



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:45 PM UTC

PDB ID : 8U9L / pdb_00008u9l
Title : Crystal Structure of RelA-cRel chimera complex with DNA
Authors : Chang, A.; Wu, Y.; Li, S.X.; Smale, S.; Chen, L.
Deposited on : 2023-09-19
Resolution : 3.09 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:

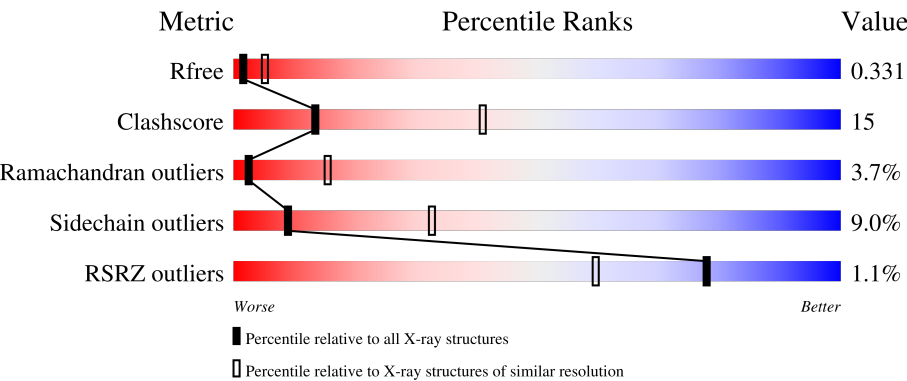
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 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	C	20	15% 40% 60%
1	E	20	25% 30% 70%
1	I	20	5% 15% 85%
1	M	20	5% 100%
2	D	20	25% 35% 65%

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Mol	Chain	Length	Quality of chain
2	F	20	20% 15% 85%
2	J	20	95% 5%
2	N	20	10% 85% 5%
3	A	277	66% 29% 5%
3	B	277	66% 27% 5%
3	G	277	69% 27%
3	H	277	71% 22% 6%
3	K	277	66% 31%
3	L	277	63% 30% 6%
3	O	277	70% 26%
3	P	277	66% 27% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20864 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 (5'-D(P*TP*TP*GP*AP*TP*GP*GP*GP*AP*AP*TP*TP*TP*CP*CP*GP*AP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	20	Total	C	N	O	P	0	0	0
			412	197	70	125	20			
1	C	20	Total	C	N	O	P	0	0	0
			412	197	70	125	20			
1	I	20	Total	C	N	O	P	0	0	0
			412	197	70	125	20			
1	M	20	Total	C	N	O	P	0	0	0
			412	197	70	125	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	20	Total	C	N	O	P	0	0	0
			410	195	78	117	20			
2	D	20	Total	C	N	O	P	0	0	0
			410	195	78	117	20			
2	J	20	Total	C	N	O	P	0	0	0
			410	195	78	117	20			
2	N	20	Total	C	N	O	P	0	0	0
			410	195	78	117	20			

- Molecule 3 is a protein called Transcription factor p65,Proto-oncogene c-Rel chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	276	Total	C	N	O	S	0	0	0
			2203	1388	394	410	11			
3	B	274	Total	C	N	O	S	0	0	0
			2191	1382	391	407	11			
3	G	276	Total	C	N	O	S	0	0	0
			2203	1388	394	410	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	274	Total	C	N	O	S	0	0	0
			2191	1382	391	407	11			
3	K	276	Total	C	N	O	S	0	0	0
			2203	1388	394	410	11			
3	L	274	Total	C	N	O	S	0	0	0
			2191	1382	391	407	11			
3	O	276	Total	C	N	O	S	0	0	0
			2203	1388	394	410	11			
3	P	274	Total	C	N	O	S	0	0	0
			2191	1382	391	407	11			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q04207
A	111	GLU	GLY	conflict	UNP P15307
A	127	PRO	GLY	conflict	UNP P15307
A	144	LEU	CYS	conflict	UNP P15307
A	145	CYS	VAL	conflict	UNP P15307
A	147	GLN	MET	conflict	UNP P15307
A	148	VAL	PHE	conflict	UNP P15307
A	154	HIS	ASP	conflict	UNP P15307
A	171	ASP	-	linker	UNP P15307
A	172	ASN	-	linker	UNP P15307
A	173	ARG	-	linker	UNP P15307
A	174	ALA	-	linker	UNP P15307
A	175	PRO	-	linker	UNP P15307
A	176	ASN	-	linker	UNP P15307
B	1	MET	-	initiating methionine	UNP Q04207
B	111	GLU	GLY	conflict	UNP P15307
B	127	PRO	GLY	conflict	UNP P15307
B	144	LEU	CYS	conflict	UNP P15307
B	145	CYS	VAL	conflict	UNP P15307
B	147	GLN	MET	conflict	UNP P15307
B	148	VAL	PHE	conflict	UNP P15307
B	154	HIS	ASP	conflict	UNP P15307
B	171	ASP	-	linker	UNP P15307
B	172	ASN	-	linker	UNP P15307
B	173	ARG	-	linker	UNP P15307
B	174	ALA	-	linker	UNP P15307
B	175	PRO	-	linker	UNP P15307
B	176	ASN	-	linker	UNP P15307
G	1	MET	-	initiating methionine	UNP Q04207

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Chain	Residue	Modelled	Actual	Comment	Reference
G	111	GLU	GLY	conflict	UNP P15307
G	127	PRO	GLY	conflict	UNP P15307
G	144	LEU	CYS	conflict	UNP P15307
G	145	CYS	VAL	conflict	UNP P15307
G	147	GLN	MET	conflict	UNP P15307
G	148	VAL	PHE	conflict	UNP P15307
G	154	HIS	ASP	conflict	UNP P15307
G	171	ASP	-	linker	UNP P15307
G	172	ASN	-	linker	UNP P15307
G	173	ARG	-	linker	UNP P15307
G	174	ALA	-	linker	UNP P15307
G	175	PRO	-	linker	UNP P15307
G	176	ASN	-	linker	UNP P15307
H	1	MET	-	initiating methionine	UNP Q04207
H	111	GLU	GLY	conflict	UNP P15307
H	127	PRO	GLY	conflict	UNP P15307
H	144	LEU	CYS	conflict	UNP P15307
H	145	CYS	VAL	conflict	UNP P15307
H	147	GLN	MET	conflict	UNP P15307
H	148	VAL	PHE	conflict	UNP P15307
H	154	HIS	ASP	conflict	UNP P15307
H	171	ASP	-	linker	UNP P15307
H	172	ASN	-	linker	UNP P15307
H	173	ARG	-	linker	UNP P15307
H	174	ALA	-	linker	UNP P15307
H	175	PRO	-	linker	UNP P15307
H	176	ASN	-	linker	UNP P15307
K	1	MET	-	initiating methionine	UNP Q04207
K	111	GLU	GLY	conflict	UNP P15307
K	127	PRO	GLY	conflict	UNP P15307
K	144	LEU	CYS	conflict	UNP P15307
K	145	CYS	VAL	conflict	UNP P15307
K	147	GLN	MET	conflict	UNP P15307
K	148	VAL	PHE	conflict	UNP P15307
K	154	HIS	ASP	conflict	UNP P15307
K	171	ASP	-	linker	UNP P15307
K	172	ASN	-	linker	UNP P15307
K	173	ARG	-	linker	UNP P15307
K	174	ALA	-	linker	UNP P15307
K	175	PRO	-	linker	UNP P15307
K	176	ASN	-	linker	UNP P15307
L	1	MET	-	initiating methionine	UNP Q04207

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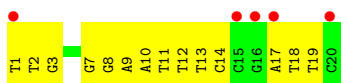
Chain	Residue	Modelled	Actual	Comment	Reference
L	111	GLU	GLY	conflict	UNP P15307
L	127	PRO	GLY	conflict	UNP P15307
L	144	LEU	CYS	conflict	UNP P15307
L	145	CYS	VAL	conflict	UNP P15307
L	147	GLN	MET	conflict	UNP P15307
L	148	VAL	PHE	conflict	UNP P15307
L	154	HIS	ASP	conflict	UNP P15307
L	171	ASP	-	linker	UNP P15307
L	172	ASN	-	linker	UNP P15307
L	173	ARG	-	linker	UNP P15307
L	174	ALA	-	linker	UNP P15307
L	175	PRO	-	linker	UNP P15307
L	176	ASN	-	linker	UNP P15307
O	1	MET	-	initiating methionine	UNP Q04207
O	111	GLU	GLY	conflict	UNP P15307
O	127	PRO	GLY	conflict	UNP P15307
O	144	LEU	CYS	conflict	UNP P15307
O	145	CYS	VAL	conflict	UNP P15307
O	147	GLN	MET	conflict	UNP P15307
O	148	VAL	PHE	conflict	UNP P15307
O	154	HIS	ASP	conflict	UNP P15307
O	171	ASP	-	linker	UNP P15307
O	172	ASN	-	linker	UNP P15307
O	173	ARG	-	linker	UNP P15307
O	174	ALA	-	linker	UNP P15307
O	175	PRO	-	linker	UNP P15307
O	176	ASN	-	linker	UNP P15307
P	1	MET	-	initiating methionine	UNP Q04207
P	111	GLU	GLY	conflict	UNP P15307
P	127	PRO	GLY	conflict	UNP P15307
P	144	LEU	CYS	conflict	UNP P15307
P	145	CYS	VAL	conflict	UNP P15307
P	147	GLN	MET	conflict	UNP P15307
P	148	VAL	PHE	conflict	UNP P15307
P	154	HIS	ASP	conflict	UNP P15307
P	171	ASP	-	linker	UNP P15307
P	172	ASN	-	linker	UNP P15307
P	173	ARG	-	linker	UNP P15307
P	174	ALA	-	linker	UNP P15307
P	175	PRO	-	linker	UNP P15307
P	176	ASN	-	linker	UNP P15307

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA (5'-D(P*TP*TP*GP*AP*TP*GP*GP*GP*AP*AP*TP*TP*TP*CP*CP*GP*AP*TP*TP*C)-3')

Chain E: 



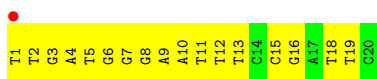
- Molecule 1: DNA (5'-D(P*TP*TP*GP*AP*TP*GP*GP*GP*AP*AP*TP*TP*TP*CP*CP*GP*AP*TP*TP*C)-3')

Chain C: 

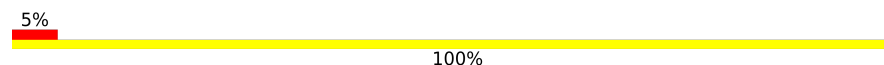


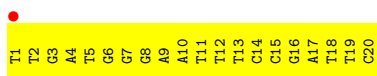
- Molecule 1: DNA (5'-D(P*TP*TP*GP*AP*TP*GP*GP*GP*AP*AP*TP*TP*TP*CP*CP*GP*AP*TP*TP*C)-3')

Chain I: 



- Molecule 1: DNA (5'-D(P*TP*TP*GP*AP*TP*GP*GP*GP*AP*AP*TP*TP*TP*CP*CP*GP*AP*TP*TP*C)-3')

Chain M: 

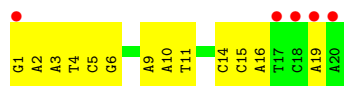


- Molecule 2: DNA (5'-D(P*GP*AP*AP*TP*CP*GP*GP*AP*AP*AP*TP*TP*CP*CP*CP*A*P*TP*CP*AP*A)-3')

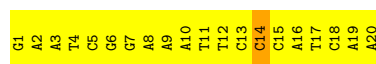
Chain F: 



- Molecule 2: DNA (5'-D(P*GP*AP*AP*TP*CP*GP*GP*AP*AP*AP*TP*TP*CP*CP*CP*A P*TP*CP*AP*A)-3')



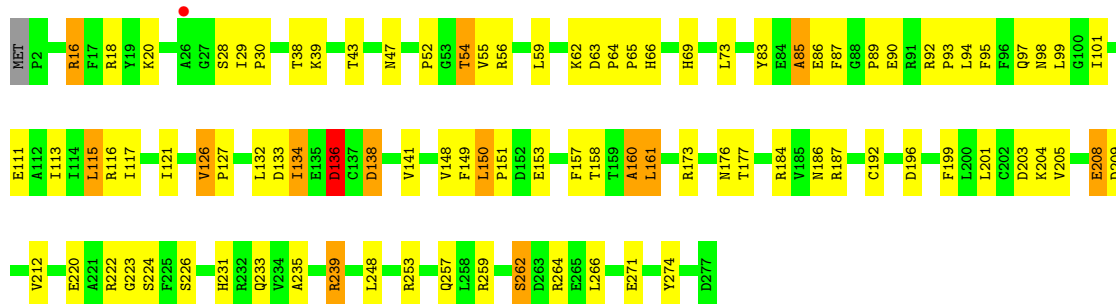
- Molecule 2: DNA (5'-D(P*GP*AP*AP*TP*CP*GP*GP*AP*AP*AP*TP*TP*CP*CP*CP*A P*TP*CP*AP*A)-3')



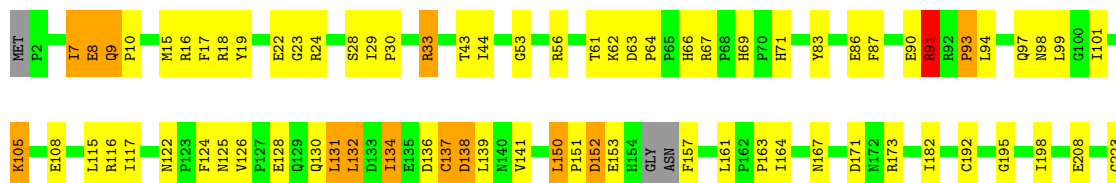
- Molecule 2: DNA (5'-D(P*GP*AP*AP*TP*CP*GP*GP*AP*AP*AP*TP*TP*CP*CP*CP*A P*TP*CP*AP*A)-3')



- Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera



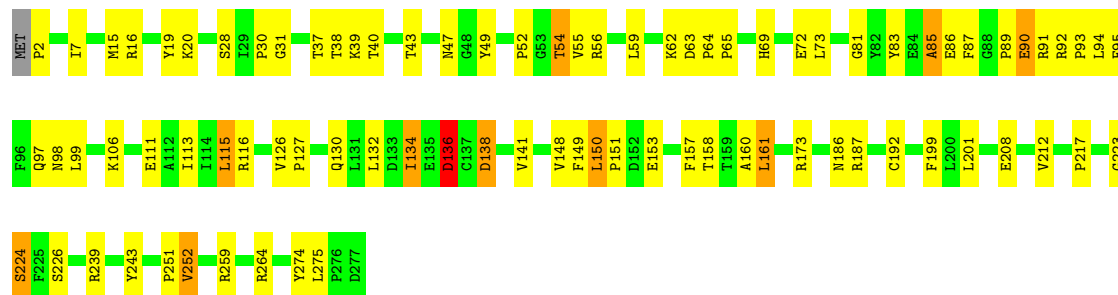
- Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera





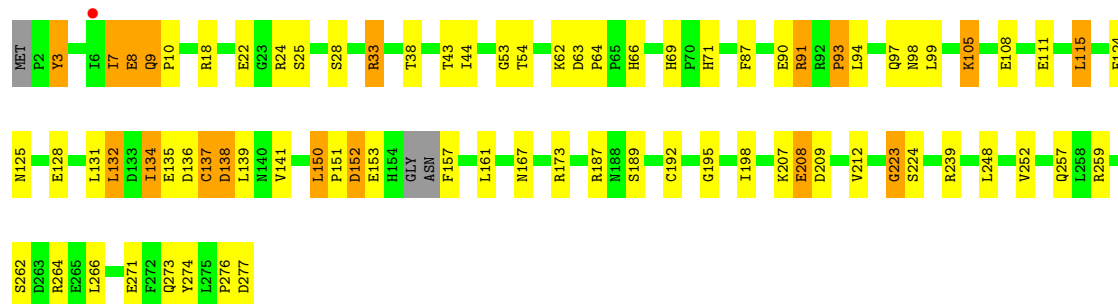
- Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera

Chain G: 69% 27% .



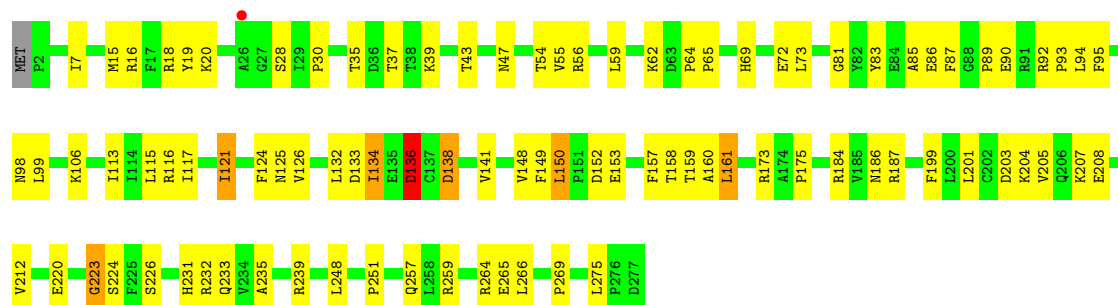
- Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera

Chain H: 71% 22% 6% .



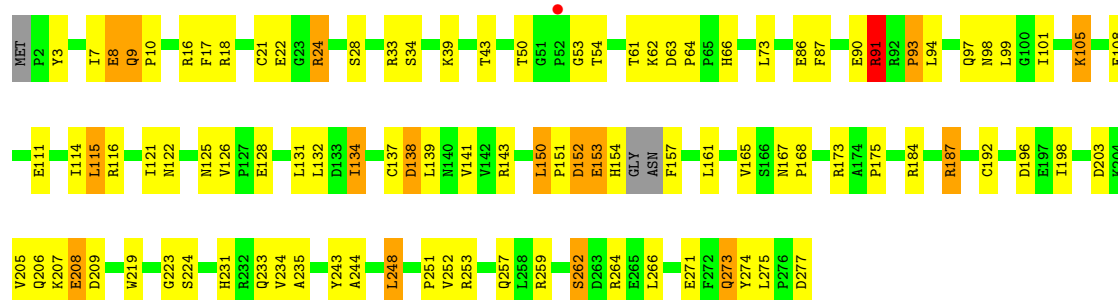
- Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera

Chain K: 66% 31% .



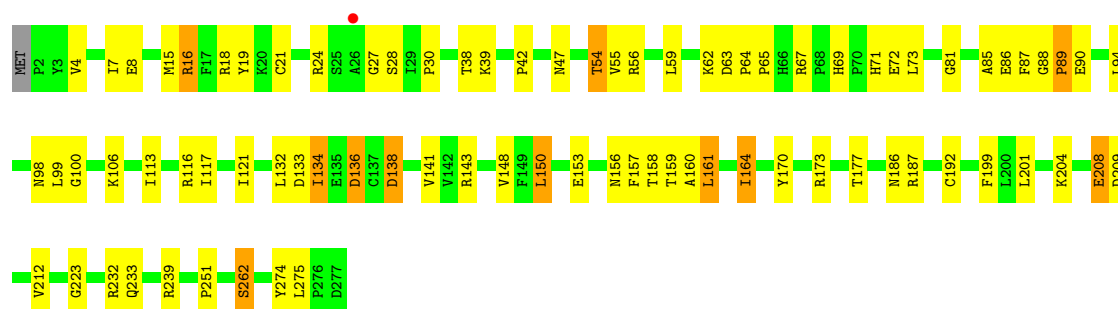
- Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera

Chain L: 63% 30% 6% .



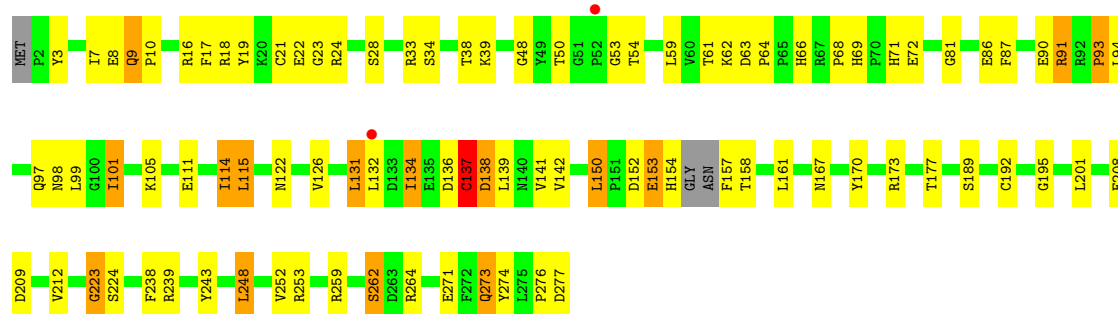
- Molecule 3: Transcription factor p55,Proto-oncogene c-Rel chimera

Chain O: 70% 26%



- Molecule 3: Transcription factor p55,Proto-oncogene c-Rel chimera

Chain P: 66% 27% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.91Å 110.46Å 162.84Å 82.20° 77.98° 72.81°	Depositor
Resolution (Å)	47.92 – 3.09 47.92 – 3.09	Depositor EDS
% Data completeness (in resolution range)	96.0 (47.92-3.09) 94.6 (47.92-3.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.277 , 0.329 0.278 , 0.331	Depositor DCC
R_{free} test set	2024 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 101.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20864	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 79.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3229e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [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	0.59	0/460	0.74	0/707
1	E	0.55	0/460	0.66	0/707
1	I	0.76	0/460	0.86	0/707
1	M	0.76	0/460	0.88	0/707
2	D	0.60	0/460	0.77	0/705
2	F	0.56	0/460	0.71	0/705
2	J	0.80	0/460	1.03	1/705 (0.1%)
2	N	0.84	0/460	1.01	1/705 (0.1%)
3	A	0.39	0/2258	0.73	0/3061
3	B	0.38	0/2245	0.70	0/3042
3	G	0.41	0/2258	0.75	0/3061
3	H	0.40	0/2245	0.74	1/3042 (0.0%)
3	K	0.43	0/2258	0.77	0/3061
3	L	0.42	0/2245	0.75	0/3042
3	O	0.44	0/2258	0.76	0/3061
3	P	0.41	0/2245	0.75	2/3042 (0.1%)
All	All	0.47	0/21692	0.76	5/30060 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	14	DC	O5'-P-OP2	-6.94	87.19	108.00
3	H	135	GLU	CB-CA-C	-5.27	108.84	116.54
3	P	137	CYS	CA-C-N	5.25	131.57	121.54
3	P	137	CYS	C-N-CA	5.25	131.57	121.54
2	N	12	DT	OP2-P-O3'	5.13	123.38	108.00

There are no chirality outliers.

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	C	412	0	229	15	0
1	E	412	0	229	20	0
1	I	412	0	229	29	0
1	M	412	0	229	44	0
2	D	410	0	225	22	0
2	F	410	0	225	28	0
2	J	410	0	225	56	0
2	N	410	0	225	64	0
3	A	2203	0	2175	45	0
3	B	2191	0	2165	62	0
3	G	2203	0	2175	40	0
3	H	2191	0	2165	47	0
3	K	2203	0	2175	44	0
3	L	2191	0	2165	63	0
3	O	2203	0	2175	49	0
3	P	2191	0	2165	56	0
All	All	20864	0	19176	569	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 15.

All (569) 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)
1:M:3:DG:N1	2:N:18:DC:O2	1.86	1.06
1:M:2:DT:N3	2:N:19:DA:N1	2.06	1.04
1:M:12:DT:OP2	3:P:19:TYR:OH	1.78	1.01
1:M:17:DA:N1	2:N:4:DT:N3	2.09	1.00
1:I:8:DG:N1	2:J:13:DC:N3	2.09	0.99
2:J:5:DC:H41	3:L:24:ARG:HH22	1.12	0.98
1:M:18:DT:N3	2:N:3:DA:N1	2.13	0.97
1:M:16:DG:O6	2:N:5:DC:N4	1.98	0.96
1:M:16:DG:N1	2:N:5:DC:N3	2.14	0.95
2:N:17:DT:H2''	2:N:18:DC:C5	2.02	0.94
2:D:1:DG:H2'	2:D:2:DA:C8	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:DG:N2	2:J:13:DC:O2	1.99	0.94
1:I:8:DG:O6	2:J:13:DC:N4	2.00	0.93
3:L:9:GLN:HG3	3:L:10:PRO:HD2	1.50	0.93
1:C:6:DG:N2	2:D:15:DC:O2	2.00	0.93
3:P:9:GLN:HG3	3:P:10:PRO:HD2	1.50	0.93
1:I:9:DA:N1	2:J:12:DT:N3	2.15	0.93
1:I:7:DG:N1	2:J:14:DC:N3	2.16	0.92
1:I:7:DG:N2	2:J:14:DC:O2	2.03	0.91
2:J:15:DC:H2''	2:J:16:DA:C8	2.06	0.91
3:P:18:ARG:NH1	3:P:22:GLU:OE2	2.06	0.89
2:N:15:DC:H2''	2:N:16:DA:C8	2.09	0.88
2:N:15:DC:H2''	2:N:16:DA:N7	1.89	0.86
1:M:7:DG:O6	3:O:18:ARG:NH2	2.09	0.86
2:J:5:DC:H41	3:L:24:ARG:NH2	1.74	0.85
2:D:5:DC:H41	3:H:24:ARG:HH22	1.22	0.85
3:H:9:GLN:HG3	3:H:10:PRO:HD2	1.59	0.84
2:J:17:DT:H4'	2:J:18:DC:H5'	1.58	0.84
2:N:1:DG:H2'	2:N:2:DA:C8	2.14	0.83
2:J:1:DG:H2'	2:J:2:DA:C8	2.14	0.83
3:B:117:ILE:HG21	3:B:131:LEU:HD11	1.60	0.83
1:I:6:DG:N1	2:J:15:DC:N3	2.26	0.82
1:E:3:DG:N2	2:F:18:DC:O2	2.12	0.82
1:E:17:DA:N6	2:F:4:DT:O4	2.10	0.81
3:G:73:LEU:HD22	3:G:99:LEU:HD22	1.61	0.81
1:M:15:DC:N4	2:N:6:DG:O6	2.11	0.81
2:J:10:DA:H2''	2:J:11:DT:H5''	1.63	0.80
1:I:6:DG:N2	2:J:15:DC:O2	2.14	0.80
2:F:1:DG:H2'	2:F:2:DA:C8	2.18	0.79
1:C:7:DG:N1	2:D:14:DC:N3	2.25	0.79
3:O:28:SER:HA	3:O:99:LEU:O	1.83	0.79
3:L:248:LEU:HD21	3:L:252:VAL:HG22	1.65	0.78
1:C:7:DG:N2	2:D:14:DC:O2	2.11	0.78
3:B:9:GLN:HG3	3:B:10:PRO:HD2	1.66	0.77
3:P:248:LEU:HD21	3:P:252:VAL:HG22	1.67	0.77
1:M:8:DG:O6	3:O:16:ARG:NH2	2.18	0.77
2:J:6:DG:N7	3:L:18:ARG:NH2	2.34	0.76
3:G:150:LEU:HD22	3:G:161:LEU:HD11	1.66	0.76
1:M:17:DA:N6	2:N:4:DT:O4	2.15	0.76
3:H:128:GLU:HG2	3:O:117:ILE:HG13	1.69	0.76
3:B:128:GLU:HG2	3:K:117:ILE:HG13	1.69	0.75
3:P:150:LEU:HD22	3:P:161:LEU:HD21	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:55:VAL:HG12	3:O:148:VAL:HG22	1.67	0.75
3:H:8:GLU:HB2	3:H:43:THR:HG22	1.69	0.74
3:A:253:ARG:NH2	3:A:271:GLU:OE1	2.21	0.74
3:P:62:LYS:HD2	3:P:141:VAL:HG11	1.68	0.73
1:M:1:DT:N3	2:N:20:DA:C2	2.57	0.73
3:L:209:ASP:OD2	3:L:262:SER:OG	2.08	0.72
3:P:59:LEU:HD11	3:P:101:ILE:HG12	1.70	0.72
3:G:28:SER:HA	3:G:99:LEU:O	1.89	0.72
3:A:73:LEU:HD22	3:A:99:LEU:HD22	1.70	0.72
3:A:28:SER:HA	3:A:99:LEU:O	1.90	0.72
1:I:5:DT:H3	2:J:16:DA:H61	1.35	0.72
1:C:6:DG:N2	2:D:15:DC:C2	2.54	0.71
3:L:62:LYS:HD2	3:L:141:VAL:HG11	1.73	0.71
1:M:2:DT:N3	2:N:19:DA:C2	2.59	0.71
3:A:55:VAL:HG12	3:A:148:VAL:HG22	1.72	0.70
1:M:2:DT:C2	2:N:19:DA:C2	2.79	0.70
3:O:186:ASN:HB2	3:O:199:PHE:H	1.56	0.70
2:J:18:DC:H2''	2:J:19:DA:OP2	1.91	0.70
3:K:28:SER:HA	3:K:99:LEU:O	1.90	0.69
1:I:11:DT:H1'	1:I:12:DT:H5''	1.74	0.69
3:G:55:VAL:HG12	3:G:148:VAL:HG22	1.73	0.69
3:K:69:HIS:NE2	3:K:138:ASP:O	2.16	0.69
3:A:69:HIS:NE2	3:A:138:ASP:O	2.16	0.69
2:J:15:DC:H2''	2:J:16:DA:H8	1.55	0.69
2:N:19:DA:H8	2:N:19:DA:OP2	1.74	0.69
3:A:150:LEU:HD22	3:A:161:LEU:HD11	1.75	0.69
3:A:117:ILE:HG13	3:L:128:GLU:HG2	1.75	0.69
1:I:9:DA:OP1	3:L:207:LYS:NZ	2.24	0.69
1:M:16:DG:N2	2:N:5:DC:O2	2.20	0.69
3:H:248:LEU:HD21	3:H:252:VAL:HG22	1.74	0.68
3:H:18:ARG:NH1	3:H:22:GLU:OE2	2.26	0.68
1:C:7:DG:O6	2:D:14:DC:N4	2.21	0.67
3:K:73:LEU:HD22	3:K:99:LEU:HD22	1.75	0.67
1:E:2:DT:N3	2:F:19:DA:C2	2.63	0.66
3:B:248:LEU:HD21	3:B:252:VAL:HG22	1.77	0.66
3:L:9:GLN:HG2	3:L:167:ASN:ND2	2.10	0.66
1:M:2:DT:O2	2:N:19:DA:C2	2.48	0.66
3:G:54:THR:HG22	3:G:85:ALA:HA	1.78	0.66
2:F:17:DT:H2''	2:F:18:DC:C5	2.31	0.65
3:H:9:GLN:OE1	3:H:167:ASN:N	2.30	0.65
2:J:19:DA:OP2	2:J:19:DA:C4	2.50	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:DG:O6	3:A:16:ARG:NH2	2.30	0.64
3:K:69:HIS:O	3:K:116:ARG:NH1	2.30	0.64
3:B:8:GLU:HB2	3:B:43:THR:HG22	1.78	0.64
3:L:91:ARG:HG3	3:L:93:PRO:HA	1.79	0.64
1:I:5:DT:H3	2:J:16:DA:N6	1.96	0.64
1:E:1:DT:N3	2:F:20:DA:H2	1.96	0.63
2:J:19:DA:H1'	2:J:20:DA:O4'	1.99	0.63
3:O:209:ASP:OD2	3:O:262:SER:OG	2.16	0.63
2:N:19:DA:H2''	2:N:20:DA:C8	2.34	0.62
3:B:163:PRO:O	3:P:48:GLY:HA2	1.99	0.62
3:L:18:ARG:NH1	3:L:22:GLU:OE2	2.32	0.62
1:I:7:DG:O6	2:J:14:DC:N4	2.22	0.62
3:H:195:GLY:O	3:H:239:ARG:NH1	2.29	0.62
3:H:28:SER:HA	3:H:99:LEU:O	2.00	0.62
3:K:64:PRO:HB2	3:K:65:PRO:HD3	1.82	0.62
2:N:14:DC:H2''	2:N:15:DC:C5	2.35	0.62
1:E:12:DT:OP2	3:B:19:TYR:OH	2.12	0.61
3:H:259:ARG:NH1	3:H:264:ARG:HG2	2.16	0.61
3:A:186:ASN:HB2	3:A:199:PHE:H	1.66	0.61
3:B:62:LYS:HD2	3:B:141:VAL:HG11	1.82	0.61
3:L:66:HIS:CD2	3:L:165:VAL:HG11	2.36	0.61
3:B:91:ARG:HG3	3:B:93:PRO:HA	1.81	0.60
2:N:11:DT:H2'	2:N:12:DT:H71	1.81	0.60
2:J:5:DC:H2''	2:J:6:DG:C8	2.36	0.60
3:H:192:CYS:HB3	3:H:248:LEU:HD22	1.84	0.60
2:N:13:DC:H2''	2:N:14:DC:H6	1.65	0.60
3:O:54:THR:HG22	3:O:85:ALA:HA	1.83	0.60
3:O:150:LEU:HD22	3:O:161:LEU:HD11	1.84	0.60
3:O:64:PRO:HB2	3:O:65:PRO:HD3	1.83	0.60
3:K:55:VAL:HG12	3:K:148:VAL:HG22	1.84	0.59
1:M:4:DA:H61	2:N:17:DT:H3	1.49	0.59
3:L:61:THR:HG22	3:L:63:ASP:H	1.68	0.59
3:L:150:LEU:HD22	3:L:161:LEU:HD21	1.83	0.59
2:F:9:DA:OP2	3:A:233:GLN:NE2	2.32	0.59
2:D:10:DA:H2''	2:D:11:DT:H5''	1.84	0.59
3:B:9:GLN:OE1	3:B:167:ASN:N	2.36	0.59
1:M:1:DT:C2	2:N:20:DA:C2	2.91	0.59
2:N:9:DA:OP2	3:O:233:GLN:NE2	2.30	0.59
3:O:192:CYS:HA	3:O:274:TYR:CD2	2.37	0.59
1:M:1:DT:C2	2:N:20:DA:H2	2.20	0.59
2:N:17:DT:H2''	2:N:18:DC:C4	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:113:ILE:HD13	3:O:134:ILE:HD12	1.84	0.58
2:D:11:DT:H72	3:G:173:ARG:HD3	1.84	0.58
3:P:53:GLY:O	3:P:87:PHE:HB3	2.03	0.58
2:N:13:DC:H2''	2:N:14:DC:C6	2.38	0.58
3:O:30:PRO:HB3	3:O:39:LYS:HE2	1.86	0.58
2:F:11:DT:H72	3:A:173:ARG:HD3	1.86	0.58
3:H:150:LEU:HD22	3:H:161:LEU:HD21	1.86	0.58
3:A:113:ILE:HD13	3:A:134:ILE:HD12	1.86	0.58
2:N:12:DT:H2''	2:N:13:DC:H6	1.69	0.58
3:K:43:THR:HG23	3:K:95:PHE:HB3	1.86	0.57
2:N:7:DG:P	3:O:232:ARG:HH12	2.27	0.57
1:I:6:DG:H1	2:J:15:DC:N4	2.02	0.57
3:H:248:LEU:HB3	3:H:276:PRO:HA	1.87	0.57
3:L:192:CYS:HA	3:L:274:TYR:HD2	1.69	0.57
2:F:19:DA:OP2	2:F:19:DA:H8	1.87	0.57
2:F:15:DC:H2''	2:F:16:DA:C8	2.39	0.57
1:I:6:DG:N2	2:J:15:DC:C2	2.58	0.57
3:B:195:GLY:O	3:B:239:ARG:NH1	2.37	0.56
3:H:53:GLY:C	3:H:87:PHE:HB3	2.30	0.56
2:J:10:DA:C2'	2:J:11:DT:H5''	2.34	0.56
3:L:53:GLY:C	3:L:87:PHE:HB3	2.30	0.56
3:K:150:LEU:HD22	3:K:161:LEU:HD11	1.86	0.56
1:M:4:DA:N6	2:N:17:DT:H3	2.04	0.56
3:H:63:ASP:O	3:H:66:HIS:ND1	2.39	0.56
3:A:231:HIS:HB3	3:A:235:ALA:HB3	1.86	0.56
3:H:209:ASP:OD2	3:H:262:SER:OG	2.21	0.56
3:K:259:ARG:NH1	3:K:264:ARG:HG2	2.21	0.56
1:M:3:DG:C2	2:N:18:DC:O2	2.58	0.56
3:O:69:HIS:O	3:O:116:ARG:NH1	2.38	0.56
3:P:61:THR:HG22	3:P:63:ASP:H	1.71	0.56
1:I:13:DT:H2'	3:L:21:CYS:SG	2.45	0.55
1:C:13:DT:H2''	1:C:14:DC:H5'	1.87	0.55
3:B:29:ILE:HD11	3:B:101:ILE:HG13	1.88	0.55
3:G:64:PRO:HB2	3:G:65:PRO:HD3	1.88	0.55
3:G:43:THR:HG23	3:G:95:PHE:HB3	1.88	0.55
3:B:16:ARG:HH21	3:B:173:ARG:NH2	2.04	0.55
1:I:6:DG:C2	2:J:15:DC:N3	2.75	0.55
3:K:113:ILE:HD13	3:K:134:ILE:HD12	1.88	0.55
2:J:5:DC:N4	3:L:24:ARG:HH22	1.94	0.55
3:K:175:PRO:HG3	3:K:204:LYS:HE3	1.88	0.55
3:P:53:GLY:C	3:P:87:PHE:HB3	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:195:GLY:O	3:P:239:ARG:NH1	2.39	0.54
1:I:6:DG:O6	2:J:15:DC:N4	2.38	0.54
2:N:14:DC:H2''	2:N:15:DC:C6	2.43	0.54
1:M:17:DA:C2	1:M:18:DT:C2	2.96	0.54
3:G:52:PRO:HG2	3:G:151:PRO:HG3	1.90	0.54
2:J:15:DC:C2'	2:J:16:DA:C8	2.84	0.54
3:L:122:ASN:HD21	3:L:126:VAL:HG22	1.73	0.54
1:C:6:DG:N1	2:D:15:DC:N3	2.53	0.53
3:H:136:ASP:O	3:H:137:CYS:HB2	2.08	0.53
2:J:11:DT:OP2	3:K:19:TYR:OH	2.13	0.53
3:H:53:GLY:O	3:H:87:PHE:HB3	2.08	0.53
3:B:122:ASN:HD21	3:B:126:VAL:HG22	1.72	0.53
1:C:11:DT:H1'	1:C:12:DT:H5''	1.90	0.53
3:G:69:HIS:NE2	3:G:138:ASP:O	2.26	0.53
2:J:11:DT:H72	3:K:173:ARG:HD3	1.90	0.53
2:J:14:DC:H2''	2:J:15:DC:C5	2.44	0.53
3:L:192:CYS:HA	3:L:274:TYR:CD2	2.43	0.53
3:L:253:ARG:HG2	3:L:271:GLU:HG3	1.89	0.53
2:D:11:DT:OP1	3:G:106:LYS:HB2	2.08	0.53
3:O:4:VAL:HB	3:O:164:ILE:HD11	1.91	0.53
3:K:186:ASN:HB2	3:K:199:PHE:H	1.74	0.52
3:L:259:ARG:NH1	3:L:264:ARG:HG2	2.24	0.52
3:H:138:ASP:O	3:H:139:LEU:HB2	2.09	0.52
3:A:64:PRO:HB2	3:A:65:PRO:HD3	1.90	0.52
2:N:15:DC:C2'	2:N:16:DA:N7	2.69	0.52
3:P:253:ARG:HG2	3:P:271:GLU:HG3	1.91	0.52
3:A:149:PHE:HD1	3:A:160:ALA:HA	1.74	0.52
3:O:150:LEU:HD22	3:O:161:LEU:HD21	1.91	0.52
3:H:91:ARG:HG3	3:H:93:PRO:HA	1.91	0.52
2:J:9:DA:C2	2:J:10:DA:C4	2.97	0.52
1:M:8:DG:C2	1:M:9:DA:C4	2.98	0.52
1:E:1:DT:N3	2:F:20:DA:C2	2.68	0.52
1:E:7:DG:O6	3:A:18:ARG:NH2	2.43	0.52
2:N:11:DT:OP1	3:O:106:LYS:HB2	2.09	0.52
3:O:170:TYR:HB3	3:O:177:THR:HB	1.91	0.52
3:O:192:CYS:HA	3:O:274:TYR:HD2	1.75	0.52
3:G:2:PRO:HG3	3:G:49:TYR:HB2	1.92	0.52
3:L:28:SER:HB2	3:L:97:GLN:O	2.10	0.52
3:P:192:CYS:SG	3:P:248:LEU:HB2	2.50	0.52
3:H:209:ASP:CG	3:H:262:SER:OG	2.53	0.52
3:K:62:LYS:HD2	3:K:141:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:13:DT:H2''	1:M:14:DC:H5'	1.92	0.52
2:D:15:DC:H2''	2:D:16:DA:C8	2.45	0.52
3:P:23:GLY:C	3:P:24:ARG:HG2	2.35	0.52
1:E:13:DT:H2''	1:E:14:DC:H5'	1.92	0.51
3:O:67:ARG:HB3	3:O:134:ILE:HD11	1.92	0.51
3:H:257:GLN:CD	3:H:266:LEU:HD23	2.35	0.51
3:G:149:PHE:HD1	3:G:160:ALA:HA	1.75	0.51
2:J:18:DC:C2'	2:J:19:DA:OP2	2.58	0.51
2:D:5:DC:N4	3:H:24:ARG:HH22	1.99	0.51
1:E:3:DG:C2	2:F:19:DA:C2	2.99	0.51
3:H:105:LYS:HB2	3:H:108:GLU:HG3	1.93	0.51
1:M:3:DG:C4	2:N:19:DA:C2	2.99	0.51
3:A:62:LYS:HD2	3:A:141:VAL:HG11	1.93	0.51
3:O:251:PRO:HB3	3:O:275:LEU:HD23	1.93	0.51
3:B:18:ARG:NH1	3:B:22:GLU:OE2	2.43	0.51
3:G:136:ASP:OD1	3:G:138:ASP:HB2	2.12	0.51
1:I:1:DT:C2'	1:I:2:DT:H71	2.41	0.51
3:L:138:ASP:O	3:L:139:LEU:HB2	2.10	0.51
3:L:187:ARG:NH1	3:L:196:ASP:HB3	2.26	0.51
1:M:1:DT:O2	2:N:20:DA:C2	2.64	0.51
3:O:56:ARG:HD3	3:O:121:ILE:HD12	1.93	0.50
2:N:5:DC:H41	3:P:24:ARG:HH22	1.59	0.50
1:E:1:DT:H3	2:F:20:DA:H2	1.45	0.50
2:F:4:DT:H72	3:B:24:ARG:NH2	2.25	0.50
2:F:17:DT:H2''	2:F:18:DC:C6	2.47	0.50
1:I:18:DT:H2'	1:I:19:DT:H72	1.92	0.50
2:J:6:DG:C2	2:J:7:DG:C5	2.99	0.50
3:K:59:LEU:HD13	3:K:73:LEU:HG	1.93	0.50
3:A:136:ASP:OD1	3:A:138:ASP:HB2	2.12	0.50
1:I:15:DC:H2''	1:I:16:DG:C8	2.46	0.50
3:K:56:ARG:HD3	3:K:121:ILE:HD12	1.94	0.50
1:M:4:DA:H1'	1:M:5:DT:H5'	1.92	0.50
2:N:14:DC:C2	2:N:15:DC:C4	3.00	0.50
3:B:8:GLU:HB2	3:B:43:THR:CG2	2.41	0.50
3:B:56:ARG:HG2	3:B:83:TYR:O	2.11	0.50
3:L:73:LEU:HD22	3:L:99:LEU:HD22	1.93	0.50
1:M:1:DT:O2	2:N:20:DA:H2	1.94	0.50
2:N:19:DA:OP2	2:N:19:DA:C8	2.60	0.50
3:G:56:ARG:HA	3:G:83:TYR:O	2.12	0.50
3:P:68:PRO:HG2	3:P:131:LEU:HD21	1.93	0.50
3:O:204:LYS:HE3	3:O:233:GLN:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:92:ARG:N	3:G:93:PRO:HD2	2.26	0.50
3:K:30:PRO:HB3	3:K:39:LYS:HE2	1.94	0.50
3:A:30:PRO:HB3	3:A:39:LYS:HE2	1.94	0.49
3:G:113:ILE:HD13	3:G:134:ILE:HD12	1.94	0.49
2:N:16:DA:C4	2:N:17:DT:C5	2.99	0.49
3:B:28:SER:HA	3:B:99:LEU:O	2.11	0.49
3:O:73:LEU:HD22	3:O:99:LEU:HD22	1.94	0.49
3:P:91:ARG:HG3	3:P:93:PRO:HA	1.94	0.49
3:K:56:ARG:HA	3:K:83:TYR:O	2.12	0.49
3:O:8:GLU:O	3:O:42:PRO:HA	2.12	0.49
3:P:248:LEU:HB3	3:P:276:PRO:HA	1.94	0.49
3:O:62:LYS:HD2	3:O:141:VAL:HG11	1.93	0.49
1:I:8:DG:C6	2:J:13:DC:N3	2.79	0.49
3:A:259:ARG:NH1	3:A:264:ARG:HG2	2.27	0.49
3:K:35:THR:OG1	3:K:37:THR:HG22	2.12	0.49
3:L:53:GLY:O	3:L:87:PHE:HB3	2.13	0.49
3:A:192:CYS:HA	3:A:274:TYR:CD2	2.48	0.49
3:B:28:SER:HB2	3:B:97:GLN:O	2.13	0.49
3:B:61:THR:HG22	3:B:63:ASP:H	1.77	0.49
1:M:5:DT:P	3:O:27:GLY:HA2	2.53	0.49
3:P:28:SER:HA	3:P:99:LEU:O	2.13	0.48
3:P:243:TYR:CE1	3:P:252:VAL:HG21	2.48	0.48
3:H:151:PRO:O	3:H:152:ASP:HB2	2.13	0.48
3:P:97:GLN:HG2	3:P:98:ASN:H	1.78	0.48
3:L:97:GLN:HG2	3:L:98:ASN:H	1.77	0.48
3:L:243:TYR:CE1	3:L:252:VAL:HG21	2.48	0.48
1:M:5:DT:H2''	1:M:6:DG:C8	2.47	0.48
2:N:15:DC:C2	2:N:16:DA:C6	3.01	0.48
3:A:56:ARG:HA	3:A:83:TYR:O	2.14	0.48
1:M:18:DT:O2	2:N:3:DA:C2	2.66	0.48
3:A:209:ASP:OD2	3:A:262:SER:OG	2.26	0.48
3:K:92:ARG:N	3:K:93:PRO:HD2	2.28	0.48
3:L:28:SER:HA	3:L:99:LEU:O	2.14	0.48
3:L:63:ASP:O	3:L:66:HIS:ND1	2.40	0.48
2:F:11:DT:C2'	2:F:12:DT:H71	2.44	0.48
3:H:3:TYR:N	3:H:3:TYR:HD2	2.12	0.48
2:J:8:DA:C2	2:J:9:DA:C4	3.02	0.48
3:L:16:ARG:HH21	3:L:173:ARG:NH2	2.11	0.48
3:H:97:GLN:HG2	3:H:98:ASN:H	1.78	0.48
3:B:136:ASP:O	3:B:137:CYS:HB2	2.14	0.48
3:O:63:ASP:HB3	3:O:64:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:138:ASP:O	3:P:139:LEU:HB2	2.12	0.48
1:E:11:DT:H1'	1:E:12:DT:H5''	1.95	0.48
1:M:2:DT:C2	2:N:19:DA:H2	2.29	0.48
3:P:111:GLU:O	3:P:115:LEU:HB2	2.14	0.48
3:H:192:CYS:HA	3:H:274:TYR:CD2	2.49	0.48
3:L:205:VAL:O	3:L:233:GLN:NE2	2.43	0.48
3:K:205:VAL:O	3:K:233:GLN:NE2	2.45	0.47
3:P:259:ARG:NH1	3:P:264:ARG:HG2	2.29	0.47
3:G:212:VAL:O	3:G:223:GLY:N	2.47	0.47
3:H:24:ARG:HG3	3:H:25:SER:O	2.15	0.47
2:J:12:DT:H1'	2:J:13:DC:H5'	1.96	0.47
3:K:203:ASP:O	3:K:205:VAL:HG13	2.14	0.47
1:M:10:DA:H1'	1:M:11:DT:H5'	1.96	0.47
2:N:11:DT:H2''	2:N:12:DT:C5'	2.44	0.47
3:L:257:GLN:CD	3:L:266:LEU:HD23	2.39	0.47
3:G:192:CYS:HA	3:G:274:TYR:CD2	2.50	0.47
3:L:53:GLY:HA2	3:L:157:PHE:CD2	2.50	0.47
3:L:116:ARG:HD2	3:L:121:ILE:HB	1.95	0.47
3:L:209:ASP:CG	3:L:262:SER:OG	2.57	0.47
3:O:156:ASN:O	3:O:158:THR:N	2.47	0.47
1:C:12:DT:H72	3:H:173:ARG:HD3	1.97	0.47
1:I:3:DG:H2''	1:I:4:DA:C8	2.50	0.47
3:K:265:GLU:O	3:K:266:LEU:HD12	2.14	0.47
3:A:111:GLU:HG3	3:L:114:ILE:HD13	1.96	0.47
3:B:97:GLN:HG2	3:B:98:ASN:H	1.79	0.47
1:C:9:DA:H2''	1:C:10:DA:H8	1.78	0.47
3:G:59:LEU:HD13	3:G:73:LEU:HG	1.96	0.47
3:O:62:LYS:HA	3:O:143:ARG:HE	1.79	0.47
3:O:204:LYS:HA	3:O:233:GLN:O	2.14	0.47
3:A:69:HIS:O	3:A:116:ARG:NH1	2.48	0.47
3:A:133:ASP:O	3:A:134:ILE:HB	2.15	0.47
2:J:14:DC:H2''	2:J:15:DC:H5	1.80	0.47
3:K:136:ASP:OD1	3:K:138:ASP:HB2	2.14	0.47
3:H:8:GLU:CB	3:H:43:THR:HG22	2.43	0.47
1:I:1:DT:H2''	1:I:2:DT:H71	1.97	0.47
2:N:11:DT:C2'	2:N:12:DT:H71	2.45	0.47
3:H:53:GLY:HA2	3:H:157:PHE:CD2	2.50	0.47
3:B:94:LEU:HA	3:B:94:LEU:HD23	1.54	0.46
3:L:94:LEU:HA	3:L:94:LEU:HD23	1.66	0.46
3:L:111:GLU:O	3:L:115:LEU:HB2	2.15	0.46
2:D:10:DA:C2'	2:D:11:DT:H5''	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:30:PRO:HB3	3:G:39:LYS:HE2	1.98	0.46
3:A:126:VAL:HG12	3:A:127:PRO:HD2	1.97	0.46
3:B:243:TYR:CE1	3:B:252:VAL:HG21	2.51	0.46
3:B:253:ARG:HG2	3:B:271:GLU:HG3	1.97	0.46
1:I:6:DG:H1	2:J:15:DC:H42	1.62	0.46
3:L:8:GLU:HB2	3:L:43:THR:CG2	2.46	0.46
3:L:207:LYS:HG3	3:L:208:GLU:HG3	1.98	0.46
3:O:212:VAL:O	3:O:223:GLY:N	2.45	0.46
3:P:50:THR:HA	3:P:91:ARG:NH2	2.30	0.46
3:A:29:ILE:HD11	3:A:101:ILE:HG13	1.96	0.46
3:A:63:ASP:O	3:A:66:HIS:ND1	2.48	0.46
3:H:3:TYR:N	3:H:3:TYR:CD2	2.83	0.46
3:L:151:PRO:O	3:L:152:ASP:HB2	2.16	0.46
2:N:11:DT:H2''	2:N:12:DT:H5'	1.97	0.46
3:G:186:ASN:HB2	3:G:199:PHE:H	1.80	0.46
1:M:18:DT:O2	2:N:3:DA:H2	1.99	0.46
3:B:53:GLY:HA2	3:B:157:PHE:CD2	2.51	0.46
3:L:97:GLN:HG2	3:L:98:ASN:N	2.31	0.46
2:F:4:DT:H72	3:B:24:ARG:HH21	1.80	0.46
1:I:8:DG:N1	2:J:13:DC:C2	2.75	0.46
3:K:239:ARG:HH22	3:L:184:ARG:HH12	1.62	0.46
3:B:132:LEU:HD13	3:B:132:LEU:O	2.15	0.46
3:H:209:ASP:OD1	3:H:262:SER:OG	2.32	0.46
2:J:11:DT:H5'	3:K:19:TYR:CE2	2.51	0.46
3:K:265:GLU:C	3:K:266:LEU:HD12	2.41	0.46
2:F:5:DC:H2''	2:F:6:DG:C8	2.51	0.45
3:B:53:GLY:C	3:B:87:PHE:HB3	2.41	0.45
1:C:19:DT:H2''	1:C:20:DC:C5	2.51	0.45
3:P:17:PHE:CG	3:P:101:ILE:HD12	2.50	0.45
3:A:92:ARG:N	3:A:93:PRO:HD2	2.32	0.45
3:G:259:ARG:NH1	3:G:264:ARG:HG2	2.30	0.45
3:B:17:PHE:CE1	3:B:171:ASP:HB2	2.52	0.45
3:G:28:SER:HB2	3:G:97:GLN:O	2.16	0.45
2:N:15:DC:C2'	2:N:16:DA:C8	2.92	0.45
3:O:69:HIS:NE2	3:O:138:ASP:O	2.42	0.45
3:O:159:THR:O	3:O:160:ALA:HB3	2.17	0.45
3:P:16:ARG:HH21	3:P:173:ARG:NH2	2.15	0.45
3:B:150:LEU:HA	3:B:150:LEU:HD12	1.81	0.45
3:B:151:PRO:O	3:B:152:ASP:HB2	2.16	0.45
3:H:111:GLU:O	3:H:115:LEU:HB2	2.16	0.45
3:G:111:GLU:HG3	3:P:114:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:59:LEU:HD13	3:A:73:LEU:HG	1.99	0.45
2:J:17:DT:C6	2:J:19:DA:N1	2.85	0.45
2:N:13:DC:C2	2:N:14:DC:C5	3.05	0.45
3:B:131:LEU:O	3:B:131:LEU:HD22	2.17	0.45
3:P:209:ASP:CG	3:P:262:SER:OG	2.59	0.45
3:B:105:LYS:HD3	3:B:108:GLU:CD	2.42	0.45
3:K:251:PRO:HB3	3:K:275:LEU:HD23	1.98	0.45
3:L:219:TRP:CD1	3:L:244:ALA:HB2	2.52	0.45
3:P:9:GLN:HG2	3:P:167:ASN:ND2	2.32	0.45
3:B:44:ILE:O	3:B:94:LEU:HB2	2.17	0.45
3:A:28:SER:HB2	3:A:97:GLN:O	2.17	0.44
3:G:31:GLY:HA3	3:G:40:THR:OG1	2.17	0.44
3:P:72:GLU:HB2	3:P:81:GLY:HA2	1.99	0.44
3:P:170:TYR:HB3	3:P:177:THR:HB	1.97	0.44
1:E:10:DA:H1'	1:E:11:DT:H5'	1.99	0.44
3:B:63:ASP:O	3:B:66:HIS:ND1	2.51	0.44
3:G:90:GLU:OE1	3:G:91:ARG:HG3	2.18	0.44
3:H:187:ARG:HD3	3:H:189:SER:O	2.17	0.44
2:J:7:DG:H1'	2:J:8:DA:H5'	1.97	0.44
1:M:20:DC:O2	2:N:2:DA:C2	2.70	0.44
3:P:253:ARG:HG3	3:P:273:GLN:CD	2.42	0.44
3:H:3:TYR:HD2	3:H:3:TYR:H	1.64	0.44
3:A:208:GLU:H	3:A:208:GLU:CD	2.24	0.44
3:A:248:LEU:HA	3:A:248:LEU:HD23	1.70	0.44
3:H:44:ILE:O	3:H:94:LEU:HB2	2.16	0.44
3:O:133:ASP:O	3:O:134:ILE:HB	2.17	0.44
3:P:63:ASP:HB3	3:P:64:PRO:HD2	1.99	0.44
3:B:124:PHE:O	3:B:125:ASN:C	2.60	0.44
3:H:124:PHE:O	3:H:125:ASN:C	2.60	0.44
3:A:176:ASN:OD1	3:A:177:THR:HG23	2.17	0.44
3:B:8:GLU:OE2	3:B:33:ARG:HG3	2.18	0.44
3:L:203:ASP:O	3:L:205:VAL:HG13	2.18	0.44
3:P:122:ASN:HD21	3:P:126:VAL:HG22	1.82	0.44
3:K:212:VAL:O	3:K:223:GLY:N	2.51	0.44
1:E:8:DG:C2	1:E:9:DA:C4	3.05	0.44
3:B:150:LEU:HD22	3:B:161:LEU:HD21	1.99	0.44
3:B:164:ILE:HA	3:P:48:GLY:HA2	1.98	0.44
3:G:243:TYR:CZ	3:G:252:VAL:HG11	2.53	0.44
3:P:69:HIS:CD2	3:P:142:VAL:HG12	2.53	0.44
2:D:9:DA:C6	2:D:10:DA:C6	3.06	0.43
1:M:18:DT:C2	2:N:3:DA:N1	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:59:LEU:HD13	3:O:73:LEU:HG	1.99	0.43
3:P:53:GLY:HA2	3:P:157:PHE:CD2	2.53	0.43
3:H:207:LYS:HG3	3:H:208:GLU:HG3	2.00	0.43
3:K:149:PHE:HD1	3:K:160:ALA:HA	1.83	0.43
2:F:13:DC:H2''	2:F:14:DC:C6	2.53	0.43
3:B:69:HIS:CD2	3:B:71:HIS:H	2.36	0.43
3:O:16:ARG:HH21	3:O:173:ARG:HH21	1.66	0.43
3:A:43:THR:HG23	3:A:95:PHE:HB3	1.99	0.43
1:C:3:DG:C2	2:D:19:DA:C2	3.07	0.43
2:D:5:DC:C2	2:D:6:DG:C5	3.06	0.43
3:G:72:GLU:HB2	3:G:81:GLY:HA2	2.00	0.43
2:J:16:DA:H1'	2:J:17:DT:OP2	2.19	0.43
3:K:231:HIS:HB3	3:K:235:ALA:HB3	2.00	0.43
3:P:34:SER:OG	3:P:39:LYS:HA	2.17	0.43
1:E:7:DG:H2''	1:E:8:DG:OP2	2.19	0.43
2:F:19:DA:H2''	2:F:20:DA:C8	2.53	0.43
3:L:93:PRO:HB2	3:L:94:LEU:H	1.73	0.43
1:M:12:DT:H72	3:P:173:ARG:HD3	2.00	0.43
1:E:18:DT:H2'	1:E:19:DT:H72	2.00	0.43
3:A:52:PRO:O	3:A:151:PRO:HD3	2.19	0.43
3:B:16:ARG:HG2	3:B:173:ARG:HB2	2.01	0.43
2:N:12:DT:H5'	3:O:21:CYS:SG	2.58	0.43
2:N:12:DT:C2	2:N:13:DC:C5	3.07	0.43
3:B:192:CYS:HA	3:B:274:TYR:CD2	2.54	0.43
3:P:189:SER:HA	3:P:273:GLN:O	2.19	0.43
3:B:116:ARG:HB2	3:B:116:ARG:NH1	2.34	0.43
2:N:14:DC:C2	2:N:15:DC:C5	3.06	0.43
2:N:16:DA:C8	2:N:17:DT:C7	3.02	0.43
3:K:248:LEU:HD23	3:K:248:LEU:HA	1.75	0.43
3:A:203:ASP:O	3:A:205:VAL:HG13	2.18	0.42
3:H:8:GLU:OE2	3:H:33:ARG:HG3	2.19	0.42
1:M:13:DT:OP2	3:P:21:CYS:SG	2.69	0.42
3:B:29:ILE:HA	3:B:30:PRO:HD3	1.86	0.42
3:G:251:PRO:HB3	3:G:275:LEU:HD23	2.01	0.42
3:L:175:PRO:HB2	3:L:206:GLN:OE1	2.19	0.42
3:O:4:VAL:HB	3:O:164:ILE:CD1	2.49	0.42
3:O:73:LEU:HA	3:O:100:GLY:O	2.19	0.42
1:C:6:DG:H1	2:D:15:DC:H42	1.67	0.42
3:O:67:ARG:HD2	3:O:134:ILE:HG12	2.01	0.42
3:P:71:HIS:NE2	3:P:139:LEU:O	2.47	0.42
1:E:2:DT:C2	2:F:19:DA:H2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:7:ILE:HG13	3:H:43:THR:HG23	2.02	0.42
3:K:18:ARG:HA	3:K:18:ARG:HD2	1.80	0.42
3:K:152:ASP:OD1	3:P:264:ARG:NH1	2.53	0.42
3:K:232:ARG:HG2	3:L:234:VAL:HG11	2.00	0.42
3:L:50:THR:HA	3:L:91:ARG:NH2	2.33	0.42
3:L:153:GLU:HB3	3:L:154:HIS:H	1.63	0.42
2:F:11:DT:H1'	2:F:12:DT:H5''	2.00	0.42
3:G:63:ASP:O	3:G:64:PRO:C	2.62	0.42
3:G:69:HIS:O	3:G:116:ARG:NH1	2.52	0.42
3:H:212:VAL:O	3:H:223:GLY:N	2.52	0.42
3:K:133:ASP:O	3:K:134:ILE:HB	2.20	0.42
3:L:143:ARG:NH1	3:L:168:PRO:HD3	2.35	0.42
3:A:257:GLN:CD	3:A:266:LEU:HD23	2.45	0.42
3:B:7:ILE:HG13	3:B:43:THR:O	2.20	0.42
3:G:223:GLY:O	3:G:224:SER:HB3	2.20	0.42
3:H:62:LYS:HD2	3:H:141:VAL:HG11	2.01	0.42
3:L:66:HIS:HD2	3:L:165:VAL:HG11	1.82	0.42
1:E:2:DT:N3	2:F:19:DA:H2	2.17	0.42
2:F:19:DA:OP2	2:F:19:DA:C8	2.68	0.42
3:B:23:GLY:O	3:B:24:ARG:HG2	2.20	0.42
3:P:69:HIS:HD2	3:P:71:HIS:HB2	1.84	0.42
3:P:192:CYS:HA	3:P:274:TYR:CD2	2.55	0.42
3:B:122:ASN:HD21	3:B:126:VAL:CG2	2.32	0.42
3:B:259:ARG:NH1	3:B:264:ARG:HG2	2.35	0.42
3:H:94:LEU:HD23	3:H:94:LEU:HA	1.59	0.42
1:I:9:DA:H2''	1:I:10:DA:H8	1.85	0.42
2:J:1:DG:H2''	2:J:2:DA:H5'	2.01	0.42
2:J:18:DC:H6	2:J:19:DA:H5'	1.85	0.42
1:M:2:DT:H2''	1:M:3:DG:OP2	2.19	0.42
2:N:19:DA:H2''	2:N:20:DA:OP2	2.20	0.42
3:P:141:VAL:HG22	3:P:170:TYR:CD1	2.55	0.42
1:E:18:DT:H3	2:F:3:DA:H61	1.67	0.42
2:F:11:DT:H2''	2:F:12:DT:H5'	2.02	0.42
2:F:11:DT:H2'	2:F:12:DT:H71	2.02	0.42
3:G:127:PRO:HG2	3:G:130:GLN:OE1	2.20	0.42
3:P:209:ASP:OD2	3:P:262:SER:OG	2.34	0.42
2:F:5:DC:H41	3:B:24:ARG:HH22	1.67	0.41
3:B:138:ASP:O	3:B:139:LEU:HB2	2.19	0.41
3:A:54:THR:HG22	3:A:85:ALA:HA	2.01	0.41
2:J:3:DA:H2''	2:J:4:DT:OP2	2.19	0.41
3:L:63:ASP:HB3	3:L:64:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:19:DT:O2	2:N:2:DA:C2	2.73	0.41
3:O:72:GLU:HB2	3:O:81:GLY:CA	2.49	0.41
3:A:115:LEU:HD12	3:A:115:LEU:HA	1.81	0.41
1:M:11:DT:H1'	1:M:12:DT:H5''	2.02	0.41
3:A:212:VAL:O	3:A:223:GLY:N	2.53	0.41
2:D:9:DA:C2	2:D:10:DA:C4	3.09	0.41
3:G:148:VAL:HB	3:G:161:LEU:HD22	2.02	0.41
3:H:132:LEU:HD22	3:H:132:LEU:HA	1.93	0.41
3:L:231:HIS:HB3	3:L:235:ALA:HB3	2.03	0.41
3:O:69:HIS:HE1	3:O:71:HIS:CD2	2.39	0.41
2:D:3:DA:C2'	2:D:4:DT:H71	2.51	0.41
3:H:69:HIS:CD2	3:H:71:HIS:H	2.39	0.41
3:K:72:GLU:HB2	3:K:81:GLY:CA	2.51	0.41
1:M:19:DT:O2	2:N:3:DA:C2	2.74	0.41
3:B:16:ARG:HH21	3:B:173:ARG:HH22	1.68	0.41
1:C:3:DG:C2	1:C:4:DA:C4	3.09	0.41
1:I:10:DA:N1	2:J:11:DT:C2	2.87	0.41
2:J:6:DG:H2''	2:J:7:DG:OP2	2.21	0.41
3:K:257:GLN:HB3	3:K:269:PRO:HA	2.02	0.41
1:E:17:DA:H2'	1:E:18:DT:H72	2.03	0.41
2:D:3:DA:H2'	2:D:4:DT:H71	2.02	0.41
3:K:56:ARG:NH1	3:K:121:ILE:HD13	2.35	0.41
3:K:124:PHE:O	3:K:125:ASN:C	2.64	0.41
1:M:2:DT:O2	2:N:19:DA:H2	1.98	0.41
3:P:94:LEU:HD23	3:P:94:LEU:HA	1.66	0.41
2:D:11:DT:H5'	3:G:19:TYR:CZ	2.55	0.41
3:G:72:GLU:HB2	3:G:81:GLY:CA	2.50	0.41
1:I:1:DT:H2'	1:I:2:DT:H71	2.02	0.41
2:J:11:DT:H5'	3:K:19:TYR:CZ	2.56	0.41
3:L:251:PRO:HB3	3:L:275:LEU:HD23	2.02	0.41
3:L:273:GLN:HE21	3:L:273:GLN:HB2	1.66	0.41
3:O:88:GLY:H	3:O:89:PRO:HD2	1.86	0.41
3:B:257:GLN:OE1	3:B:266:LEU:HD23	2.21	0.41
3:L:105:LYS:HB2	3:L:108:GLU:HG3	2.03	0.41
3:P:136:ASP:O	3:P:137:CYS:HB2	2.20	0.41
3:A:196:ASP:O	3:A:239:ARG:HA	2.20	0.40
3:A:204:LYS:HE3	3:A:233:GLN:OE1	2.20	0.40
3:B:15:MET:HE3	3:B:15:MET:HB2	1.99	0.40
3:G:115:LEU:HD12	3:G:115:LEU:HA	1.90	0.40
2:J:7:DG:C2	2:J:8:DA:C4	3.09	0.40
3:L:105:LYS:HD3	3:L:108:GLU:CD	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:11:DT:H5'	3:O:19:TYR:CE2	2.56	0.40
3:P:212:VAL:HG11	3:P:238:PHE:CZ	2.56	0.40
3:B:182:ILE:HD11	3:B:257:GLN:HA	2.02	0.40
3:B:248:LEU:O	3:B:276:PRO:HB3	2.21	0.40
2:J:11:DT:C2	2:J:12:DT:C5	3.10	0.40
2:J:12:DT:C2	2:J:13:DC:C6	3.10	0.40
3:L:34:SER:OG	3:L:39:LYS:HG3	2.21	0.40
2:N:15:DC:H42	3:O:24:ARG:HH22	1.68	0.40
3:P:72:GLU:HB2	3:P:81:GLY:CA	2.51	0.40
3:B:53:GLY:O	3:B:87:PHE:HB3	2.20	0.40
3:B:67:ARG:NH1	3:B:130:GLN:O	2.54	0.40
1:C:19:DT:H2''	1:C:20:DC:C6	2.57	0.40
3:G:62:LYS:HD2	3:G:141:VAL:HG11	2.02	0.40
3:B:64:PRO:HB3	3:P:3:TYR:HB3	2.04	0.40
3:B:93:PRO:HB2	3:B:94:LEU:H	1.70	0.40
2:J:4:DT:H2''	2:J:5:DC:OP2	2.20	0.40
3:P:153:GLU:HB3	3:P:154:HIS:H	1.62	0.40
3:P:212:VAL:O	3:P:223:GLY:N	2.54	0.40
3:A:192:CYS:HA	3:A:274:TYR:HD2	1.86	0.40
3:B:248:LEU:HB3	3:B:276:PRO:HA	2.03	0.40
3:G:99:LEU:HA	3:G:99:LEU:HD23	1.86	0.40
3:K:159:THR:O	3:K:160:ALA:HB3	2.21	0.40
3:L:17:PHE:CE2	3:L:101:ILE:HD13	2.57	0.40
1:M:3:DG:C2	2:N:19:DA:C2	3.09	0.40
3:O:208:GLU:CD	3:O:208:GLU:H	2.30	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	274/277 (99%)	244 (89%)	20 (7%)	10 (4%)	2 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	270/277 (98%)	240 (89%)	20 (7%)	10 (4%)	2	15
3	G	274/277 (99%)	242 (88%)	22 (8%)	10 (4%)	2	16
3	H	270/277 (98%)	240 (89%)	20 (7%)	10 (4%)	2	15
3	K	274/277 (99%)	244 (89%)	20 (7%)	10 (4%)	2	16
3	L	270/277 (98%)	241 (89%)	17 (6%)	12 (4%)	2	12
3	O	274/277 (99%)	242 (88%)	25 (9%)	7 (3%)	4	21
3	P	270/277 (98%)	239 (88%)	20 (7%)	11 (4%)	2	13
All	All	2176/2216 (98%)	1932 (89%)	164 (8%)	80 (4%)	2	15

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	86	GLU
3	A	87	PHE
3	A	89	PRO
3	A	134	ILE
3	B	93	PRO
3	B	137	CYS
3	B	138	ASP
3	B	152	ASP
3	B	153	GLU
3	B	224	SER
3	G	86	GLU
3	G	89	PRO
3	G	134	ILE
3	G	157	PHE
3	H	93	PRO
3	H	137	CYS
3	H	138	ASP
3	H	152	ASP
3	H	153	GLU
3	H	224	SER
3	K	86	GLU
3	K	87	PHE
3	K	89	PRO
3	K	134	ILE
3	K	153	GLU
3	K	224	SER
3	L	93	PRO
3	L	137	CYS

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Mol	Chain	Res	Type
3	L	138	ASP
3	L	152	ASP
3	L	153	GLU
3	L	224	SER
3	O	86	GLU
3	O	89	PRO
3	O	134	ILE
3	O	153	GLU
3	O	157	PHE
3	P	93	PRO
3	P	137	CYS
3	P	138	ASP
3	P	152	ASP
3	P	153	GLU
3	P	224	SER
3	A	153	GLU
3	A	224	SER
3	B	90	GLU
3	B	91	ARG
3	G	87	PHE
3	G	153	GLU
3	G	224	SER
3	H	90	GLU
3	H	91	ARG
3	K	85	ALA
3	L	24	ARG
3	L	90	GLU
3	L	91	ARG
3	L	134	ILE
3	O	87	PHE
3	P	90	GLU
3	P	91	ARG
3	P	134	ILE
3	A	136	ASP
3	A	157	PHE
3	B	223	GLY
3	G	136	ASP
3	H	134	ILE
3	H	223	GLY
3	K	136	ASP
3	K	157	PHE
3	O	136	ASP

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Mol	Chain	Res	Type
3	P	66	HIS
3	G	85	ALA
3	K	223	GLY
3	A	160	ALA
3	P	223	GLY
3	A	85	ALA
3	L	125	ASN
3	B	134	ILE
3	L	223	GLY
3	G	217	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	245/246 (100%)	219 (89%)	26 (11%)	6	26
3	B	244/246 (99%)	226 (93%)	18 (7%)	13	40
3	G	245/246 (100%)	220 (90%)	25 (10%)	7	28
3	H	244/246 (99%)	225 (92%)	19 (8%)	11	38
3	K	245/246 (100%)	219 (89%)	26 (11%)	6	26
3	L	244/246 (99%)	223 (91%)	21 (9%)	10	34
3	O	245/246 (100%)	225 (92%)	20 (8%)	10	36
3	P	244/246 (99%)	222 (91%)	22 (9%)	9	33
All	All	1956/1968 (99%)	1779 (91%)	177 (9%)	9	33

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	16	ARG
3	A	20	LYS
3	A	38	THR
3	A	47	ASN
3	A	54	THR

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Mol	Chain	Res	Type
3	A	90	GLU
3	A	94	LEU
3	A	98	ASN
3	A	115	LEU
3	A	121	ILE
3	A	126	VAL
3	A	132	LEU
3	A	136	ASP
3	A	138	ASP
3	A	150	LEU
3	A	158	THR
3	A	161	LEU
3	A	184	ARG
3	A	187	ARG
3	A	201	LEU
3	A	208	GLU
3	A	220	GLU
3	A	222	ARG
3	A	226	SER
3	A	239	ARG
3	A	262	SER
3	B	7	ILE
3	B	8	GLU
3	B	9	GLN
3	B	33	ARG
3	B	86	GLU
3	B	91	ARG
3	B	105	LYS
3	B	115	LEU
3	B	131	LEU
3	B	132	LEU
3	B	134	ILE
3	B	150	LEU
3	B	198	ILE
3	B	208	GLU
3	B	248	LEU
3	B	252	VAL
3	B	273	GLN
3	B	277	ASP
3	G	7	ILE
3	G	15	MET
3	G	16	ARG

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Mol	Chain	Res	Type
3	G	20	LYS
3	G	37	THR
3	G	38	THR
3	G	47	ASN
3	G	54	THR
3	G	90	GLU
3	G	94	LEU
3	G	98	ASN
3	G	115	LEU
3	G	126	VAL
3	G	132	LEU
3	G	136	ASP
3	G	138	ASP
3	G	150	LEU
3	G	158	THR
3	G	161	LEU
3	G	187	ARG
3	G	201	LEU
3	G	208	GLU
3	G	226	SER
3	G	239	ARG
3	G	252	VAL
3	H	3	TYR
3	H	7	ILE
3	H	8	GLU
3	H	9	GLN
3	H	33	ARG
3	H	38	THR
3	H	54	THR
3	H	64	PRO
3	H	105	LYS
3	H	115	LEU
3	H	131	LEU
3	H	132	LEU
3	H	134	ILE
3	H	150	LEU
3	H	198	ILE
3	H	208	GLU
3	H	271	GLU
3	H	273	GLN
3	H	277	ASP
3	K	7	ILE

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Mol	Chain	Res	Type
3	K	15	MET
3	K	16	ARG
3	K	20	LYS
3	K	47	ASN
3	K	54	THR
3	K	90	GLU
3	K	94	LEU
3	K	98	ASN
3	K	106	LYS
3	K	115	LEU
3	K	121	ILE
3	K	126	VAL
3	K	132	LEU
3	K	136	ASP
3	K	138	ASP
3	K	150	LEU
3	K	158	THR
3	K	161	LEU
3	K	184	ARG
3	K	187	ARG
3	K	201	LEU
3	K	207	LYS
3	K	208	GLU
3	K	220	GLU
3	K	226	SER
3	L	3	TYR
3	L	7	ILE
3	L	8	GLU
3	L	9	GLN
3	L	33	ARG
3	L	54	THR
3	L	86	GLU
3	L	91	ARG
3	L	105	LYS
3	L	115	LEU
3	L	131	LEU
3	L	132	LEU
3	L	134	ILE
3	L	150	LEU
3	L	187	ARG
3	L	198	ILE
3	L	208	GLU

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Mol	Chain	Res	Type
3	L	248	LEU
3	L	262	SER
3	L	273	GLN
3	L	277	ASP
3	O	7	ILE
3	O	15	MET
3	O	16	ARG
3	O	38	THR
3	O	47	ASN
3	O	54	THR
3	O	90	GLU
3	O	94	LEU
3	O	98	ASN
3	O	132	LEU
3	O	136	ASP
3	O	138	ASP
3	O	150	LEU
3	O	161	LEU
3	O	164	ILE
3	O	187	ARG
3	O	201	LEU
3	O	208	GLU
3	O	239	ARG
3	O	262	SER
3	P	7	ILE
3	P	8	GLU
3	P	9	GLN
3	P	33	ARG
3	P	38	THR
3	P	54	THR
3	P	86	GLU
3	P	101	ILE
3	P	105	LYS
3	P	114	ILE
3	P	115	LEU
3	P	131	LEU
3	P	132	LEU
3	P	134	ILE
3	P	150	LEU
3	P	158	THR
3	P	201	LEU
3	P	208	GLU

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Mol	Chain	Res	Type
3	P	248	LEU
3	P	262	SER
3	P	273	GLN
3	P	277	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	97	GLN
3	A	257	GLN
3	B	97	GLN
3	G	98	ASN
3	G	257	GLN
3	H	97	GLN
3	K	147	GLN
3	K	257	GLN
3	K	273	GLN
3	L	41	HIS
3	L	273	GLN
3	O	41	HIS
3	P	69	HIS
3	P	206	GLN
3	P	233	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	C	20/20 (100%)	0.78	3 (15%) 5 3	58, 73, 101, 109	0
1	E	20/20 (100%)	1.12	5 (25%) 2 1	47, 100, 151, 152	0
1	I	20/20 (100%)	-0.17	1 (5%) 34 18	49, 68, 93, 96	0
1	M	20/20 (100%)	0.01	1 (5%) 34 18	46, 76, 118, 123	0
2	D	20/20 (100%)	1.50	5 (25%) 2 1	43, 97, 119, 119	0
2	F	20/20 (100%)	1.52	4 (20%) 3 1	55, 82, 118, 121	0
2	J	20/20 (100%)	-0.27	0 100 100	39, 63, 130, 143	0
2	N	20/20 (100%)	-0.11	0 100 100	51, 71, 89, 99	0
3	A	276/277 (99%)	-0.24	1 (0%) 88 76	60, 82, 133, 168	0
3	B	274/277 (98%)	-0.17	1 (0%) 88 76	56, 83, 141, 166	0
3	G	276/277 (99%)	-0.30	0 100 100	49, 79, 135, 157	0
3	H	274/277 (98%)	-0.27	1 (0%) 88 76	48, 79, 141, 164	0
3	K	276/277 (99%)	-0.36	1 (0%) 88 76	56, 84, 128, 166	0
3	L	274/277 (98%)	-0.42	1 (0%) 88 76	45, 77, 118, 170	0
3	O	276/277 (99%)	-0.31	1 (0%) 88 76	48, 83, 125, 155	0
3	P	274/277 (98%)	-0.39	2 (0%) 84 68	51, 77, 117, 173	0
All	All	2360/2376 (99%)	-0.25	27 (1%) 78 59	39, 80, 131, 173	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	20	DA	5.4
2	F	20	DA	4.5
2	F	1	DG	4.2
2	F	19	DA	3.7
2	D	1	DG	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	19	DA	3.4
1	E	1	DT	3.3
1	C	1	DT	3.2
1	E	20	DC	3.1
2	F	18	DC	3.1
3	P	52	PRO	3.0
3	O	26	ALA	3.0
1	E	16	DG	2.7
2	D	17	DT	2.7
2	D	18	DC	2.7
1	M	1	DT	2.6
3	L	52	PRO	2.5
1	C	4	DA	2.5
1	I	1	DT	2.4
3	H	6	ILE	2.2
3	B	275	LEU	2.2
3	K	26	ALA	2.2
1	E	17	DA	2.1
1	E	15	DC	2.1
1	C	15	DC	2.1
3	A	26	ALA	2.1
3	P	132	LEU	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.