A:2057:TRP:HE3	2.37	0.41
4:B:250:ILE:HG12	4:B:331:LEU:HD13	2.03	0.41
3:A:2095:ASP:C	3:A:2097:SER:H	2.23	0.41
4:B:47:GLN:OE1	4:B:235:ASP:N	2.53	0.41
4:B:42:LEU:CD2	4:B:82:VAL:HB	2.36	0.41
4:B:165:PRO:C	4:B:167:LEU:HD13	2.41	0.41
3:A:1102:THR:HG23	3:A:1104:ARG:HB2	2.02	0.41
3:A:86:HIS:ND1	3:A:87:PRO:CD	2.84	0.41
3:A:144:PRO:HG2	3:A:147:GLU:OE1	2.20	0.41
4:B:304:HIS:CE1	4:B:305:ARG:HD3	2.55	0.41
3:A:2047:GLN:HG2	3:A:2049:GLU:H	1.85	0.41
4:B:319:ILE:HB	4:B:320:ASN:H	1.67	0.41
4:B:49:LYS:HD3	4:B:51:ARG:O	2.20	0.41
3:A:2073:LEU:N	3:A:2074:PRO:HD2	2.35	0.41
3:A:84:ARG:HG2	3:A:143:VAL:HG11	2.03	0.41
3:A:2011:TRP:CE3	3:A:2057:TRP:CE3	3.08	0.41
2:F:23:DC:H2"	2:F:24:DT:H6	1.85	0.41
1:E:29:DT:H2"	1:E:30:DC:H5"	2.03	0.41
3:A:1027:TYR:O	3:A:1028:GLU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:DA:H1'	1:E:13:DA:H5''	2.03	0.41
3:A:2093:ALA:N	3:A:2106:ILE:O	2.53	0.41
4:B:255:ARG:HD3	4:B:266:ILE:HD13	2.02	0.41
4:B:98:VAL:HG11	4:B:213:MET:HE1	2.02	0.41
4:B:218:LEU:HB2	4:B:227:ARG:HB2	2.02	0.41
3:A:186:ASN:HD21	3:A:193:GLU:H	1.68	0.41
4:B:143:THR:CG2	4:B:144:LYS:N	2.83	0.40
3:A:46:ILE:HA	3:A:47:PRO:HD3	1.97	0.40
3:A:228:PHE:HB2	3:A:235:ALA:HB3	2.02	0.40
3:A:2086:ARG:HG2	3:A:2086:ARG:H	1.54	0.40
1:E:4:DA:H2''	1:E:5:DA:C5'	2.51	0.40
3:A:263:GLN:HA	3:A:263:GLN:NE2	2.36	0.40
4:B:125:ALA:CB	4:B:132:VAL:HG22	2.52	0.40
2:F:12:DT:H2''	2:F:13:DC:C5'	2.51	0.40
4:B:72:SER:N	4:B:78:SER:OG	2.55	0.40
1:E:11:DG:C6	3:A:2086:ARG:NH2	2.69	0.40
4:B:332:ARG:CG	4:B:339:THR:HG22	2.38	0.40
1:E:6:DA:H4'	3:A:2042:LEU:HG	2.03	0.40
3:A:190:ASN:CB	3:A:220:GLN:HE22	2.33	0.40
3:A:2024:VAL:HG12	3:A:2037:PRO:HD3	2.04	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	490/540 (91%)	399 (81%)	60 (12%)	31 (6%)	2 4
4	B	312/314 (99%)	264 (85%)	37 (12%)	11 (4%)	4 15
All	All	802/854 (94%)	663 (83%)	97 (12%)	42 (5%)	2 7

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	81	PRO
3	A	169	SER
3	A	191	THR
3	A	1074	SER
3	A	1128	LEU
3	A	2032	THR
3	A	2085	ASN
3	A	2088	GLU
3	A	2110	VAL
4	B	74	LYS
4	B	87	TYR
4	B	114	LYS
4	B	165	PRO
4	B	173	LEU
4	B	183	ASP
4	B	319	ILE
3	A	41	ARG
3	A	83	HIS
3	A	145	ILE
3	A	165	VAL
3	A	1127	SER
3	A	2025	ALA
3	A	2038	TRP
4	B	63	SER
4	B	88	VAL
4	B	175	TYR
3	A	168	PRO
3	A	246	ARG
3	A	1072	PRO
3	A	2031	ARG
4	B	322	THR
3	A	44	GLY
3	A	49	GLU
3	A	221	LYS
3	A	231	PRO
3	A	1126	GLY
3	A	1131	ASP
3	A	2020	GLN
3	A	171	ARG
3	A	2019	GLY
3	A	1114	ASP
3	A	2041	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	423/463 (91%)	384 (91%)	39 (9%)	11	32
4	B	269/269 (100%)	244 (91%)	25 (9%)	11	32
All	All	692/732 (94%)	628 (91%)	64 (9%)	11	32

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	28	LYS
3	A	30	ARG
3	A	76	LEU
3	A	81	PRO
3	A	90	LEU
3	A	107	ASP
3	A	124	ARG
3	A	133	ARG
3	A	135	GLN
3	A	138	ASN
3	A	139	ASN
3	A	175	LEU
3	A	190	ASN
3	A	200	ASN
3	A	222	GLU
3	A	224	ILE
3	A	246	ARG
3	A	269	SER
3	A	272	LEU
3	A	284	MET
3	A	1013	LEU
3	A	1018	LEU
3	A	1030	LEU
3	A	1054	GLU
3	A	1058	ARG
3	A	1102	THR
3	A	1104	ARG

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Mol	Chain	Res	Type
3	A	1114	ASP
3	A	1131	ASP
3	A	2012	LEU
3	A	2028	ASN
3	A	2029	LYS
3	A	2031	ARG
3	A	2035	ARG
3	A	2053	ILE
3	A	2073	LEU
3	A	2086	ARG
3	A	2094	GLU
3	A	2109	PHE
4	B	37	MET
4	B	42	LEU
4	B	47	GLN
4	B	74	LYS
4	B	77	LYS
4	B	87	TYR
4	B	98	VAL
4	B	117	GLU
4	B	130	MET
4	B	143	THR
4	B	146	LYS
4	B	167	LEU
4	B	168	LEU
4	B	176	LEU
4	B	192	GLU
4	B	210	VAL
4	B	228	ARG
4	B	247	ASN
4	B	255	ARG
4	B	275	LYS
4	B	285	GLU
4	B	305	ARG
4	B	322	THR
4	B	329	VAL
4	B	331	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	29	GLN

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Mol	Chain	Res	Type
3	A	111	HIS
3	A	114	GLN
3	A	128	GLN
3	A	138	ASN
3	A	139	ASN
3	A	148	GLN
3	A	162	GLN
3	A	186	ASN
3	A	190	ASN
3	A	200	ASN
3	A	220	GLN
3	A	263	GLN
3	A	271	GLN
3	A	287	GLN
3	A	1111	ASN
3	A	2028	ASN
3	A	2044	GLN
3	A	2047	GLN
4	B	109	HIS
4	B	185	GLN
4	B	247	ASN
4	B	279	GLN
4	B	288	ASN
4	B	304	HIS
4	B	320	ASN
4	B	330	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 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	E	36/36 (100%)	0.14	3 (8%) 14 7	30, 51, 124, 142	0
2	F	34/34 (100%)	0.01	1 (2%) 55 43	27, 48, 71, 123	0
3	A	498/540 (92%)	0.22	33 (6%) 22 13	27, 60, 122, 139	0
4	B	314/314 (100%)	0.18	16 (5%) 32 21	28, 63, 116, 140	0
All	All	882/924 (95%)	0.20	53 (6%) 25 15	27, 60, 121, 142	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	1132	SER	8.5
4	B	181	GLY	6.8
3	A	2016	LEU	6.4
4	B	176	LEU	6.1
4	B	180	GLY	5.3
3	A	1079	PRO	5.0
3	A	2110	VAL	4.6
3	A	1081	PRO	4.3
3	A	2092	LEU	4.3
4	B	177	GLN	3.9
3	A	2033	ARG	3.9
3	A	2034	PHE	3.8
3	A	1080	PRO	3.7
4	B	182	GLY	3.7
4	B	175	TYR	3.7
3	A	2012	LEU	3.6
3	A	2111	ASN	3.2
4	B	162	GLY	3.2
3	A	2085	ASN	3.0
3	A	2045	ASP	3.0
3	A	2051	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
3	A	2088	GLU	2.9
3	A	2025	ALA	2.7
4	B	126	GLY	2.7
3	A	42	SER	2.7
4	B	74	LYS	2.6
3	A	2043	ARG	2.5
1	E	1	DT	2.5
3	A	1075	ARG	2.5
3	A	2042	LEU	2.5
3	A	2031	ARG	2.4
2	F	2	DC	2.4
3	A	2046	ALA	2.4
3	A	2091	ARG	2.4
3	A	147	GLU	2.4
3	A	2030	SER	2.4
3	A	2011	TRP	2.4
4	B	321	ILE	2.3
3	A	81	PRO	2.3
3	A	291	ASP	2.3
1	E	35	DG	2.3
4	B	87	TYR	2.3
4	B	222	THR	2.3
3	A	2086	ARG	2.2
3	A	2023	GLY	2.2
3	A	2044	GLN	2.2
4	B	164	ASN	2.2
3	A	266	VAL	2.1
1	E	36	DT	2.1
3	A	1131	ASP	2.1
4	B	37	MET	2.1
4	B	163	TYR	2.0
4	B	168	LEU	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 ⓘ

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.