



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:18 PM UTC

PDB ID : 2F8X / pdb_00002f8x
Title : Crystal structure of activated Notch, CSL and MAML on HES-1 promoter DNA sequence
Authors : Nam, Y.; Sliz, P.; Blacklow, S.C.
Deposited on : 2005-12-04
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

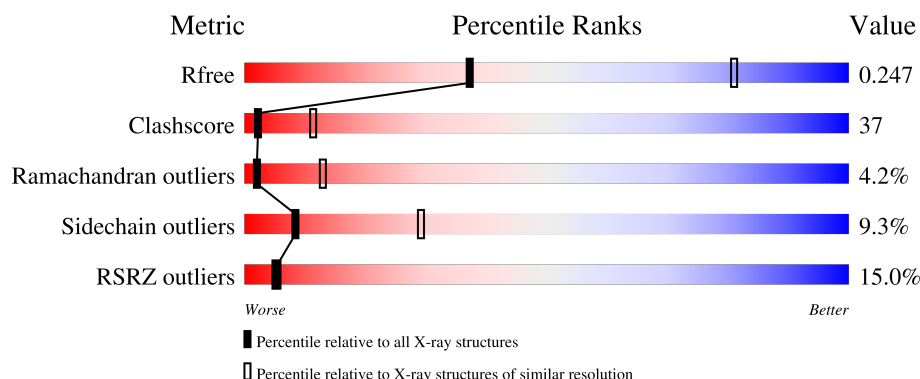
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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 $\leq 5\%$. 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	X	18	33% 6% 67% 22% 6%
2	Y	18	28% 83% 17%
3	C	434	17% 38% 47% 13% .
4	K	256	7% 46% 34% 5% 15%
5	M	63	11% 48% 30% 10% 13%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6236 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(*GP*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	18	Total	C	N	O	P	0	0	0
			375	179	76	103	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	18	Total	C	N	O	P	0	0	0
			357	174	57	109	17			

- Molecule 3 is a protein called Recombining binding protein suppressor of hairless, isoform 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	424	Total	C	N	O	S	0	0	0
			3369	2133	580	631	25			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	MET	-	initiating methionine	UNP Q06330
C	436	HIS	-	expression tag	UNP Q06330
C	437	HIS	-	expression tag	UNP Q06330
C	438	HIS	-	expression tag	UNP Q06330
C	439	HIS	-	expression tag	UNP Q06330
C	440	HIS	-	expression tag	UNP Q06330
C	441	HIS	-	expression tag	UNP Q06330

- Molecule 4 is a protein called Neurogenic locus notch homolog protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	218	Total	C	N	O	S	0	0	0
			1658	1014	312	324	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1872	GLY	-	cloning artifact	UNP P46531

- Molecule 5 is a protein called Mastermind-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	M	55	Total	C	N	O	S	0	0	0
			467	282	103	78	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	12	GLY	-	cloning artifact	UNP Q92585

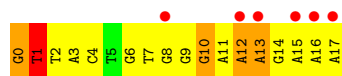
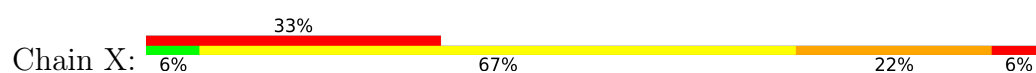
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	4	Total	O	0	0
			4	4		
6	K	4	Total	O	0	0
			4	4		
6	M	2	Total	O	0	0
			2	2		

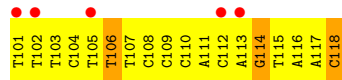
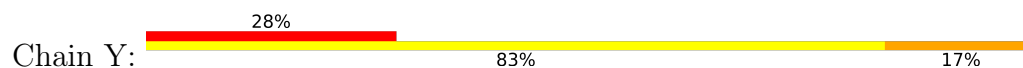
3 Residue-property plots

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.

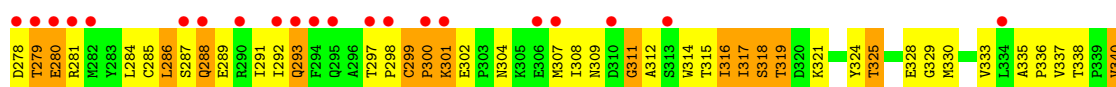
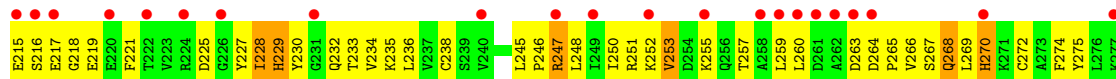
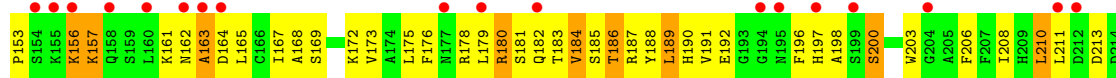
- Molecule 1: 5'-D(*GP*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*AP*AP*A)-3'

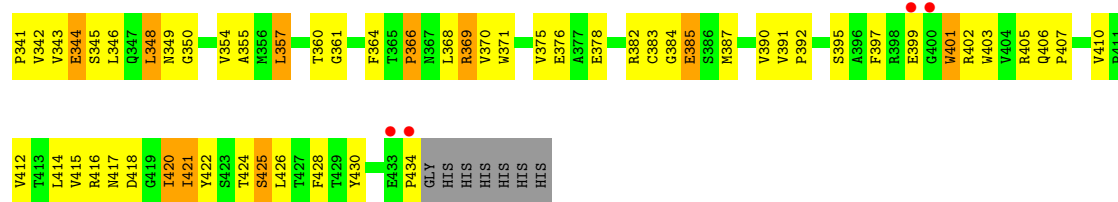


- Molecule 2: 5'-D(*TP*TP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*TP*AP*AP*C)-3'

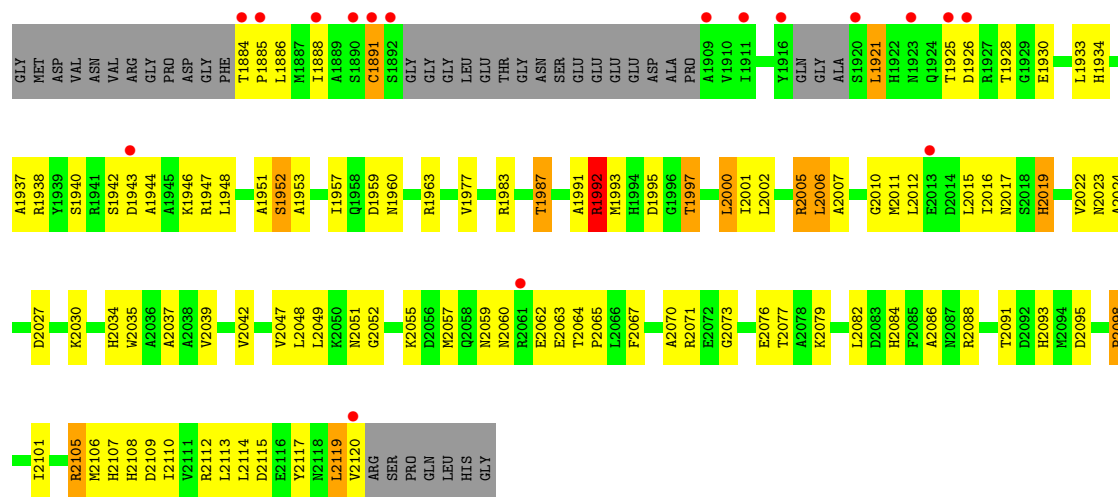


- Molecule 3: Recombining binding protein suppressor of hairless, isoform 4

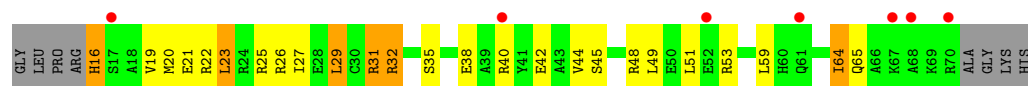




• Molecule 4: Neurogenic locus notch homolog protein 1



• Molecule 5: Mastermind-like protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	273.87Å 273.87Å 121.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.82 – 3.25 44.82 – 3.25	Depositor EDS
% Data completeness (in resolution range)	91.1 (44.82-3.25) 97.6 (44.82-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.25Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.257 0.220 , 0.247	Depositor DCC
R_{free} test set	3688 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	83.1	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 72.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6236	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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, 0.333 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	X	0.46	0/423	0.98	2/653 (0.3%)
2	Y	0.51	0/397	1.09	3/609 (0.5%)
3	C	0.60	0/3444	1.13	28/4655 (0.6%)
4	K	0.74	0/1678	1.18	15/2275 (0.7%)
5	M	0.76	0/474	0.99	0/631
All	All	0.64	0/6416	1.12	48/8823 (0.5%)

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	X	0	4
2	Y	0	1
All	All	0	5

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	LYS	N-CA-C	-10.37	102.80	114.62
3	C	80	GLU	N-CA-C	-9.84	100.41	111.82
3	C	200	SER	N-CA-C	-9.43	101.09	112.59
4	K	2005	ARG	N-CA-C	8.95	121.12	111.36
3	C	112	LYS	N-CA-C	8.03	122.17	112.38
3	C	391	VAL	CA-C-N	7.96	127.72	119.76
3	C	391	VAL	C-N-CA	7.96	127.72	119.76
2	Y	118	DC	C4'-C3'-O3'	-7.89	98.17	110.00
3	C	137	ASP	N-CA-C	-7.62	99.75	110.50
4	K	2019	HIS	N-CA-C	7.06	121.40	111.52
3	C	228	ILE	N-CA-C	6.63	117.41	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2024	ALA	N-CA-C	-6.43	102.05	110.53
3	C	369	ARG	N-CA-C	-6.18	99.73	109.50
1	X	1	DT	N1-C1'-C2'	6.16	122.73	113.50
3	C	38	HIS	N-CA-C	6.02	117.28	108.14
3	C	402	ARG	N-CA-C	-6.01	105.90	113.72
3	C	180	ARG	N-CA-C	5.87	119.75	112.47
4	K	2115	ASP	N-CA-C	5.87	118.63	111.82
3	C	390	VAL	N-CA-C	5.85	116.23	107.51
3	C	382	ARG	N-CA-C	-5.77	103.83	111.96
3	C	12	PRO	CA-C-N	5.71	123.83	119.66
3	C	12	PRO	C-N-CA	5.71	123.83	119.66
3	C	113	THR	N-CA-C	5.68	118.15	110.88
4	K	2098	PRO	N-CA-C	-5.66	106.01	113.65
4	K	1942	SER	N-CA-C	5.64	117.43	111.28
3	C	319	THR	N-CA-C	5.57	118.31	109.50
2	Y	106	DT	N1-C1'-C2'	5.45	121.68	113.50
4	K	2108	HIS	N-CA-C	5.44	117.21	111.28
3	C	420	ILE	CB-CA-C	-5.35	102.69	111.51
4	K	1891	CYS	N-CA-C	5.35	118.02	111.82
4	K	2117	TYR	N-CA-C	5.34	117.44	108.73
4	K	2064	THR	CA-C-N	-5.30	113.57	119.19
4	K	2064	THR	C-N-CA	-5.30	113.57	119.19
2	Y	118	DC	C2'-C3'-O3'	-5.30	103.55	111.50
3	C	350	GLY	N-CA-C	-5.29	104.26	112.45
3	C	279	THR	N-CA-C	-5.28	105.52	111.28
3	C	32	GLN	N-CA-C	-5.24	101.16	109.59
4	K	2010	GLY	N-CA-C	5.22	125.56	113.18
1	X	10	DG	N9-C1'-C2'	5.17	121.25	113.50
4	K	2052	GLY	N-CA-C	5.15	125.39	113.18
4	K	1992	ARG	N-CA-C	5.15	117.80	108.69
3	C	369	ARG	CA-C-N	-5.13	115.57	122.91
3	C	369	ARG	C-N-CA	-5.13	115.57	122.91
3	C	344	GLU	N-CA-C	5.12	116.94	111.36
4	K	2119	LEU	N-CA-C	5.12	116.58	109.31
3	C	145	LYS	N-CA-C	-5.08	103.34	110.50
3	C	420	ILE	CA-C-N	-5.03	116.55	123.14
3	C	420	ILE	C-N-CA	-5.03	116.55	123.14

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	0	DG	Sidechain
1	X	1	DT	Sidechain
1	X	12	DA	Sidechain
1	X	13	DA	Sidechain
2	Y	114	DG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	375	0	204	18	0
2	Y	357	0	207	29	0
3	C	3369	0	3348	294	0
4	K	1658	0	1606	90	0
5	M	467	0	472	26	0
6	C	4	0	0	0	0
6	K	4	0	0	0	0
6	M	2	0	0	0	0
All	All	6236	0	5837	443	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 37.

All (443) 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:C:299:CYS:H	3:C:300:PRO:HD2	1.19	1.05
2:Y:112:DC:H2''	2:Y:113:DA:H5'	1.39	1.04
3:C:157:LYS:H	3:C:157:LYS:HD2	1.34	0.92
4:K:1963:ARG:HH11	4:K:1993:MET:HE1	1.35	0.92
3:C:41:VAL:HG21	3:C:268:GLN:HG2	1.52	0.91
3:C:401:TRP:HD1	3:C:401:TRP:H	1.17	0.91
3:C:173:VAL:HG12	3:C:318:SER:HA	1.52	0.91
3:C:187:ARG:HB3	3:C:198:ALA:O	1.72	0.89
3:C:34:VAL:HG12	3:C:35:LEU:H	1.37	0.89
3:C:33:THR:HB	3:C:325:THR:HB	1.53	0.89
2:Y:117:DA:H2''	2:Y:118:DC:H5''	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:2106:MET:HE1	5:M:48:ARG:HB2	1.56	0.88
3:C:401:TRP:H	3:C:401:TRP:CD1	1.85	0.86
3:C:229:HIS:HA	3:C:265:PRO:HA	1.58	0.85
3:C:143:LEU:HD12	3:C:143:LEU:H	1.40	0.85
4:K:1963:ARG:HD2	4:K:1993:MET:HE2	1.60	0.84
3:C:297:THR:HB	3:C:298:PRO:HD3	1.60	0.83
2:Y:108:DC:H2''	2:Y:109:DC:H5'	1.58	0.83
3:C:189:LEU:HD21	3:C:196:PHE:HD2	1.44	0.82
4:K:1963:ARG:HD2	4:K:1993:MET:CE	2.10	0.82
5:M:32:ARG:HG2	5:M:32:ARG:HH11	1.44	0.82
1:X:13:DA:H2''	1:X:14:DG:H5''	1.59	0.81
3:C:211:LEU:HD13	3:C:215:GLU:HG2	1.63	0.79
4:K:2005:ARG:HD2	4:K:2035:TRP:CE3	2.16	0.79
3:C:61:LEU:HD13	3:C:66:TRP:CZ2	2.18	0.79
3:C:131:MET:O	3:C:139:ILE:HB	1.82	0.79
4:K:2109:ASP:HA	4:K:2112:ARG:NH1	1.96	0.79
3:C:250:ILE:HD12	3:C:266:VAL:HG21	1.63	0.78
3:C:74:GLU:C	3:C:76:ASP:H	1.90	0.77
2:Y:113:DA:H4'	2:Y:114:DG:OP1	1.85	0.77
2:Y:103:DT:H2''	2:Y:104:DC:H5''	1.66	0.77
3:C:268:GLN:OE1	3:C:318:SER:HB2	1.85	0.77
3:C:424:THR:O	3:C:425:SER:HB2	1.86	0.76
3:C:421:ILE:C	3:C:421:ILE:HD12	2.11	0.76
3:C:157:LYS:H	3:C:157:LYS:CD	1.99	0.76
3:C:89:ILE:HD13	3:C:114:LEU:HD11	1.68	0.76
3:C:18:THR:HG23	3:C:330:MET:HE1	1.68	0.75
4:K:2109:ASP:HA	4:K:2112:ARG:HH12	1.50	0.75
3:C:34:VAL:HG12	3:C:35:LEU:N	2.01	0.75
5:M:20:MET:HE3	5:M:23:LEU:HD12	1.68	0.75
4:K:1997:THR:HG21	4:K:2002:LEU:HD21	1.68	0.74
2:Y:113:DA:H1'	2:Y:114:DG:C8	2.22	0.74
4:K:2016:ILE:HG21	4:K:2051:ASN:ND2	2.01	0.74
2:Y:101:DT:H2'	2:Y:102:DT:C7	2.17	0.74
3:C:135:ASN:HD22	3:C:135:ASN:H	1.35	0.74
3:C:299:CYS:N	3:C:300:PRO:HD2	1.98	0.74
3:C:180:ARG:O	3:C:181:SER:HB3	1.88	0.74
3:C:89:ILE:HG21	3:C:114:LEU:HD11	1.70	0.73
1:X:3:DA:H1'	1:X:4:DC:H5''	1.71	0.72
3:C:135:ASN:HD22	3:C:135:ASN:N	1.85	0.72
3:C:308:ILE:HD12	3:C:309:ASN:H	1.55	0.72
1:X:6:DG:H2''	1:X:7:DT:C5'	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:ALA:C	3:C:165:LEU:H	1.97	0.71
4:K:2005:ARG:HD2	4:K:2035:TRP:CZ3	2.25	0.71
3:C:299:CYS:H	3:C:300:PRO:CD	1.99	0.71
3:C:301:LYS:O	3:C:302:GLU:HG3	1.91	0.70
4:K:2105:ARG:HG2	4:K:2105:ARG:HH11	1.55	0.70
3:C:143:LEU:HD12	3:C:143:LEU:N	2.06	0.70
3:C:269:LEU:HD23	3:C:317:ILE:HG12	1.72	0.70
3:C:51:ARG:HG3	3:C:51:ARG:HH11	1.57	0.69
4:K:2055:LYS:HD2	4:K:2086:ALA:HA	1.73	0.69
3:C:49:GLU:OE2	3:C:51:ARG:NH1	2.26	0.69
3:C:228:ILE:CG2	3:C:250:ILE:HD11	2.23	0.69
3:C:401:TRP:CD1	3:C:401:TRP:N	2.57	0.68
3:C:169:SER:HB2	3:C:210:LEU:HB2	1.74	0.68
3:C:279:THR:O	3:C:280:GLU:HG2	1.94	0.68
4:K:2071:ARG:HG2	4:K:2071:ARG:HH11	1.58	0.68
1:X:6:DG:H2''	1:X:7:DT:H5'	1.75	0.68
1:X:13:DA:C2'	1:X:14:DG:H5''	2.23	0.68
3:C:344:GLU:HG3	3:C:361:GLY:HA2	1.76	0.67
3:C:175:LEU:HD21	3:C:316:ILE:HG12	1.75	0.67
4:K:2016:ILE:HG21	4:K:2051:ASN:HD22	1.56	0.67
3:C:341:PRO:HB2	3:C:414:LEU:HD12	1.76	0.66
1:X:7:DT:H2''	1:X:8:DG:C8	2.30	0.66
3:C:257:THR:HG22	3:C:307:MET:HG2	1.78	0.66
4:K:1963:ARG:NH1	4:K:1993:MET:HE1	2.10	0.66
3:C:229:HIS:CA	3:C:265:PRO:HA	2.27	0.65
4:K:1959:ASP:OD2	4:K:1963:ARG:HG3	1.96	0.65
3:C:416:ARG:HG2	3:C:417:ASN:H	1.62	0.65
3:C:124:HIS:CE1	3:C:146:ARG:NH2	2.64	0.65
3:C:176:PHE:HB3	3:C:188:TYR:CD2	2.32	0.65
4:K:2098:PRO:O	4:K:2101:ILE:HG22	1.97	0.65
2:Y:112:DC:C2'	2:Y:113:DA:H5'	2.22	0.65
3:C:354:VAL:HG12	3:C:354:VAL:O	1.97	0.64
2:Y:115:DT:H1'	2:Y:116:DA:H5'	1.80	0.64
3:C:236:LEU:HD11	3:C:274:PHE:HE2	1.62	0.64
3:C:148:LYS:HB2	3:C:148:LYS:HZ2	1.63	0.64
3:C:35:LEU:HD21	3:C:37:LEU:HD21	1.80	0.64
2:Y:101:DT:H2'	2:Y:102:DT:H72	1.80	0.64
5:M:51:LEU:O	5:M:51:LEU:HD12	1.97	0.63
3:C:285:CYS:HB2	3:C:312:ALA:HB2	1.79	0.63
3:C:190:HIS:CG	3:C:191:VAL:H	2.16	0.63
4:K:2112:ARG:HH11	4:K:2112:ARG:HB2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:HIS:CD2	3:C:147:ILE:HD11	2.34	0.62
3:C:280:GLU:HB3	3:C:281:ARG:HD2	1.80	0.62
3:C:89:ILE:HG13	3:C:129:VAL:HG22	1.80	0.62
3:C:38:HIS:CE1	3:C:144:SER:HB2	2.34	0.62
3:C:269:LEU:CD2	3:C:317:ILE:HG12	2.30	0.62
3:C:18:THR:HG23	3:C:330:MET:CE	2.30	0.62
4:K:2106:MET:HE1	5:M:48:ARG:CB	2.30	0.62
4:K:1884:THR:N	4:K:1885:PRO:HD2	2.15	0.62
3:C:371:TRP:CD1	3:C:415:VAL:HG21	2.35	0.61
3:C:208:ILE:HG23	3:C:208:ILE:O	1.98	0.61
3:C:340:VAL:HG13	3:C:422:TYR:CD2	2.35	0.61
3:C:236:LEU:HD11	3:C:274:PHE:CE2	2.36	0.61
4:K:1983:ARG:HG3	4:K:1983:ARG:HH11	1.64	0.61
3:C:34:VAL:O	3:C:35:LEU:HB2	2.00	0.61
3:C:298:PRO:HB2	3:C:307:MET:HB2	1.82	0.61
2:Y:103:DT:C2'	2:Y:104:DC:H5''	2.31	0.60
3:C:406:GLN:CG	3:C:407:PRO:HD2	2.30	0.60
4:K:2034:HIS:CD2	4:K:2065:PRO:HG3	2.36	0.60
3:C:217:GLU:HG3	3:C:218:GLY:H	1.66	0.60
3:C:74:GLU:O	3:C:76:ASP:N	2.35	0.60
3:C:345:SER:HB3	3:C:360:THR:OG1	2.02	0.60
2:Y:117:DA:C2'	2:Y:118:DC:H5''	2.29	0.60
2:Y:107:DT:H1'	2:Y:108:DC:H5''	1.83	0.60
3:C:33:THR:HB	3:C:325:THR:CB	2.30	0.60
3:C:434:PRO:HG2	4:K:1891:CYS:SG	2.42	0.60
3:C:179:LEU:HD21	3:C:288:GLN:HE21	1.68	0.59
3:C:37:LEU:HD22	3:C:321:LYS:HB2	1.85	0.59
4:K:2039:VAL:HG12	4:K:2039:VAL:O	2.01	0.59
4:K:2105:ARG:HH11	4:K:2105:ARG:CG	2.15	0.59
3:C:206:PHE:CD2	3:C:238:CYS:HA	2.37	0.59
3:C:74:GLU:C	3:C:76:ASP:N	2.59	0.58
1:X:0:DG:H1'	1:X:1:DT:H5'	1.85	0.58
3:C:368:LEU:C	3:C:369:ARG:HD3	2.29	0.58
3:C:151:SER:O	3:C:152:LYS:HB2	2.03	0.58
3:C:196:PHE:HB3	3:C:291:ILE:HD12	1.84	0.58
4:K:1963:ARG:HB3	4:K:1993:MET:HE3	1.84	0.58
4:K:2011:MET:O	4:K:2015:LEU:HD12	2.04	0.58
2:Y:107:DT:H2''	2:Y:108:DC:C5'	2.34	0.58
3:C:337:VAL:HG12	3:C:420:ILE:HD12	1.86	0.58
2:Y:108:DC:H2''	2:Y:109:DC:C5'	2.31	0.58
4:K:1963:ARG:HB3	4:K:1993:MET:CE	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:364:PHE:HD1	3:C:387:MET:HB2	1.69	0.58
3:C:91:ILE:O	3:C:92:GLY:C	2.47	0.57
3:C:139:ILE:O	3:C:337:VAL:HG22	2.04	0.57
4:K:1997:THR:CG2	4:K:2002:LEU:HD21	2.33	0.57
3:C:55:PRO:HD3	3:C:317:ILE:HG21	1.85	0.57
3:C:38:HIS:HD2	3:C:147:ILE:HD11	1.70	0.57
2:Y:107:DT:H2''	2:Y:108:DC:H5'	1.85	0.57
3:C:54:CYS:SG	3:C:188:TYR:HE2	2.27	0.57
4:K:2106:MET:HB2	5:M:44:VAL:HG11	1.85	0.57
3:C:328:GLU:O	3:C:330:MET:N	2.38	0.57
3:C:346:LEU:HD12	3:C:426:LEU:CD1	2.34	0.57
3:C:348:LEU:HD23	3:C:349:ASN:H	1.69	0.57
3:C:392:PRO:O	3:C:430:TYR:OH	2.19	0.56
3:C:11:ARG:HD2	3:C:11:ARG:O	2.04	0.56
3:C:228:ILE:HG22	3:C:250:ILE:HD11	1.87	0.56
3:C:41:VAL:CG2	3:C:268:GLN:HG2	2.33	0.56
3:C:192:GLU:HB3	3:C:197:HIS:NE2	2.21	0.56
3:C:337:VAL:HG12	3:C:420:ILE:CD1	2.35	0.56
3:C:250:ILE:CD1	3:C:266:VAL:HG21	2.34	0.56
3:C:385:GLU:N	3:C:385:GLU:CD	2.63	0.56
4:K:1928:THR:HB	4:K:1930:GLU:HG3	1.87	0.56
3:C:189:LEU:HD21	3:C:196:PHE:CD2	2.33	0.56
3:C:230:TYR:CD1	3:C:252:LYS:HB2	2.41	0.56
5:M:32:ARG:HD3	5:M:32:ARG:O	2.05	0.56
1:X:16:DA:H2''	1:X:17:DA:O5'	2.06	0.56
3:C:285:CYS:CB	3:C:312:ALA:HB2	2.35	0.56
4:K:2006:LEU:N	4:K:2006:LEU:HD23	2.20	0.55
3:C:161:LYS:HD2	3:C:162:ASN:N	2.22	0.55
3:C:337:VAL:HA	3:C:416:ARG:NH2	2.21	0.55
3:C:89:ILE:CG2	3:C:114:LEU:HD11	2.36	0.55
3:C:253:VAL:HG13	3:C:272:CYS:HA	1.89	0.55
3:C:416:ARG:NH1	3:C:418:ASP:OD2	2.39	0.55
3:C:366:PRO:HB2	5:M:38:GLU:HA	1.89	0.54
3:C:285:CYS:SG	3:C:311:GLY:C	2.90	0.54
5:M:16:HIS:O	5:M:20:MET:HB2	2.07	0.54
3:C:86:CYS:O	3:C:87:ALA:HB2	2.06	0.54
4:K:2120:VAL:HG13	4:K:2120:VAL:O	2.07	0.54
3:C:41:VAL:HG11	3:C:150:ILE:HD13	1.88	0.54
3:C:135:ASN:H	3:C:135:ASN:ND2	2.02	0.54
3:C:210:LEU:HD11	3:C:232:GLN:NE2	2.23	0.54
3:C:341:PRO:HD2	3:C:422:TYR:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:229:HIS:CB	3:C:265:PRO:HA	2.38	0.54
3:C:190:HIS:CG	3:C:191:VAL:N	2.75	0.53
4:K:2071:ARG:HG2	4:K:2071:ARG:NH1	2.23	0.53
3:C:284:LEU:HD22	3:C:314:TRP:HE1	1.72	0.53
3:C:123:LYS:HB2	3:C:124:HIS:CD2	2.43	0.53
1:X:6:DG:H2''	1:X:7:DT:H5''	1.89	0.53
3:C:333:VAL:HG21	3:C:420:ILE:HD11	1.91	0.53
4:K:2082:LEU:HD22	4:K:2088:ARG:NH2	2.23	0.53
3:C:34:VAL:CG1	3:C:35:LEU:H	2.17	0.53
3:C:229:HIS:CD2	3:C:265:PRO:HB3	2.42	0.53
3:C:406:GLN:HG2	3:C:407:PRO:HD2	1.91	0.53
3:C:371:TRP:CE2	3:C:376:GLU:HG3	2.44	0.53
1:X:10:DG:C2	1:X:11:DA:C5	2.97	0.53
4:K:2082:LEU:HD22	4:K:2088:ARG:HH21	1.74	0.53
4:K:2091:THR:HB	4:K:2095:ASP:HA	1.91	0.53
3:C:86:CYS:O	3:C:131:MET:HG3	2.09	0.52
3:C:260:LEU:HD12	3:C:304:ASN:HA	1.91	0.52
3:C:348:LEU:C	3:C:349:ASN:HD22	2.16	0.52
3:C:324:TYR:N	3:C:324:TYR:CD1	2.77	0.52
3:C:41:VAL:HG12	3:C:42:ALA:N	2.23	0.52
3:C:66:TRP:CH2	3:C:131:MET:CE	2.93	0.52
3:C:156:LYS:HB3	3:C:157:LYS:HD2	1.90	0.52
3:C:180:ARG:O	3:C:181:SER:CB	2.58	0.52
3:C:354:VAL:O	3:C:355:ALA:C	2.50	0.52
4:K:2007:ALA:HB1	5:M:29:LEU:HD12	1.92	0.52
5:M:19:VAL:HG13	5:M:20:MET:N	2.23	0.52
4:K:2005:ARG:HB3	4:K:2006:LEU:HD23	1.92	0.52
3:C:88:PHE:CD1	3:C:88:PHE:N	2.78	0.52
3:C:371:TRP:CD1	3:C:415:VAL:CG2	2.93	0.52
3:C:130:LYS:HG3	3:C:131:MET:N	2.25	0.51
3:C:66:TRP:HH2	3:C:131:MET:CE	2.23	0.51
3:C:251:ARG:NH1	3:C:260:LEU:HA	2.24	0.51
3:C:397:PHE:CZ	3:C:410:VAL:HG11	2.46	0.51
5:M:16:HIS:HA	5:M:19:VAL:HG12	1.92	0.51
3:C:125:PHE:CD1	3:C:125:PHE:C	2.87	0.51
3:C:281:ARG:HD2	3:C:281:ARG:N	2.26	0.51
3:C:292:ILE:HG22	3:C:293:GLN:N	2.25	0.51
5:M:49:LEU:HD12	5:M:49:LEU:O	2.10	0.51
1:X:6:DG:H1'	1:X:7:DT:H5''	1.92	0.51
3:C:340:VAL:HG13	3:C:422:TYR:HD2	1.76	0.51
3:C:142:PHE:N	3:C:142:PHE:CD1	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:21:GLU:HG2	5:M:25:ARG:HH12	1.75	0.50
3:C:16:ARG:O	3:C:330:MET:HE2	2.12	0.50
3:C:176:PHE:HB3	3:C:188:TYR:HD2	1.76	0.50
4:K:2016:ILE:HD11	4:K:2048:LEU:HD23	1.93	0.50
4:K:2049:LEU:HD13	4:K:2084:HIS:ND1	2.26	0.50
3:C:178:ARG:NH2	3:C:186:THR:OG1	2.45	0.50
3:C:167:ILE:HD12	3:C:167:ILE:N	2.27	0.50
3:C:179:LEU:HD11	3:C:288:GLN:HG3	1.92	0.50
4:K:1944:ALA:O	4:K:1948:LEU:HG	2.12	0.50
3:C:17:LEU:HD21	3:C:22:MET:HB2	1.93	0.50
2:Y:114:DG:H2''	2:Y:115:DT:H5'	1.94	0.50
4:K:2012:LEU:C	4:K:2012:LEU:HD23	2.37	0.50
4:K:2105:ARG:CG	4:K:2105:ARG:NH1	2.75	0.50
3:C:416:ARG:HG2	3:C:417:ASN:N	2.28	0.49
4:K:2016:ILE:HD12	4:K:2047:VAL:HG12	1.94	0.49
4:K:2073:GLY:O	5:M:40:ARG:NH1	2.45	0.49
2:Y:104:DC:H2'	2:Y:105:DT:H72	1.93	0.49
3:C:58:CYS:SG	3:C:60:TYR:CE1	2.95	0.49
4:K:2000:LEU:HD21	4:K:2012:LEU:HG	1.95	0.49
4:K:2059:ASN:O	4:K:2062:GLU:N	2.41	0.49
3:C:299:CYS:N	3:C:300:PRO:CD	2.68	0.49
3:C:392:PRO:HG2	3:C:430:TYR:OH	2.13	0.49
4:K:1963:ARG:HH11	4:K:1993:MET:CE	2.16	0.49
3:C:428:PHE:HE2	3:C:430:TYR:CE1	2.30	0.49
3:C:129:VAL:HG12	3:C:129:VAL:O	2.13	0.49
4:K:1937:ALA:HA	4:K:1977:VAL:HG11	1.93	0.49
1:X:12:DA:C2	1:X:13:DA:C5	3.01	0.49
3:C:133:TYR:CE2	3:C:139:ILE:HD11	2.47	0.49
3:C:96:GLN:HA	3:C:96:GLN:NE2	2.28	0.49
3:C:230:TYR:CD2	3:C:252:LYS:N	2.81	0.49
3:C:108:TYR:C	3:C:108:TYR:CD2	2.90	0.48
3:C:163:ALA:C	3:C:165:LEU:N	2.64	0.48
3:C:206:PHE:CE2	3:C:238:CYS:HA	2.48	0.48
5:M:32:ARG:HG2	5:M:32:ARG:NH1	2.20	0.48
3:C:34:VAL:HG21	3:C:142:PHE:CZ	2.48	0.48
3:C:343:VAL:HG12	3:C:343:VAL:O	2.14	0.48
3:C:405:ARG:HG3	3:C:405:ARG:HH11	1.78	0.48
3:C:87:ALA:C	3:C:88:PHE:CD1	2.91	0.48
4:K:1886:LEU:HD21	4:K:1921:LEU:HD12	1.96	0.48
3:C:41:VAL:HG13	3:C:150:ILE:HG23	1.95	0.48
3:C:267:SER:HB3	3:C:270:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:ILE:CG2	3:C:114:LEU:HD21	2.43	0.48
3:C:173:VAL:HG21	3:C:316:ILE:HD11	1.96	0.48
4:K:1938:ARG:C	4:K:1940:SER:H	2.20	0.48
2:Y:101:DT:H2'	2:Y:102:DT:H73	1.93	0.47
3:C:167:ILE:HD12	3:C:167:ILE:H	1.79	0.47
4:K:2005:ARG:CD	4:K:2035:TRP:CE3	2.95	0.47
4:K:2022:VAL:HG23	4:K:2023:ASN:OD1	2.14	0.47
4:K:1928:THR:C	4:K:1960:ASN:ND2	2.72	0.47
3:C:50:LYS:HD2	3:C:52:PHE:HE2	1.78	0.47
4:K:1925:THR:HG22	4:K:1926:ASP:N	2.29	0.47
4:K:1947:ARG:HH11	4:K:1947:ARG:HG2	1.79	0.47
3:C:44:LYS:HG2	3:C:151:SER:HA	1.96	0.47
3:C:221:PHE:CZ	3:C:235:LYS:HD3	2.50	0.47
3:C:100:GLN:HG2	3:C:101:LEU:N	2.30	0.47
3:C:297:THR:HB	3:C:298:PRO:CD	2.36	0.47
4:K:2059:ASN:OD1	4:K:2063:GLU:N	2.44	0.47
3:C:179:LEU:HB2	3:C:185:SER:HB2	1.95	0.47
4:K:1948:LEU:O	4:K:1953:ALA:HB2	2.14	0.47
3:C:250:ILE:HG22	3:C:274:PHE:CZ	2.50	0.47
4:K:1884:THR:O	4:K:1888:ILE:HG13	2.14	0.47
1:X:6:DG:C2'	1:X:7:DT:H5''	2.45	0.47
3:C:364:PHE:CD1	3:C:387:MET:HB2	2.48	0.47
3:C:287:SER:O	3:C:289:GLU:N	2.48	0.46
3:C:335:ALA:HB1	3:C:336:PRO:CD	2.46	0.46
3:C:378:GLU:OE2	5:M:31:ARG:NH1	2.47	0.46
4:K:2110:ILE:O	4:K:2114:LEU:HG	2.15	0.46
3:C:157:LYS:HD2	3:C:157:LYS:N	2.16	0.46
3:C:49:GLU:CD	3:C:51:ARG:HH12	2.22	0.46
3:C:52:PHE:CE1	3:C:113:THR:HG22	2.51	0.46
3:C:346:LEU:HD12	3:C:426:LEU:HD13	1.97	0.46
4:K:2039:VAL:O	4:K:2039:VAL:CG1	2.63	0.46
3:C:89:ILE:HD13	3:C:114:LEU:CD1	2.44	0.46
3:C:340:VAL:HA	3:C:341:PRO:HD3	1.75	0.46
3:C:368:LEU:HD23	3:C:416:ARG:HA	1.98	0.46
3:C:152:LYS:HG3	3:C:153:PRO:HD2	1.97	0.46
3:C:17:LEU:HD23	3:C:371:TRP:CZ2	2.51	0.46
3:C:285:CYS:SG	3:C:311:GLY:O	2.74	0.46
3:C:341:PRO:CB	3:C:414:LEU:HD12	2.45	0.46
3:C:17:LEU:HA	3:C:330:MET:HE2	1.96	0.45
3:C:143:LEU:O	3:C:324:TYR:OH	2.31	0.45
4:K:2017:ASN:C	4:K:2019:HIS:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:ARG:HG3	3:C:51:ARG:NH1	2.30	0.45
3:C:406:GLN:HG3	3:C:407:PRO:HD2	1.98	0.45
3:C:34:VAL:CG1	3:C:35:LEU:N	2.73	0.45
3:C:185:SER:O	3:C:187:ARG:HG3	2.16	0.45
3:C:89:ILE:HG23	3:C:114:LEU:HD21	1.98	0.45
3:C:227:TYR:N	3:C:227:TYR:CD1	2.84	0.45
4:K:2037:ALA:HA	4:K:2077:THR:HG21	1.99	0.45
3:C:178:ARG:HD3	3:C:186:THR:OG1	2.15	0.45
3:C:196:PHE:CE2	3:C:245:LEU:HG	2.51	0.45
4:K:2070:ALA:HA	4:K:2110:ILE:HG21	1.99	0.45
3:C:173:VAL:HG12	3:C:318:SER:CA	2.34	0.45
3:C:378:GLU:CD	5:M:31:ARG:NH1	2.75	0.45
3:C:34:VAL:HG21	3:C:142:PHE:CE1	2.51	0.45
3:C:371:TRP:NE1	3:C:376:GLU:HG3	2.32	0.45
3:C:378:GLU:CD	5:M:31:ARG:HH11	2.24	0.45
3:C:229:HIS:HB3	3:C:265:PRO:HA	1.98	0.45
3:C:287:SER:C	3:C:289:GLU:N	2.75	0.45
3:C:79:SER:HB2	3:C:82:GLU:HG3	1.99	0.45
3:C:227:TYR:N	3:C:227:TYR:HD1	2.15	0.45
4:K:1930:GLU:HB3	4:K:1934:HIS:CB	2.47	0.45
3:C:88:PHE:CG	5:M:59:LEU:HD13	2.52	0.44
3:C:104:GLU:C	3:C:106:LYS:H	2.23	0.44
3:C:234:VAL:HG21	3:C:250:ILE:HG23	1.98	0.44
3:C:54:CYS:HA	3:C:55:PRO:C	2.42	0.44
3:C:184:VAL:O	3:C:184:VAL:CG2	2.64	0.44
3:C:346:LEU:HD12	3:C:426:LEU:HD12	2.00	0.44
4:K:2001:ILE:O	4:K:2002:LEU:C	2.59	0.44
4:K:1987:THR:O	4:K:1987:THR:HG22	2.17	0.44
4:K:1995:ASP:C	4:K:1995:ASP:OD2	2.61	0.44
2:Y:102:DT:H2'	2:Y:103:DT:C7	2.48	0.44
3:C:56:PRO:HD2	3:C:203:TRP:CD1	2.53	0.44
3:C:190:HIS:O	3:C:191:VAL:HG23	2.17	0.44
3:C:217:GLU:H	3:C:217:GLU:HG2	1.68	0.44
3:C:308:ILE:HD12	3:C:309:ASN:N	2.28	0.44
3:C:428:PHE:CE2	3:C:430:TYR:CE1	3.05	0.44
4:K:2042:VAL:HG21	4:K:2076:GLU:HB3	1.98	0.44
1:X:3:DA:H1'	1:X:4:DC:C5'	2.43	0.44
3:C:284:LEU:O	3:C:312:ALA:HB1	2.17	0.44
3:C:292:ILE:CG2	3:C:293:GLN:N	2.81	0.44
2:Y:107:DT:C2'	2:Y:108:DC:H5''	2.48	0.44
3:C:157:LYS:CD	3:C:157:LYS:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:385:GLU:CD	3:C:385:GLU:H	2.25	0.44
4:K:1991:ALA:O	4:K:1992:ARG:HG3	2.18	0.44
4:K:2067:PHE:HA	4:K:2098:PRO:HB3	2.00	0.44
3:C:285:CYS:SG	3:C:286:LEU:N	2.91	0.44
3:C:421:ILE:HD12	3:C:422:TYR:N	2.33	0.44
3:C:30:GLY:O	3:C:65:GLY:HA3	2.17	0.43
3:C:217:GLU:CG	3:C:218:GLY:H	2.27	0.43
3:C:168:ALA:O	3:C:169:SER:C	2.59	0.43
3:C:172:LYS:HA	3:C:206:PHE:O	2.18	0.43
3:C:342:VAL:O	3:C:342:VAL:HG23	2.19	0.43
3:C:187:ARG:HA	3:C:200:SER:HA	1.99	0.43
3:C:340:VAL:HG13	3:C:422:TYR:CE2	2.52	0.43
2:Y:102:DT:H2'	2:Y:103:DT:H72	2.00	0.43
3:C:246:PRO:O	3:C:248:LEU:CD1	2.66	0.43
3:C:251:ARG:HH11	3:C:260:LEU:HA	1.82	0.43
4:K:1995:ASP:C	4:K:2027:ASP:OD2	2.62	0.43
3:C:91:ILE:HG22	3:C:122:ARG:HH22	1.84	0.43
3:C:124:HIS:CE1	3:C:146:ARG:HH21	2.36	0.43
3:C:230:TYR:CE1	3:C:252:LYS:HB2	2.54	0.43
3:C:246:PRO:O	3:C:247:ARG:O	2.37	0.43
3:C:364:PHE:N	3:C:364:PHE:CD2	2.87	0.43
4:K:1933:LEU:HA	4:K:1948:LEU:HD12	2.01	0.43
4:K:1951:ALA:O	4:K:1952:SER:C	2.61	0.43
3:C:354:VAL:O	3:C:354:VAL:CG1	2.67	0.43
5:M:32:ARG:HH11	5:M:32:ARG:CG	2.19	0.43
3:C:257:THR:HA	3:C:307:MET:HA	2.01	0.43
3:C:395:SER:C	3:C:397:PHE:H	2.26	0.43
4:K:2000:LEU:O	4:K:2000:LEU:HD22	2.19	0.43
3:C:275:TYR:OH	3:C:278:ASP:HA	2.19	0.43
4:K:2112:ARG:HH11	4:K:2112:ARG:CB	2.30	0.43
3:C:172:LYS:O	3:C:173:VAL:HG13	2.19	0.43
3:C:268:GLN:OE1	3:C:318:SER:N	2.43	0.43
3:C:360:THR:HA	3:C:385:GLU:O	2.18	0.43
1:X:1:DT:H2''	1:X:2:DT:H5'	2.00	0.42
1:X:9:DG:H2''	1:X:10:DG:H8	1.84	0.42
3:C:182:GLN:NE2	3:C:182:GLN:HA	2.34	0.42
4:K:1884:THR:N	4:K:1885:PRO:CD	2.79	0.42
4:K:2082:LEU:HD23	4:K:2082:LEU:HA	1.88	0.42
5:M:49:LEU:O	5:M:53:ARG:HG3	2.19	0.42
3:C:156:LYS:HB3	3:C:157:LYS:H	1.70	0.42
3:C:229:HIS:HA	3:C:266:VAL:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:27:ILE:O	5:M:31:ARG:HB2	2.19	0.42
3:C:187:ARG:HD3	3:C:286:LEU:HD11	2.00	0.42
3:C:39:ALA:HB2	3:C:55:PRO:HD2	2.01	0.42
3:C:228:ILE:HG21	3:C:250:ILE:HD11	1.99	0.42
3:C:248:LEU:CD2	3:C:274:PHE:HB3	2.49	0.42
3:C:251:ARG:HD3	3:C:259:LEU:O	2.20	0.42
3:C:383:CYS:O	3:C:384:GLY:C	2.62	0.42
3:C:418:ASP:OD1	3:C:418:ASP:C	2.61	0.42
3:C:175:LEU:HA	3:C:315:THR:O	2.19	0.42
3:C:281:ARG:HG3	3:C:281:ARG:HH11	1.85	0.42
3:C:346:LEU:HB2	3:C:426:LEU:HD13	2.02	0.42
3:C:378:GLU:OE1	5:M:31:ARG:NH1	2.53	0.42
4:K:2057:MET:O	4:K:2065:PRO:HD3	2.20	0.42
3:C:250:ILE:O	3:C:250:ILE:HG13	2.20	0.42
4:K:1934:HIS:CE1	4:K:1957:ILE:O	2.73	0.42
4:K:2062:GLU:HB2	4:K:2093:HIS:N	2.35	0.42
3:C:116:ILE:HD11	3:C:120:ASP:CB	2.49	0.42
5:M:44:VAL:O	5:M:44:VAL:HG12	2.19	0.42
3:C:179:LEU:HB2	3:C:185:SER:CB	2.49	0.42
3:C:211:LEU:HB2	3:C:233:THR:O	2.20	0.42
3:C:54:CYS:SG	3:C:188:TYR:CE2	3.11	0.41
3:C:175:LEU:CD2	3:C:316:ILE:HG12	2.47	0.41
3:C:348:LEU:HD23	3:C:349:ASN:N	2.33	0.41
3:C:37:LEU:CD2	3:C:321:LYS:HB2	2.48	0.41
3:C:88:PHE:N	3:C:88:PHE:HD1	2.17	0.41
3:C:385:GLU:HG3	4:K:2030:LYS:NZ	2.35	0.41
3:C:187:ARG:HG2	3:C:200:SER:HB3	2.00	0.41
3:C:35:LEU:C	3:C:35:LEU:HD23	2.45	0.41
3:C:246:PRO:O	3:C:247:ARG:C	2.62	0.41
3:C:369:ARG:HD3	3:C:369:ARG:N	2.35	0.41
4:K:1930:GLU:HB3	4:K:1934:HIS:HB2	2.02	0.41
4:K:2000:LEU:HA	4:K:2000:LEU:HD23	1.77	0.41
3:C:255:LYS:HG3	3:C:255:LYS:O	2.20	0.41
3:C:126:MET:HE3	3:C:144:SER:O	2.20	0.41
2:Y:112:DC:H2'	2:Y:113:DA:C8	2.56	0.41
3:C:248:LEU:HD23	3:C:274:PHE:HB3	2.02	0.41
3:C:284:LEU:C	3:C:284:LEU:HD23	2.45	0.41
2:Y:107:DT:C1'	2:Y:108:DC:H5''	2.48	0.41
2:Y:114:DG:C8	2:Y:115:DT:H72	2.55	0.41
3:C:135:ASN:HD21	3:C:137:ASP:HB2	1.85	0.41
3:C:148:LYS:NZ	3:C:164:ASP:OD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:0:DG:H2'	1:X:1:DT:H71	2.03	0.41
2:Y:110:DC:H2''	2:Y:111:DA:C8	2.56	0.41
3:C:55:PRO:HB2	3:C:203:TRP:CE2	2.55	0.41
3:C:293:GLN:H	3:C:293:GLN:HG2	1.72	0.41
4:K:1946:LYS:HE3	4:K:1946:LYS:HB2	1.82	0.41
4:K:1983:ARG:HG3	4:K:1983:ARG:NH1	2.33	0.41
4:K:2059:ASN:O	4:K:2060:ASN:C	2.63	0.41
5:M:64:ILE:HG22	5:M:65:GLN:N	2.36	0.41
3:C:84:GLN:O	3:C:85:PRO:C	2.64	0.41
3:C:346:LEU:HD21	3:C:357:LEU:HD21	2.03	0.41
2:Y:106:DT:H1'	2:Y:107:DT:H5''	2.01	0.40
3:C:206:PHE:HD2	3:C:238:CYS:HA	1.84	0.40
3:C:217:GLU:O	3:C:247:ARG:NH1	2.53	0.40
2:Y:104:DC:P	3:C:157:LYS:HD3	2.62	0.40
3:C:263:ASP:O	3:C:264:ASP:C	2.65	0.40
1:X:15:DA:H2''	1:X:16:DA:OP2	2.21	0.40
2:Y:114:DG:H2''	2:Y:115:DT:C5'	2.51	0.40
3:C:403:TRP:CZ3	3:C:405:ARG:HG2	2.57	0.40
4:K:2088:ARG:NH1	4:K:2119:LEU:HD21	2.37	0.40
3:C:179:LEU:HD21	3:C:288:GLN:NE2	2.33	0.40
3:C:188:TYR:CG	3:C:203:TRP:HB3	2.57	0.40
4:K:2071:ARG:O	4:K:2107:HIS:CE1	2.74	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	C	422/434 (97%)	329 (78%)	66 (16%)	27 (6%)	1	7
4	K	212/256 (83%)	195 (92%)	15 (7%)	2 (1%)	14	42
5	M	53/63 (84%)	53 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	687/753 (91%)	577 (84%)	81 (12%)	29 (4%)	2	13

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	219	GLU
3	C	225	ASP
3	C	247	ARG
3	C	299	CYS
3	C	329	GLY
3	C	425	SER
3	C	49	GLU
3	C	75	ARG
3	C	163	ALA
3	C	280	GLU
3	C	288	GLN
3	C	293	GLN
3	C	401	TRP
3	C	29	ARG
3	C	50	LYS
3	C	183	THR
3	C	213	ASP
3	C	216	SER
4	K	1921	LEU
3	C	35	LEU
3	C	152	LYS
3	C	156	LYS
3	C	186	THR
3	C	399	GLU
4	K	1952	SER
3	C	92	GLY
3	C	366	PRO
3	C	300	PRO
3	C	311	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	C	374/382 (98%)	339 (91%)	35 (9%)	8	29
4	K	170/204 (83%)	161 (95%)	9 (5%)	20	48
5	M	49/54 (91%)	38 (78%)	11 (22%)	1	4
All	All	593/640 (93%)	538 (91%)	55 (9%)	8	29

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	16	ARG
3	C	26	LEU
3	C	33	THR
3	C	43	GLN
3	C	50	LYS
3	C	61	LEU
3	C	88	PHE
3	C	117	SER
3	C	126	MET
3	C	135	ASN
3	C	143	LEU
3	C	148	LYS
3	C	157	LYS
3	C	184	VAL
3	C	189	LEU
3	C	210	LEU
3	C	229	HIS
3	C	253	VAL
3	C	268	GLN
3	C	270	HIS
3	C	286	LEU
3	C	316	ILE
3	C	317	ILE
3	C	318	SER
3	C	319	THR
3	C	325	THR
3	C	338	THR
3	C	340	VAL
3	C	348	LEU
3	C	357	LEU
3	C	370	VAL
3	C	375	VAL

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Mol	Chain	Res	Type
3	C	385	GLU
3	C	412	VAL
3	C	421	ILE
4	K	1943	ASP
4	K	1987	THR
4	K	1992	ARG
4	K	1997	THR
4	K	2000	LEU
4	K	2006	LEU
4	K	2079	LYS
4	K	2105	ARG
4	K	2113	LEU
5	M	16	HIS
5	M	22	ARG
5	M	23	LEU
5	M	26	ARG
5	M	29	LEU
5	M	31	ARG
5	M	32	ARG
5	M	35	SER
5	M	42	GLU
5	M	45	SER
5	M	64	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	24	ASN
3	C	43	GLN
3	C	48	ASN
3	C	93	ASN
3	C	96	GLN
3	C	124	HIS
3	C	135	ASN
3	C	162	ASN
3	C	182	GLN
3	C	190	HIS
3	C	288	GLN
3	C	293	GLN
3	C	304	ASN
3	C	349	ASN
4	K	1923	ASN

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Mol	Chain	Res	Type
4	K	1984	ASN
4	K	1994	HIS
4	K	2093	HIS
4	K	2107	HIS
5	M	54	GLN

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 oligosaccharides 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

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	X	18/18 (100%)	1.32	6 (33%)  	69, 100, 192, 200	0
2	Y	18/18 (100%)	1.18	5 (27%)  	61, 98, 201, 201	0
3	C	424/434 (97%)	0.88	75 (17%)  	19, 81, 196, 201	1 (0%)
4	K	218/256 (85%)	0.11	17 (7%)  	21, 54, 179, 201	0
5	M	55/63 (87%)	0.53	7 (12%)  	24, 68, 182, 201	0
All	All	733/789 (92%)	0.65	110 (15%)  	19, 71, 194, 201	1 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	297	THR	6.8
3	C	306	GLU	6.2
4	K	2120	VAL	5.7
3	C	434	PRO	5.3
3	C	96	GLN	5.2
3	C	281	ARG	5.1
4	K	1920	SER	4.9
3	C	292	ILE	4.6
4	K	1891	CYS	4.6
3	C	154	SER	4.6
3	C	155	LYS	4.6
5	M	67	LYS	4.5
3	C	287	SER	4.5
4	K	1888	ILE	4.4
3	C	92	GLY	4.4
3	C	301	LYS	4.3
3	C	433	GLU	4.3
3	C	278	ASP	4.3
3	C	255	LYS	4.1
4	K	1892	SER	4.0

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Mol	Chain	Res	Type	RSRZ
3	C	290	ARG	4.0
5	M	40	ARG	4.0
1	X	17	DA	3.9
3	C	194	GLY	3.9
3	C	300	PRO	3.8
4	K	1911	ILE	3.6
3	C	259	LEU	3.5
3	C	216	SER	3.5
3	C	258	ALA	3.5
3	C	156	LYS	3.5
3	C	264	ASP	3.4
4	K	1916	TYR	3.4
3	C	293	GLN	3.3
4	K	1885	PRO	3.3
3	C	277	LYS	3.3
3	C	263	ASP	3.2
3	C	307	MET	3.2
1	X	15	DA	3.1
4	K	1890	SER	3.0
3	C	247	ARG	3.0
3	C	197	HIS	3.0
3	C	81	GLN	3.0
1	X	16	DA	2.9
3	C	217	GLU	2.9
4	K	1909	ALA	2.9
3	C	288	GLN	2.9
3	C	222	THR	2.9
3	C	211	LEU	2.9
3	C	204	GLY	2.8
3	C	262	ALA	2.8
3	C	282	MET	2.8
3	C	240	VAL	2.8
3	C	215	GLU	2.8
3	C	220	GLU	2.7
3	C	252	LYS	2.7
3	C	310	ASP	2.7
3	C	279	THR	2.6
3	C	179	LEU	2.6
4	K	1926	ASP	2.6
3	C	195	ASN	2.6
3	C	400	GLY	2.6
3	C	313	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	231	GLY	2.5
3	C	295	GLN	2.5
2	Y	105	DT	2.5
4	K	1943	ASP	2.4
5	M	68	ALA	2.4
5	M	61	GLN	2.4
4	K	1925	THR	2.4
3	C	20	GLU	2.4
3	C	74	GLU	2.4
4	K	1884	THR	2.3
4	K	1923	ASN	2.3
3	C	294	PHE	2.3
1	X	13	DA	2.3
3	C	280	GLU	2.3
5	M	52	GLU	2.3
3	C	77	GLY	2.3
3	C	11	ARG	2.3
3	C	212	ASP	2.3
3	C	93	ASN	2.3
3	C	224	ARG	2.3
1	X	12	DA	2.2
3	C	270	HIS	2.2
3	C	107	ASN	2.2
3	C	249	ILE	2.2
3	C	298	PRO	2.2
3	C	158	GLN	2.2
3	C	260	LEU	2.2
3	C	399	GLU	2.2
3	C	164	ASP	2.2
3	C	261	ASP	2.2
3	C	199	SER	2.2
2	Y	101	DT	2.2
3	C	226	GLY	2.1
3	C	162	ASN	2.1
2	Y	102	DT	2.1
4	K	2061	ARG	2.1
2	Y	112	DC	2.1
3	C	151	SER	2.1
5	M	17	SER	2.1
3	C	334	LEU	2.1
5	M	70	ARG	2.1
3	C	163	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	160	LEU	2.1
1	X	8	DG	2.1
2	Y	113	DA	2.0
3	C	177	ASN	2.0
4	K	2013	GLU	2.0
3	C	182	GLN	2.0

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 oligosaccharides 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.