Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:23 am BST

PDB ID	:	5DQT
Title	:	Crystal Structure of Cas-DNA-22 complex
Authors	:	Wang, J.; Li, J.; Zhao, H.; Sheng, G.; Wang, M.; Yin, M.; Wang, Y.
Deposited on	:	2015-09-15
Resolution	:	3.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

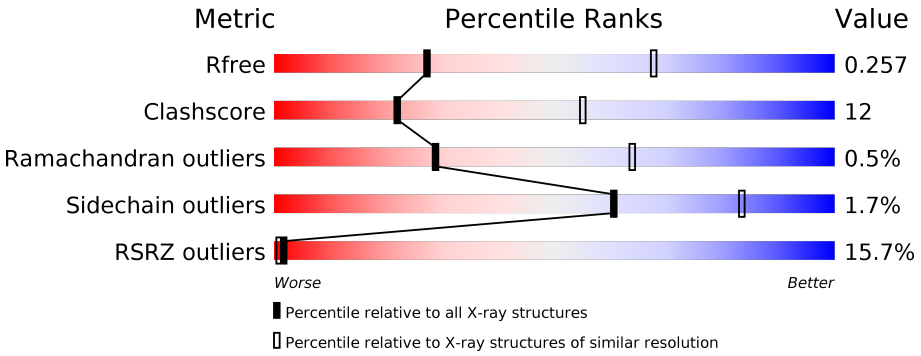
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	14% 65% 21% • 12%
1	B	305	14% 72% 18% • 9%
1	C	305	12% 70% 19% • 9%
1	D	305	16% 60% 21% •• 16%
1	I	305	20% 65% 22% 12%
1	J	305	13% 68% 23% • 8%

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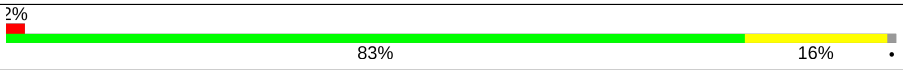
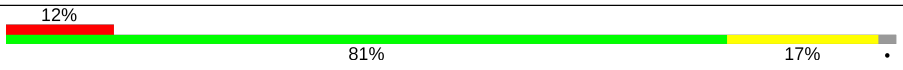
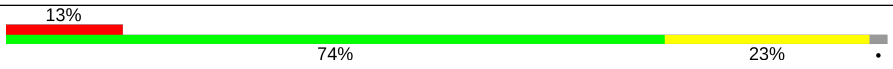
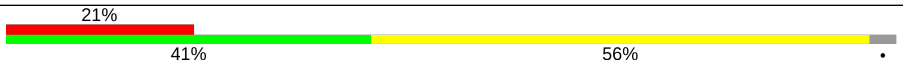
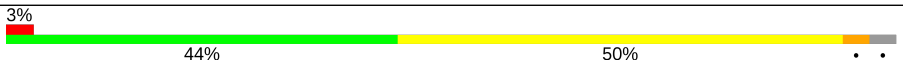
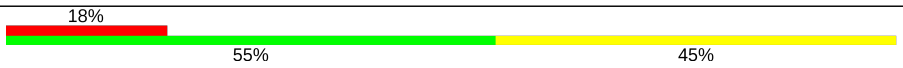
Mol	Chain	Length	Quality of chain
1	K	305	
1	L	305	
2	E	94	
2	F	94	
2	M	94	
2	N	94	
3	G	34	
3	O	34	
4	H	33	
4	P	33	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21956 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 protein called CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	255	Total	C	N	O	S	0	0	0
			1920	1230	336	347	7			
1	C	278	Total	C	N	O	S	0	0	0
			2076	1329	361	379	7			
1	A	267	Total	C	N	O	S	0	0	0
			2028	1298	356	367	7			
1	B	279	Total	C	N	O	S	0	0	0
			2128	1363	379	379	7			
1	L	267	Total	C	N	O	S	0	0	0
			1988	1272	351	358	7			
1	K	278	Total	C	N	O	S	0	0	0
			2111	1354	374	376	7			
1	I	267	Total	C	N	O	S	0	0	0
			2022	1296	355	364	7			
1	J	280	Total	C	N	O	S	0	0	0
			2121	1360	377	377	7			

- Molecule 2 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	93	Total	C	N	O	S	0	0	0
			732	470	127	131	4			
2	E	93	Total	C	N	O	S	0	0	0
			732	470	127	131	4			
2	N	92	Total	C	N	O	S	0	0	0
			722	464	126	128	4			
2	M	92	Total	C	N	O	S	0	0	0
			708	457	123	124	4			

- Molecule 3 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	33	Total	C	N	O	P	0	0	0
			671	321	106	211	33			
3	O	33	Total	C	N	O	P	0	0	0
			672	322	106	211	33			

- Molecule 4 is a DNA chain called DNA (33-MER).

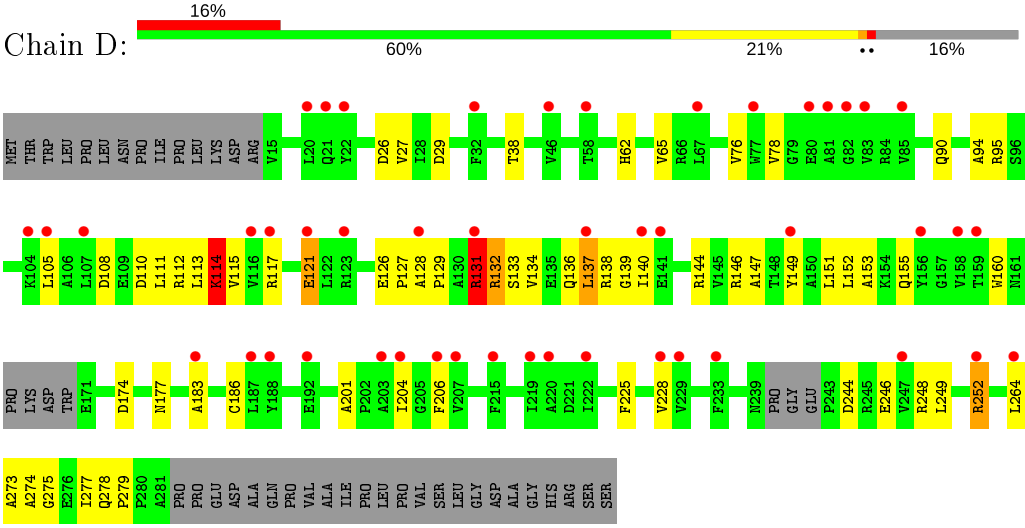
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	33	Total	C	N	O	P	0	0	0
			662	318	104	207	33			
4	P	33	Total	C	N	O	P	0	0	0
			663	319	104	207	33			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

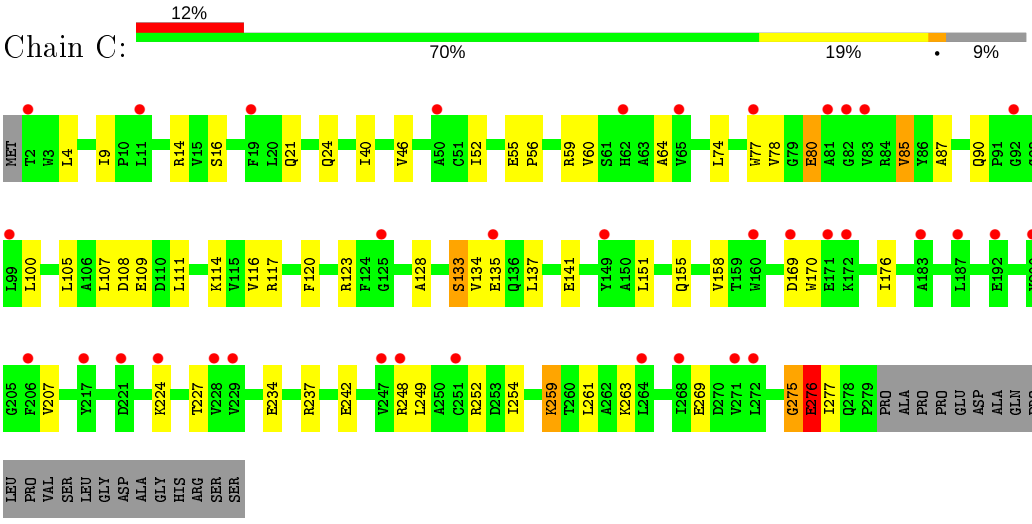
- Molecule 1: CRISPR-associated endonuclease Cas1

Chain D:



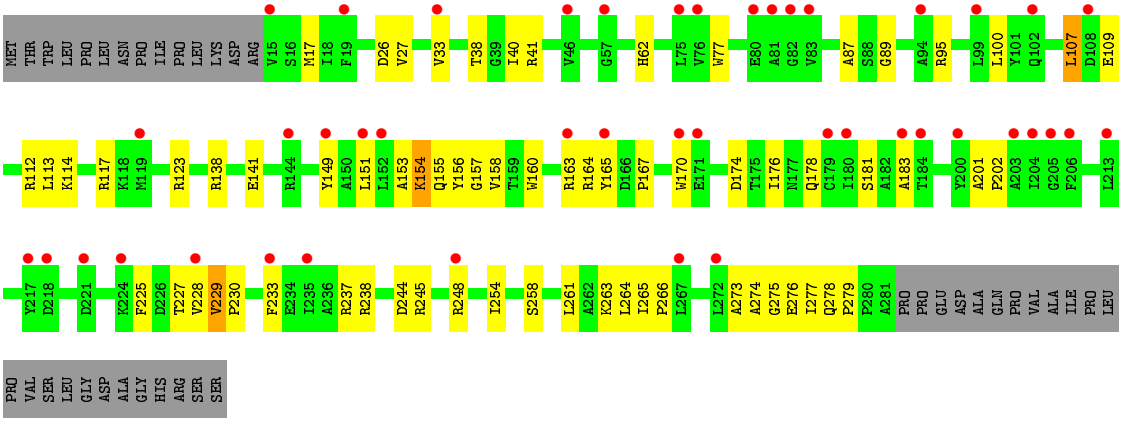
- Molecule 1: CRISPR-associated endonuclease Cas1

Chain C:



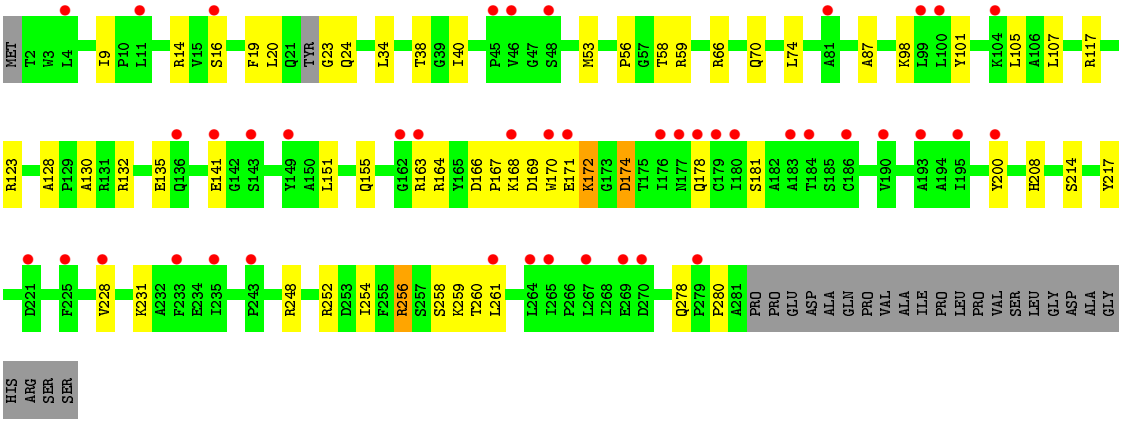
- Molecule 1: CRISPR-associated endonuclease Cas1

Chain A:



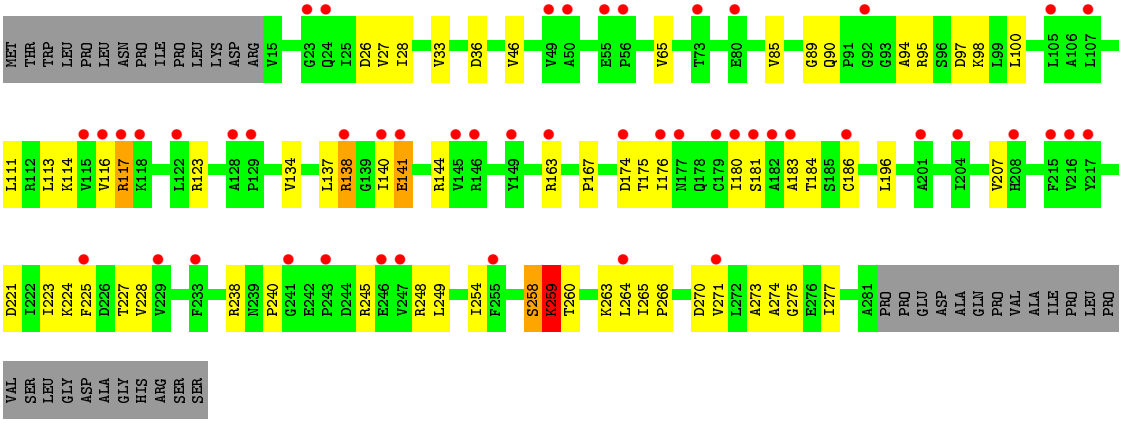
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain B:



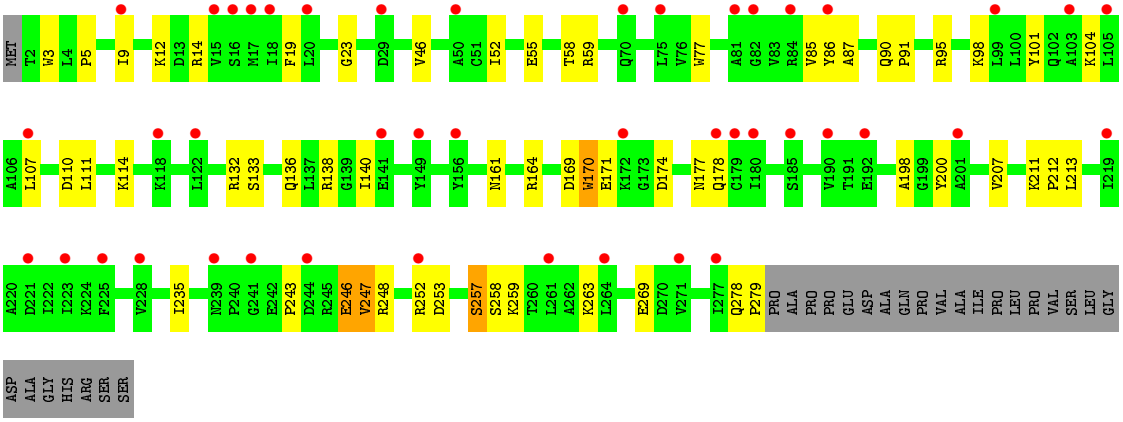
• Molecule 1: CRISPR-associated endonuclease Cas1

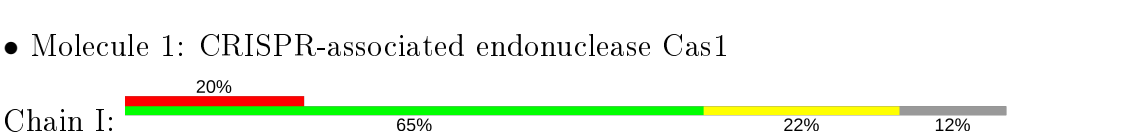
Chain L:

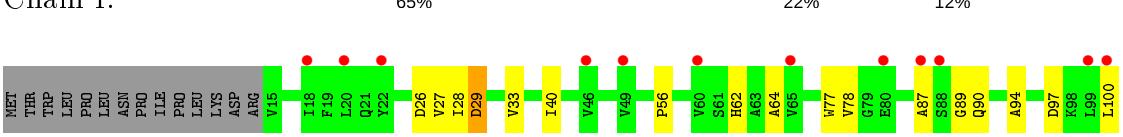


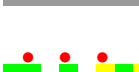
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain K:







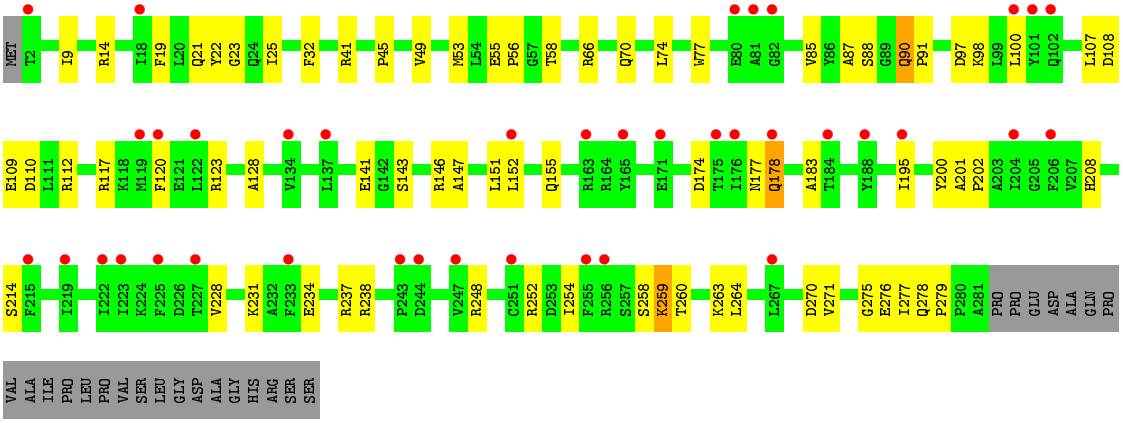


• Molecule 1: CRISPR-associated endonuclease Cas1

Chain I:

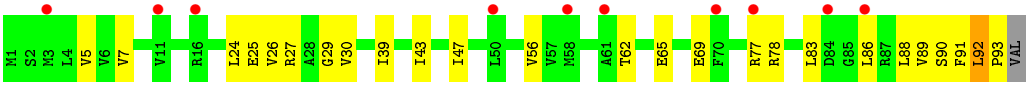
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain J:

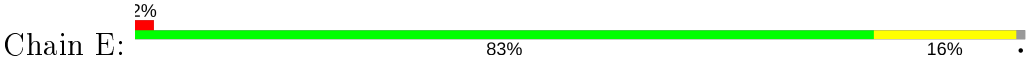


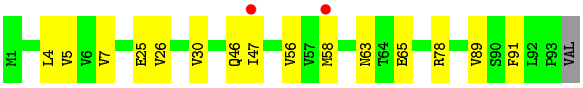
• Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain F:

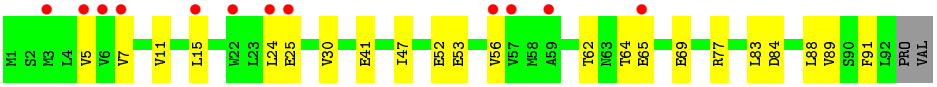


• Molecule 2: CRISPR-associated endoribonuclease Cas2

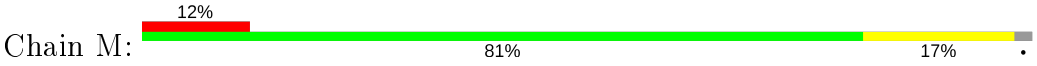


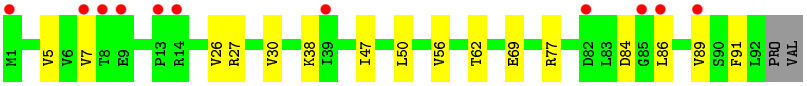


• Molecule 2: CRISPR-associated endoribonuclease Cas2

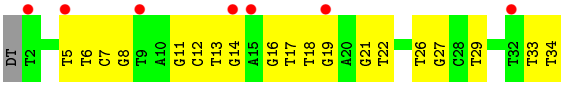


• Molecule 2: CRISPR-associated endoribonuclease Cas2

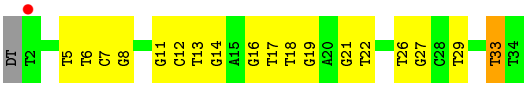




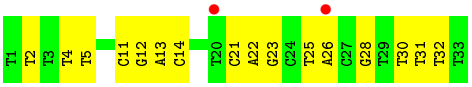
• Molecule 3: DNA (34-MER)



• Molecule 3: DNA (34-MER)

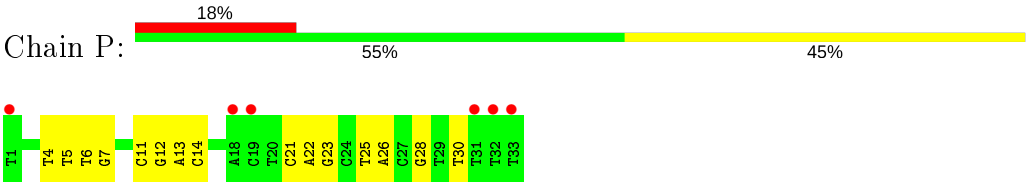


• Molecule 4: DNA (33-MER)



• Molecule 4: DNA (33-MER)

Chain P:


18%
55%
45%
T1
T4
T5
T6
G7
C11
G12
A13
C14
A18
C19
T20
C21
A22
G23
C24
T25
A26
C27
G28
T29
T30
T31
T32
T33

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.43Å 194.96Å 195.20Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	48.80 – 3.10 49.68 – 3.07	Depositor EDS
% Data completeness (in resolution range)	93.2 (48.80-3.10) 92.2 (49.68-3.07)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.211 , 0.258 0.208 , 0.257	Depositor DCC
R_{free} test set	4578 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	98.4	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 84.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.368 for -h,l,k 0.387 for -h,-l,-k 0.408 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21956	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/2068	0.66	1/2809 (0.0%)
1	B	0.42	0/2171	0.67	1/2950 (0.0%)
1	C	0.39	0/2115	0.65	4/2878 (0.1%)
1	D	0.47	0/1953	0.80	6/2650 (0.2%)
1	I	0.38	0/2062	0.70	2/2801 (0.1%)
1	J	0.37	0/2164	0.67	1/2943 (0.0%)
1	K	0.35	0/2154	0.60	0/2929
1	L	0.36	0/2025	0.68	2/2753 (0.1%)
2	E	0.37	0/746	0.62	0/1014
2	F	0.37	0/746	0.61	0/1014
2	M	0.34	0/721	0.59	0/981
2	N	0.35	0/735	0.60	0/998
3	G	0.69	0/748	1.10	0/1152
3	O	0.70	0/749	1.11	1/1154 (0.1%)
4	H	0.77	0/737	1.06	0/1132
4	P	0.70	0/738	1.04	0/1134
All	All	0.44	0/22632	0.74	18/31292 (0.1%)

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	A	0	1
1	D	0	1
1	L	0	1
All	All	0	3

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	132	ARG	NE-CZ-NH2	-10.81	114.90	120.30
1	C	275	GLY	N-CA-C	7.98	133.06	113.10
1	D	114	LYS	CD-CE-NZ	7.62	129.23	111.70
1	B	164	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	D	137	LEU	CA-CB-CG	6.41	130.05	115.30
1	L	138	ARG	NE-CZ-NH2	6.00	123.30	120.30
3	O	33	DT	P-O3'-C3'	5.89	126.77	119.70
1	C	276	GLU	C-N-CA	5.74	136.06	121.70
1	D	131	ARG	CB-CG-CD	5.67	126.35	111.60
1	C	105	LEU	CB-CG-CD2	-5.61	101.47	111.00
1	D	131	ARG	CA-CB-CG	-5.49	101.32	113.40
1	L	138	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	C	276	GLU	N-CA-C	5.42	125.63	111.00
1	D	132	ARG	N-CA-C	5.37	125.50	111.00
1	I	138	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	107	LEU	CA-CB-CG	5.31	127.52	115.30
1	I	29	ASP	CB-CG-OD1	5.18	122.97	118.30
1	J	178	GLN	CA-CB-CG	5.07	124.55	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	LYS	Peptide
1	D	131	ARG	Peptide
1	L	258	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2028	0	2063	55	0
1	B	2128	0	2173	44	1
1	C	2076	0	2100	56	0
1	D	1920	0	1961	85	0
1	I	2022	0	2061	53	0
1	J	2121	0	2167	48	0
1	K	2111	0	2156	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1988	0	2014	59	0
2	E	732	0	747	16	0
2	F	732	0	747	21	0
2	M	708	0	719	16	0
2	N	722	0	738	16	0
3	G	671	0	366	13	0
3	O	672	0	369	12	0
4	H	662	0	367	11	1
4	P	663	0	370	11	0
All	All	21956	0	21118	504	1

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 12.

All (504) 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:K:211:LYS:HD2	1:K:212:PRO:HD2	1.33	1.09
1:L:138:ARG:HA	1:L:141:GLU:HG3	1.36	1.07
1:D:114:LYS:HG2	1:D:115:VAL:N	1.73	1.03
1:L:138:ARG:HE	1:L:207:VAL:HG11	1.25	0.96
1:B:166:ASP:HB3	1:B:172:LYS:HG3	1.48	0.93
1:D:132:ARG:NH1	1:D:136:GLN:OE1	2.01	0.92
1:D:132:ARG:HH21	1:D:137:LEU:HB2	1.36	0.91
1:B:170:TRP:HE1	1:B:178:GLN:HE22	0.92	0.91
1:D:114:LYS:HD2	1:D:275:GLY:HA2	1.52	0.91
1:L:259:LYS:HE3	1:L:263:LYS:HD2	1.51	0.90
1:D:132:ARG:HH22	1:D:134:VAL:C	1.73	0.90
1:D:132:ARG:NH2	1:D:134:VAL:O	2.04	0.88
1:K:55:GLU:OE2	1:K:248:ARG:NH2	2.07	0.88
1:D:149:TYR:HE1	1:D:225:PHE:HE1	1.21	0.87
1:C:111:LEU:HD13	1:C:276:GLU:HG3	1.57	0.86
2:F:5:VAL:HG21	2:E:5:VAL:HG21	1.56	0.86
1:D:132:ARG:CZ	1:D:137:LEU:H	1.89	0.85
1:B:252:ARG:NH1	2:E:65:GLU:OE1	2.12	0.82
1:B:170:TRP:HE1	1:B:178:GLN:NE2	1.76	0.82
1:K:246:GLU:O	1:K:248:ARG:N	2.14	0.81
1:B:258:SER:O	1:B:260:THR:N	2.14	0.81
1:I:132:ARG:HH22	1:I:140:ILE:HG13	1.47	0.80
1:L:248:ARG:NH2	3:O:29:DT:OP1	2.15	0.80
1:C:276:GLU:HG2	1:C:277:ILE:HG12	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:252:ARG:NH1	2:N:84:ASP:O	2.15	0.79
1:J:41:ARG:HH12	2:M:91:PHE:HD2	1.31	0.79
1:C:276:GLU:CD	1:C:277:ILE:H	1.87	0.78
1:D:132:ARG:NH1	1:D:136:GLN:H	1.82	0.78
1:K:138:ARG:NH2	1:K:207:VAL:O	2.16	0.78
1:A:229:VAL:HG23	1:A:230:PRO:HD3	1.63	0.77
1:D:248:ARG:NH2	3:G:29:DT:OP1	2.17	0.77
1:D:114:LYS:CD	1:D:275:GLY:HA2	2.13	0.77
1:J:275:GLY:O	1:J:277:ILE:N	2.16	0.77
1:I:248:ARG:NH2	4:P:28:DG:OP1	2.18	0.76
1:C:111:LEU:HD22	1:C:276:GLU:HB3	1.67	0.76
3:O:26:DT:H2"	3:O:27:DG:H5'	1.66	0.76
3:G:26:DT:H2"	3:G:27:DG:H5'	1.68	0.76
1:A:248:ARG:NH2	4:H:28:DG:OP1	2.20	0.74
1:L:138:ARG:HA	1:L:141:GLU:CG	2.17	0.73
1:I:150:ALA:O	1:I:154:LYS:HG3	1.89	0.73
1:B:123:ARG:NH1	1:B:141:GLU:OE2	2.20	0.73
2:N:5:VAL:HG21	2:M:5:VAL:HG21	1.70	0.72
1:A:151:LEU:HG	1:A:155:GLN:HE21	1.52	0.72
1:K:98:LYS:NZ	1:K:269:GLU:OE1	2.19	0.71
1:D:132:ARG:HE	1:D:137:LEU:HB2	1.54	0.71
1:D:132:ARG:NH2	1:D:137:LEU:H	1.89	0.71
1:I:100:LEU:HB3	1:J:107:LEU:HD21	1.70	0.71
1:C:98:LYS:NZ	1:C:269:GLU:OE1	2.22	0.70
1:D:249:LEU:HB2	1:D:252:ARG:NH1	2.07	0.70
1:C:275:GLY:O	1:C:276:GLU:HB3	1.89	0.70
1:A:154:LYS:HA	1:A:157:GLY:H	1.56	0.70
1:K:170:TRP:CE3	1:K:171:GLU:HG2	2.26	0.70
1:K:211:LYS:HD2	1:K:212:PRO:CD	2.18	0.69
1:D:132:ARG:NH2	1:D:134:VAL:C	2.44	0.68
1:L:26:ASP:OD1	1:L:27:VAL:N	2.25	0.68
1:C:276:GLU:CG	1:C:277:ILE:H	2.06	0.68
1:D:249:LEU:HB2	1:D:252:ARG:HH11	1.57	0.68
1:D:149:TYR:HE1	1:D:225:PHE:CE1	2.10	0.68
4:P:4:DT:H4'	4:P:5:DT:H5'	1.75	0.68
1:C:276:GLU:OE1	1:C:276:GLU:N	2.27	0.68
1:D:132:ARG:NH2	1:D:137:LEU:HB2	2.06	0.68
1:D:246:GLU:HA	1:D:249:LEU:HG	1.75	0.68
1:I:138:ARG:HD2	1:I:138:ARG:O	1.94	0.68
1:J:9:ILE:O	1:J:14:ARG:NH1	2.28	0.67
1:C:252:ARG:NH1	2:F:65:GLU:OE1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:258:SER:O	1:L:260:THR:N	2.27	0.67
1:L:113:LEU:O	1:L:117:ARG:HG2	1.95	0.66
1:L:114:LYS:HE2	1:L:275:GLY:HA2	1.78	0.66
1:B:166:ASP:HB3	1:B:172:LYS:CG	2.25	0.66
1:J:55:GLU:OE2	1:J:248:ARG:NH2	2.23	0.65
1:B:231:LYS:HD2	1:B:254:ILE:HD11	1.77	0.65
1:D:136:GLN:OE1	1:D:136:GLN:N	2.28	0.65
1:A:157:GLY:O	1:A:237:ARG:HD3	1.97	0.65
1:D:114:LYS:HG2	1:D:115:VAL:H	1.59	0.64
1:D:129:PRO:HG2	1:D:131:ARG:HD2	1.79	0.64
1:L:275:GLY:C	1:L:277:ILE:H	1.99	0.64
1:L:174:ASP:OD1	1:L:175:THR:N	2.31	0.64
1:C:123:ARG:NH1	1:C:141:GLU:OE2	2.32	0.63
1:K:12:LYS:O	1:K:12:LYS:HD2	1.98	0.63
1:C:259:LYS:HB2	1:C:263:LYS:HE3	1.81	0.63
1:K:169:ASP:OD1	1:K:170:TRP:N	2.30	0.63
1:D:117:ARG:HG3	1:D:128:ALA:HB3	1.81	0.62
1:J:174:ASP:OD1	1:J:177:ASN:ND2	2.31	0.62
1:I:126:GLU:OE2	1:I:144:ARG:NH1	2.32	0.62
1:B:9:ILE:O	1:B:14:ARG:NH1	2.33	0.62
2:F:26:VAL:HA	2:E:89:VAL:HG11	1.83	0.61
1:A:154:LYS:HB3	1:A:157:GLY:HA2	1.82	0.61
1:B:166:ASP:O	1:B:172:LYS:HE2	2.00	0.61
1:A:154:LYS:HE3	1:A:157:GLY:HA2	1.82	0.61
1:L:114:LYS:HD2	1:L:274:ALA:O	1.99	0.61
2:F:89:VAL:HG11	2:E:26:VAL:HA	1.81	0.61
1:I:113:LEU:HD13	1:I:133:SER:HA	1.83	0.61
1:L:123:ARG:HH11	1:L:225:PHE:HE2	1.47	0.61
1:C:117:ARG:NH2	1:C:128:ALA:O	2.31	0.60
1:D:132:ARG:HG3	1:D:133:SER:N	2.15	0.60
2:F:83:LEU:HD13	2:F:88:LEU:HD12	1.82	0.60
1:D:132:ARG:HH12	1:D:136:GLN:H	1.46	0.60
1:D:132:ARG:HE	1:D:137:LEU:CB	2.14	0.60
1:D:26:ASP:OD1	1:D:27:VAL:N	2.33	0.60
1:I:156:TYR:CE2	1:I:234:GLU:HB2	2.37	0.60
1:A:138:ARG:HA	1:A:141:GLU:HG2	1.83	0.60
1:A:33:VAL:HG13	1:A:40:ILE:HG23	1.82	0.60
1:L:270:ASP:HA	1:L:273:ALA:HB3	1.84	0.60
1:D:90:GLN:HB3	1:D:94:ALA:HB2	1.84	0.59
2:F:92:LEU:HB2	2:F:93:PRO:HD3	1.83	0.59
1:D:152:LEU:HA	1:D:155:GLN:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:VAL:HG21	1:I:134:VAL:HG22	1.85	0.59
1:I:26:ASP:OD1	1:I:27:VAL:N	2.32	0.59
1:B:98:LYS:HE2	1:B:200:TYR:CZ	2.37	0.59
1:A:244:ASP:OD1	1:A:245:ARG:N	2.35	0.59
1:C:234:GLU:O	1:C:237:ARG:HG2	2.02	0.59
1:L:114:LYS:CE	1:L:275:GLY:HA2	2.32	0.58
1:J:252:ARG:HH12	2:M:86:LEU:HG	1.67	0.58
1:C:16:SER:HA	1:C:261:LEU:HD11	1.83	0.58
1:J:120:PHE:HD2	1:J:128:ALA:HB2	1.68	0.58
1:I:196:LEU:HD11	1:J:91:PRO:HB3	1.85	0.58
1:I:90:GLN:HB3	1:I:94:ALA:HB2	1.85	0.58
3:G:33:DT:H5"	3:G:34:DT:H72	1.86	0.58
1:I:33:VAL:HG13	1:I:40:ILE:HG23	1.86	0.58
1:A:174:ASP:N	1:A:174:ASP:OD1	2.32	0.58
1:I:149:TYR:HE2	1:I:163:ARG:HD3	1.68	0.58
1:K:252:ARG:NH2	2:N:65:GLU:OE1	2.29	0.58
3:O:16:DG:H1'	3:O:17:DT:H5'	1.86	0.58
3:G:16:DG:H1'	3:G:17:DT:H5'	1.85	0.57
2:N:77:ARG:HH21	2:N:91:PHE:HZ	1.50	0.57
1:B:20:LEU:HD22	1:B:34:LEU:HD22	1.86	0.57
1:A:153:ALA:HA	1:A:233:PHE:CE2	2.38	0.57
1:C:133:SER:O	1:C:137:LEU:HG	2.05	0.57
2:N:41:GLU:HG3	2:N:41:GLU:O	2.05	0.57
1:A:40:ILE:O	1:K:164:ARG:NH2	2.37	0.56
2:E:47:ILE:HD13	2:E:56:VAL:HG11	1.87	0.56
1:D:111:LEU:O	1:D:114:LYS:N	2.39	0.56
1:B:278:GLN:H	1:B:278:GLN:CD	2.08	0.56
1:C:111:LEU:HD22	1:C:275:GLY:O	2.05	0.56
4:H:13:DA:H1'	4:H:14:DC:H5'	1.87	0.56
1:J:98:LYS:HG2	1:J:200:TYR:CZ	2.41	0.56
1:D:146:ARG:HG3	1:D:147:ALA:N	2.21	0.56
1:I:151:LEU:HA	1:I:154:LYS:HD2	1.87	0.56
2:N:89:VAL:HG11	2:M:26:VAL:HA	1.88	0.56
1:I:143:SER:HA	1:I:146:ARG:HE	1.70	0.56
1:A:114:LYS:HE3	1:A:274:ALA:C	2.27	0.55
1:B:74:LEU:HD11	1:B:87:ALA:HB1	1.87	0.55
1:J:258:SER:O	1:J:260:THR:N	2.39	0.55
1:D:149:TYR:CE1	1:D:225:PHE:HE1	2.13	0.55
1:I:143:SER:O	1:I:146:ARG:HG2	2.05	0.55
1:J:98:LYS:NZ	1:J:200:TYR:OH	2.40	0.55
1:B:130:ALA:O	1:B:132:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:258:SER:C	1:L:259:LYS:HG3	2.26	0.55
1:A:151:LEU:O	1:A:155:GLN:HG3	2.06	0.55
1:C:108:ASP:OD1	1:C:111:LEU:HG	2.06	0.55
1:D:132:ARG:NE	1:D:137:LEU:HB2	2.22	0.55
1:C:109:GLU:OE1	1:C:109:GLU:N	2.40	0.55
1:K:9:ILE:O	1:K:14:ARG:NH1	2.39	0.55
1:B:98:LYS:HG2	1:B:280:PRO:HG2	1.89	0.55
1:C:276:GLU:CG	1:C:277:ILE:N	2.70	0.55
1:L:95:ARG:NH1	1:L:98:LYS:HE3	2.22	0.55
1:C:249:LEU:HD12	1:C:252:ARG:HH21	1.72	0.54
1:A:163:ARG:NH2	1:A:181:SER:OG	2.39	0.54
1:B:166:ASP:CB	1:B:172:LYS:HG3	2.30	0.54
1:A:154:LYS:HA	1:A:157:GLY:N	2.21	0.54
1:C:24:GLN:HB3	1:C:59:ARG:HH21	1.73	0.54
1:I:77:TRP:HB2	1:I:87:ALA:HB3	1.88	0.54
1:J:21:GLN:HG3	1:J:22:TYR:HB2	1.90	0.54
1:D:121:GLU:HG2	1:D:127:PRO:HA	1.89	0.54
1:J:110:ASP:OD1	1:J:110:ASP:N	2.40	0.54
1:D:132:ARG:NH2	1:D:137:LEU:N	2.56	0.54
1:L:36:ASP:OD2	4:P:5:DT:H4'	2.07	0.54
1:L:85:VAL:HG12	1:K:91:PRO:HG2	1.89	0.53
1:L:90:GLN:HB3	1:L:94:ALA:HB2	1.90	0.53
1:L:97:ASP:OD1	1:L:97:ASP:N	2.42	0.53
2:N:47:ILE:HD13	2:N:56:VAL:HG11	1.91	0.53
2:N:83:LEU:HD13	2:N:88:LEU:HD12	1.91	0.53
1:C:176:ILE:HD12	1:C:176:ILE:H	1.72	0.53
2:N:25:GLU:O	2:M:89:VAL:HG21	2.08	0.53
4:P:21:DC:H2"	4:P:22:DA:C8	2.44	0.53
4:H:25:DT:H2"	4:H:26:DA:H5"	1.91	0.53
1:I:132:ARG:HH12	1:I:140:ILE:HD11	1.73	0.53
1:L:265:ILE:HB	1:L:266:PRO:HD3	1.90	0.53
1:B:40:ILE:HG23	2:E:91:PHE:O	2.09	0.53
1:D:38:THR:HG21	4:H:5:DT:H5"	1.90	0.53
1:A:167:PRO:HA	4:H:32:DT:C4	2.44	0.53
1:B:256:ARG:NH2	2:E:63:ASN:O	2.26	0.53
3:G:33:DT:H3'	3:G:34:DT:H71	1.89	0.53
3:G:5:DT:H4'	3:G:6:DT:O5'	2.09	0.53
4:H:4:DT:H4'	4:H:5:DT:H5'	1.91	0.53
2:N:30:VAL:HG11	2:M:7:VAL:HG21	1.91	0.52
1:D:151:LEU:HG	1:D:155:GLN:NE2	2.24	0.52
1:I:123:ARG:HH11	1:I:225:PHE:HE2	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:167:PRO:HA	3:O:33:DT:N3	2.23	0.52
1:C:55:GLU:OE2	1:C:248:ARG:NH2	2.43	0.52
1:D:131:ARG:CG	1:D:132:ARG:HB2	2.40	0.52
1:I:132:ARG:NH2	1:I:137:LEU:HA	2.25	0.52
2:F:62:THR:HG21	2:F:69:GLU:HG3	1.92	0.52
1:D:275:GLY:C	1:D:277:ILE:H	2.13	0.52
1:J:183:ALA:HB1	1:J:228:VAL:CG1	2.40	0.52
1:A:77:TRP:HB2	1:A:87:ALA:HB3	1.92	0.52
1:C:46:VAL:HG23	1:C:52:ILE:HD11	1.91	0.52
2:F:7:VAL:HG21	2:E:30:VAL:HG11	1.92	0.52
1:A:237:ARG:HB3	1:A:238:ARG:HH11	1.74	0.51
1:D:137:LEU:O	1:D:140:ILE:N	2.43	0.51
1:L:137:LEU:HB3	1:L:141:GLU:OE2	2.10	0.51
1:B:163:ARG:NH2	1:B:181:SER:OG	2.38	0.51
1:I:258:SER:O	1:I:263:LYS:HE3	2.11	0.51
1:I:156:TYR:HE2	1:I:234:GLU:HB2	1.74	0.51
1:I:28:ILE:O	1:I:29:ASP:HB3	2.11	0.51
4:P:13:DA:H1'	4:P:14:DC:H5'	1.93	0.51
1:B:24:GLN:OE1	1:B:59:ARG:NH2	2.44	0.51
1:D:132:ARG:HE	1:D:137:LEU:CG	2.24	0.51
2:F:47:ILE:HD13	2:F:56:VAL:HG11	1.93	0.51
2:M:47:ILE:HD13	2:M:56:VAL:HG11	1.93	0.51
1:B:66:ARG:O	1:B:70:GLN:HG3	2.11	0.51
1:C:133:SER:OG	1:C:134:VAL:N	2.39	0.51
1:C:111:LEU:CD1	1:C:276:GLU:HG3	2.35	0.51
3:G:33:DT:H4'	3:G:34:DT:OP2	2.11	0.51
4:P:11:DC:H2"	4:P:12:DG:C8	2.46	0.51
1:K:211:LYS:HG3	1:K:213:LEU:H	1.76	0.51
1:J:252:ARG:NH1	2:M:86:LEU:HG	2.26	0.51
1:D:111:LEU:O	1:D:114:LYS:HD3	2.11	0.50
1:I:265:ILE:HB	1:I:266:PRO:HD3	1.93	0.50
1:A:123:ARG:HH11	1:A:225:PHE:HE2	1.59	0.50
1:C:151:LEU:O	1:C:155:GLN:HG3	2.11	0.50
1:I:131:ARG:NE	1:I:132:ARG:HD3	2.26	0.50
2:F:30:VAL:HG11	2:E:7:VAL:HG21	1.93	0.50
2:N:24:LEU:HD11	2:M:89:VAL:H	1.77	0.50
1:D:132:ARG:NH1	1:D:136:GLN:N	2.58	0.50
4:P:4:DT:H4'	4:P:5:DT:C5'	2.40	0.50
1:K:278:GLN:CD	1:K:279:PRO:HD2	2.32	0.50
1:L:245:ARG:NH2	1:L:249:LEU:HD11	2.26	0.50
4:H:30:DT:H4'	4:H:31:DT:O5'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:132:ARG:HH12	1:I:140:ILE:CD1	2.25	0.50
1:L:254:ILE:O	1:L:258:SER:OG	2.27	0.50
4:P:25:DT:H2"	4:P:26:DA:H5"	1.94	0.50
4:H:21:DC:H2"	4:H:22:DA:C8	2.47	0.50
1:B:24:GLN:HB3	1:B:59:ARG:HH21	1.75	0.49
4:P:6:DT:H2"	4:P:7:DG:C8	2.47	0.49
1:D:126:GLU:OE1	1:D:144:ARG:NH1	2.43	0.49
1:D:117:ARG:HH21	1:D:132:ARG:HB3	1.76	0.49
1:J:231:LYS:HB2	1:J:254:ILE:HD11	1.93	0.49
1:J:19:PHE:HB2	2:M:84:ASP:OD2	2.12	0.49
1:D:133:SER:OG	1:D:134:VAL:N	2.44	0.49
1:L:100:LEU:HB3	1:K:107:LEU:HD21	1.95	0.49
1:A:113:LEU:O	1:A:117:ARG:HG3	2.13	0.49
1:A:154:LYS:HG2	1:A:158:VAL:O	2.12	0.49
1:A:183:ALA:HB1	1:A:228:VAL:HG13	1.94	0.49
2:F:89:VAL:HG21	2:E:25:GLU:O	2.12	0.49
1:I:97:ASP:N	1:I:97:ASP:OD1	2.46	0.49
1:I:129:PRO:C	1:I:131:ARG:H	2.15	0.49
2:N:62:THR:HG21	2:N:69:GLU:HG3	1.94	0.49
1:A:258:SER:O	1:A:263:LYS:HE2	2.12	0.48
1:L:94:ALA:O	1:K:212:PRO:HG3	2.12	0.48
4:H:11:DC:H2"	4:H:12:DG:C8	2.48	0.48
1:J:25:ILE:HG21	1:J:32:PHE:CZ	2.49	0.48
1:K:101:TYR:CZ	1:K:279:PRO:HG3	2.48	0.48
1:B:231:LYS:HB2	1:B:254:ILE:HD11	1.95	0.48
1:B:16:SER:HA	1:B:261:LEU:HD11	1.96	0.48
1:J:74:LEU:HD11	1:J:87:ALA:HB1	1.95	0.48
1:A:164:ARG:HA	1:A:164:ARG:HD2	1.50	0.48
1:I:174:ASP:OD1	1:I:174:ASP:N	2.39	0.48
1:D:114:LYS:HG3	1:D:274:ALA:O	2.13	0.48
2:F:25:GLU:O	2:E:89:VAL:HG21	2.13	0.48
1:I:150:ALA:HB1	1:I:154:LYS:HE3	1.95	0.48
1:J:123:ARG:NH1	1:J:141:GLU:OE1	2.47	0.48
1:L:181:SER:HA	1:L:184:THR:H	1.79	0.48
1:L:270:ASP:OD1	1:L:271:VAL:N	2.47	0.48
1:A:201:ALA:HA	1:A:202:PRO:HD3	1.79	0.47
1:C:276:GLU:HG2	1:C:277:ILE:CG1	2.39	0.47
1:I:109:GLU:HA	1:I:112:ARG:HB3	1.96	0.47
1:L:28:ILE:HD12	1:L:33:VAL:HG21	1.96	0.47
1:D:204:ILE:HG23	1:C:100:LEU:HD21	1.96	0.47
2:M:62:THR:HG21	2:M:69:GLU:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASP:OD1	1:A:27:VAL:N	2.39	0.47
1:D:105:LEU:HD13	1:D:114:LYS:HZ3	1.79	0.47
3:O:7:DC:H2"	3:O:8:DG:C8	2.49	0.47
1:A:225:PHE:CD1	1:A:229:VAL:HG21	2.49	0.47
1:J:234:GLU:O	1:J:237:ARG:HG2	2.14	0.47
1:D:95:ARG:HB3	1:D:97:ASP:OD1	2.15	0.47
1:I:138:ARG:HA	1:I:141:GLU:CD	2.35	0.47
1:K:46:VAL:HG23	1:K:52:ILE:HD11	1.96	0.47
1:L:183:ALA:HB1	1:L:228:VAL:HG13	1.97	0.47
1:A:265:ILE:HB	1:A:266:PRO:HD3	1.97	0.47
1:C:227:THR:HB	1:C:254:ILE:HG21	1.96	0.47
1:K:178:GLN:HE21	1:K:243:PRO:HG3	1.80	0.47
1:D:273:ALA:C	1:D:275:GLY:H	2.18	0.46
1:I:27:VAL:HG23	1:I:64:ALA:HA	1.97	0.46
1:A:38:THR:HG22	1:K:161:ASN:O	2.15	0.46
1:D:275:GLY:O	1:D:277:ILE:N	2.44	0.46
1:J:143:SER:HA	1:J:146:ARG:NH1	2.30	0.46
1:L:95:ARG:NH2	1:L:97:ASP:OD2	2.47	0.46
1:B:23:GLY:O	1:B:58:THR:HA	2.14	0.46
1:B:19:PHE:CZ	1:B:53:MET:HG3	2.51	0.46
1:C:275:GLY:O	1:C:276:GLU:CB	2.59	0.46
1:C:9:ILE:O	1:C:14:ARG:NH1	2.48	0.46
1:I:183:ALA:HB1	1:I:228:VAL:CG1	2.45	0.46
1:K:278:GLN:OE1	1:K:279:PRO:HD2	2.15	0.46
2:M:38:LYS:HG2	2:M:38:LYS:H	1.56	0.46
1:B:248:ARG:O	1:B:252:ARG:HG3	2.14	0.46
1:J:23:GLY:O	1:J:58:THR:HA	2.16	0.46
1:J:74:LEU:HD12	1:J:88:SER:O	2.16	0.46
1:D:131:ARG:HG3	1:D:132:ARG:HB2	1.98	0.46
1:D:111:LEU:CA	1:D:114:LYS:HD3	2.46	0.46
2:F:27:ARG:HB2	2:F:30:VAL:HB	1.98	0.46
1:D:186:CYS:SG	1:D:248:ARG:HG3	2.56	0.46
1:D:174:ASP:OD1	1:D:177:ASN:HB2	2.16	0.46
2:F:24:LEU:HD11	2:E:89:VAL:HG22	1.97	0.46
1:I:132:ARG:NH2	1:I:140:ILE:HG13	2.23	0.46
1:C:116:VAL:HG13	1:C:207:VAL:HG22	1.98	0.45
1:C:74:LEU:HD11	1:C:87:ALA:HB1	1.98	0.45
1:D:131:ARG:HH12	1:D:140:ILE:HD11	1.81	0.45
1:L:163:ARG:NH2	1:L:181:SER:OG	2.49	0.45
4:H:22:DA:H2"	4:H:23:DG:C8	2.51	0.45
1:I:62:HIS:CG	1:J:56:PRO:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:TYR:O	1:A:237:ARG:HG2	2.16	0.45
3:O:21:DG:H2"	3:O:22:DT:O5'	2.17	0.45
1:I:231:LYS:HD2	1:I:231:LYS:H	1.82	0.45
1:J:147:ALA:O	1:J:151:LEU:HD13	2.16	0.45
1:J:19:PHE:CZ	1:J:53:MET:HG3	2.51	0.45
1:D:114:LYS:HG3	1:D:275:GLY:HA2	1.99	0.45
1:D:183:ALA:HB1	1:D:228:VAL:CG1	2.46	0.45
1:J:152:LEU:HA	1:J:155:GLN:OE1	2.16	0.45
1:L:196:LEU:HD11	1:K:91:PRO:HB3	1.97	0.45
1:C:158:VAL:HG11	1:C:176:ILE:HG12	1.98	0.45
1:K:132:ARG:HG3	1:K:133:SER:H	1.81	0.45
1:K:23:GLY:O	1:K:58:THR:HA	2.16	0.45
1:C:60:VAL:HG12	1:C:64:ALA:HB3	1.98	0.45
2:N:64:THR:HG21	2:N:69:GLU:OE2	2.17	0.45
1:A:114:LYS:HE2	1:A:276:GLU:HB2	1.98	0.45
1:D:114:LYS:HD2	1:D:275:GLY:CA	2.34	0.45
1:D:97:ASP:N	1:D:97:ASP:OD1	2.49	0.45
1:K:110:ASP:N	1:K:110:ASP:OD1	2.47	0.45
1:B:151:LEU:O	1:B:155:GLN:HG3	2.17	0.45
1:K:248:ARG:O	1:K:252:ARG:HG3	2.16	0.45
1:L:223:ILE:HD13	1:L:264:LEU:HD21	1.98	0.45
1:I:149:TYR:HE1	1:I:225:PHE:CE1	2.35	0.45
1:A:100:LEU:HB3	1:B:107:LEU:HD21	2.00	0.44
1:A:165:TYR:CD1	1:A:167:PRO:HD3	2.53	0.44
1:K:235:ILE:HD13	1:K:247:VAL:H	1.82	0.44
1:B:117:ARG:NH2	1:B:128:ALA:O	2.45	0.44
1:C:116:VAL:HG11	1:C:137:LEU:HD11	2.00	0.44
1:D:114:LYS:CG	1:D:275:GLY:HA2	2.47	0.44
2:F:77:ARG:CZ	2:F:93:PRO:HD2	2.48	0.44
3:G:18:DT:H2"	3:G:19:DG:H5'	2.00	0.44
1:A:170:TRP:CZ2	1:A:178:GLN:HB2	2.52	0.44
1:A:17:MET:SD	1:A:261:LEU:HD22	2.58	0.44
1:K:95:ARG:NH1	1:K:98:LYS:HD2	2.32	0.44
1:A:165:TYR:HD1	1:A:167:PRO:HD3	1.83	0.44
1:A:275:GLY:C	1:A:277:ILE:H	2.21	0.44
1:B:166:ASP:HB3	1:B:172:LYS:CD	2.48	0.44
2:E:78:ARG:NH2	2:E:91:PHE:HZ	2.15	0.44
1:J:55:GLU:HG2	1:J:56:PRO:HD2	1.99	0.44
1:K:258:SER:O	1:K:263:LYS:HE3	2.18	0.44
1:L:180:ILE:O	1:L:184:THR:HG23	2.16	0.44
1:A:227:THR:HB	1:A:254:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:GLN:HB3	1:C:59:ARG:NH2	2.32	0.44
1:I:151:LEU:HA	1:I:154:LYS:CD	2.47	0.44
1:L:123:ARG:NH1	1:L:225:PHE:HE2	2.12	0.44
1:C:120:PHE:CD1	1:C:128:ALA:HB2	2.52	0.44
1:I:149:TYR:HD2	1:I:160:TRP:CZ2	2.36	0.44
1:L:264:LEU:HA	1:L:264:LEU:HD23	1.68	0.44
1:A:278:GLN:HA	1:A:279:PRO:HD3	1.63	0.44
1:D:153:ALA:HB1	1:D:160:TRP:HB2	1.99	0.44
1:J:183:ALA:HB1	1:J:228:VAL:HG13	2.00	0.44
2:N:7:VAL:HG21	2:M:30:VAL:HG11	1.99	0.44
1:A:151:LEU:HG	1:A:155:GLN:NE2	2.25	0.44
3:G:33:DT:H5"	3:G:34:DT:C7	2.47	0.44
1:I:56:PRO:HD3	1:I:78:VAL:O	2.17	0.44
1:A:149:TYR:HD2	1:A:160:TRP:CZ2	2.36	0.44
1:B:169:ASP:O	1:B:172:LYS:HE3	2.17	0.44
1:C:135:GLU:H	1:C:135:GLU:CD	2.21	0.44
3:G:13:DT:H2"	3:G:14:DG:C8	2.53	0.44
3:O:5:DT:H4'	3:O:6:DT:O5'	2.18	0.44
1:D:99:LEU:HD22	1:D:201:ALA:HB2	2.00	0.43
1:A:41:ARG:CZ	1:K:164:ARG:HD3	2.48	0.43
1:D:131:ARG:HD3	1:D:132:ARG:HD3	2.01	0.43
1:D:62:HIS:CG	1:C:56:PRO:HA	2.53	0.43
1:D:110:ASP:O	1:D:113:LEU:HB3	2.18	0.43
1:D:265:ILE:HB	1:D:266:PRO:HD3	2.00	0.43
1:I:180:ILE:O	1:I:184:THR:HG23	2.18	0.43
1:I:264:LEU:HD23	1:I:264:LEU:HA	1.75	0.43
1:L:114:LYS:NZ	1:L:275:GLY:HA2	2.34	0.43
1:A:154:LYS:HE3	1:A:157:GLY:CA	2.46	0.43
1:C:55:GLU:OE2	1:C:248:ARG:CZ	2.67	0.43
1:D:264:LEU:HA	1:D:264:LEU:HD23	1.75	0.43
1:L:176:ILE:O	1:L:180:ILE:HG13	2.18	0.43
1:A:225:PHE:HA	1:A:229:VAL:CG2	2.48	0.43
2:F:39:ILE:O	2:F:43:ILE:HG13	2.18	0.43
1:K:111:LEU:HA	1:K:114:LYS:HG3	1.99	0.43
1:K:174:ASP:OD1	1:K:177:ASN:HB2	2.18	0.43
2:E:78:ARG:CZ	2:E:91:PHE:CZ	3.01	0.43
1:J:117:ARG:NH2	1:J:128:ALA:O	2.49	0.43
1:L:245:ARG:NH2	3:O:29:DT:OP1	2.52	0.43
1:J:195:ILE:HG23	1:J:200:TYR:HB2	2.01	0.43
1:J:77:TRP:O	1:J:85:VAL:HB	2.18	0.43
1:K:132:ARG:HG3	1:K:133:SER:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:30:DT:O2	4:P:30:DT:H2'	2.18	0.43
1:C:201:ALA:HA	1:C:202:PRO:HD3	1.90	0.43
1:C:97:ASP:N	1:C:97:ASP:OD1	2.52	0.43
2:F:78:ARG:CZ	2:F:91:PHE:CZ	3.02	0.43
1:L:65:VAL:HG11	1:K:77:TRP:CG	2.54	0.43
1:L:95:ARG:HB3	1:L:97:ASP:OD1	2.19	0.43
1:D:278:GLN:HA	1:D:279:PRO:HD3	1.84	0.43
1:J:259:LYS:O	1:J:263:LYS:HG3	2.19	0.43
1:B:171:GLU:N	1:B:171:GLU:CD	2.72	0.43
1:L:89:GLY:HA3	1:K:86:TYR:CE1	2.53	0.43
1:J:109:GLU:HG3	1:J:112:ARG:HD3	2.01	0.42
2:E:4:LEU:HD11	2:E:58:MET:HG3	2.01	0.42
1:L:89:GLY:HA2	1:K:87:ALA:O	2.19	0.42
1:L:263:LYS:HA	1:L:266:PRO:HD2	2.01	0.42
1:D:132:ARG:NE	1:D:137:LEU:H	2.16	0.42
3:G:7:DC:H2"	3:G:8:DG:C8	2.54	0.42
1:I:138:ARG:HA	1:I:141:GLU:OE1	2.19	0.42
1:K:19:PHE:CD1	1:K:248:ARG:HD3	2.54	0.42
2:N:11:VAL:HG21	2:N:15:LEU:HD23	2.01	0.42
2:N:52:GLU:HB3	2:N:53:GLU:H	1.48	0.42
4:P:22:DA:H2"	4:P:23:DG:C8	2.55	0.42
1:L:227:THR:HB	1:L:254:ILE:HD13	2.01	0.42
1:D:101:TYR:O	1:D:105:LEU:HG	2.20	0.42
1:J:66:ARG:O	1:J:70:GLN:HG3	2.20	0.42
1:B:105:LEU:HA	1:B:105:LEU:HD23	1.92	0.42
1:D:131:ARG:NH1	1:D:140:ILE:HD11	2.35	0.42
1:K:3:TRP:HA	2:M:50:LEU:HD21	2.01	0.42
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.76	0.42
1:B:101:TYR:CZ	1:B:105:LEU:HD11	2.55	0.42
1:C:158:VAL:CG1	1:C:176:ILE:HG12	2.50	0.42
1:J:208:HIS:O	1:J:214:SER:HB3	2.19	0.42
1:K:3:TRP:HZ3	1:K:5:PRO:HA	1.84	0.42
1:L:140:ILE:O	1:L:144:ARG:HG3	2.20	0.42
3:O:18:DT:H2"	3:O:19:DG:H5'	2.00	0.42
1:D:95:ARG:NH1	1:D:98:LYS:HE3	2.34	0.42
1:L:111:LEU:O	1:L:114:LYS:HE3	2.20	0.42
1:L:221:ASP:HA	1:L:224:LYS:HB2	2.01	0.42
2:M:77:ARG:O	2:M:91:PHE:HA	2.19	0.42
1:A:114:LYS:HE2	1:A:276:GLU:N	2.35	0.42
1:B:166:ASP:HA	1:B:167:PRO:HD3	1.68	0.42
1:C:169:ASP:OD1	1:C:170:TRP:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:LEU:HD12	2:E:46:GLN:HA	2.01	0.42
1:J:278:GLN:HA	1:J:279:PRO:HD3	1.69	0.42
1:K:98:LYS:HD3	1:K:198:ALA:O	2.19	0.42
1:D:65:VAL:HG11	1:C:77:TRP:CG	2.54	0.42
1:D:111:LEU:O	1:D:112:ARG:C	2.58	0.42
1:D:76:VAL:HG12	1:D:78:VAL:HG13	2.02	0.42
2:F:78:ARG:HA	2:F:90:SER:O	2.19	0.42
1:J:201:ALA:HA	1:J:202:PRO:HD3	1.87	0.42
1:L:137:LEU:O	1:L:141:GLU:HG3	2.19	0.42
1:I:244:ASP:OD1	1:I:244:ASP:N	2.53	0.41
1:K:136:GLN:O	1:K:140:ILE:HG13	2.20	0.41
1:K:77:TRP:O	1:K:85:VAL:HB	2.19	0.41
1:A:158:VAL:HG11	1:A:176:ILE:HB	2.02	0.41
1:D:105:LEU:HD22	1:D:114:LYS:HZ3	1.85	0.41
1:J:264:LEU:HD23	1:J:264:LEU:HA	1.89	0.41
1:J:45:PRO:O	1:J:49:VAL:HG23	2.19	0.41
1:J:98:LYS:HG2	1:J:200:TYR:CE1	2.56	0.41
1:K:259:LYS:HA	1:K:259:LYS:HD2	1.94	0.41
1:L:186:CYS:SG	1:L:248:ARG:HG3	2.61	0.41
3:G:21:DG:H2"	3:G:22:DT:O5'	2.21	0.41
1:K:58:THR:C	1:K:59:ARG:HG3	2.41	0.41
1:B:208:HIS:O	1:B:214:SER:HB3	2.21	0.41
1:C:80:GLU:H	1:C:80:GLU:CD	2.24	0.41
1:A:167:PRO:HA	4:H:32:DT:N3	2.36	0.41
1:J:252:ARG:HE	1:J:252:ARG:HB2	1.66	0.41
3:O:13:DT:H2"	3:O:14:DG:C8	2.56	0.41
1:A:154:LYS:HE3	1:A:157:GLY:C	2.41	0.41
1:D:108:ASP:OD2	1:D:111:LEU:HG	2.21	0.41
2:F:7:VAL:HA	2:F:29:GLY:O	2.20	0.41
1:D:100:LEU:HB3	1:C:107:LEU:HD21	2.02	0.41
1:D:137:LEU:C	1:D:139:GLY:N	2.73	0.41
1:B:174:ASP:OD1	1:B:174:ASP:N	2.54	0.41
1:C:78:VAL:HA	1:C:85:VAL:HG13	2.02	0.41
1:I:132:ARG:HE	1:I:136:GLN:HB3	1.84	0.41
1:K:90:GLN:HA	1:K:91:PRO:HD3	1.84	0.41
1:L:167:PRO:HA	3:O:33:DT:H3	1.84	0.41
3:G:11:DG:H2"	3:G:12:DC:O5'	2.20	0.41
1:L:116:VAL:HG21	1:L:134:VAL:HG13	2.03	0.41
1:B:135:GLU:OE1	1:B:135:GLU:N	2.39	0.41
1:A:62:HIS:CG	1:B:56:PRO:HA	2.55	0.41
1:C:252:ARG:NH1	2:F:86:LEU:HD11	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:27:ARG:HB2	2:M:30:VAL:HB	2.02	0.41
1:A:89:GLY:HA2	1:B:87:ALA:O	2.21	0.41
1:B:168:LYS:HB2	1:B:168:LYS:HE3	1.71	0.41
1:C:40:ILE:HG23	2:F:91:PHE:O	2.21	0.41
1:B:38:THR:OG1	1:B:40:ILE:HG12	2.20	0.40
1:C:111:LEU:HA	1:C:114:LYS:HG3	2.02	0.40
1:I:89:GLY:HA2	1:J:87:ALA:O	2.21	0.40
1:L:238:ARG:HG2	1:L:240:PRO:HD3	2.03	0.40
1:L:28:ILE:HB	1:L:33:VAL:HG11	2.03	0.40
1:C:248:ARG:O	1:C:252:ARG:HG3	2.20	0.40
1:D:149:TYR:CE1	1:D:225:PHE:CE1	3.00	0.40
1:D:244:ASP:OD1	1:D:244:ASP:N	2.54	0.40
1:J:270:ASP:OD1	1:J:271:VAL:N	2.55	0.40
1:J:90:GLN:HA	1:J:91:PRO:HD3	1.82	0.40
1:K:253:ASP:O	1:K:257:SER:HB3	2.21	0.40
1:L:263:LYS:C	1:L:266:PRO:HD2	2.41	0.40
1:L:275:GLY:C	1:L:277:ILE:N	2.68	0.40
1:A:109:GLU:HA	1:A:112:ARG:HB3	2.04	0.40
1:A:273:ALA:C	1:A:275:GLY:H	2.24	0.40
1:C:55:GLU:HB3	1:C:56:PRO:HD2	2.03	0.40
1:D:113:LEU:HD13	1:D:133:SER:HA	2.04	0.40
1:D:206:PHE:N	1:D:206:PHE:CD1	2.90	0.40
1:I:111:LEU:HA	1:I:114:LYS:HG3	2.02	0.40
1:I:147:ALA:O	1:I:150:ALA:HB3	2.21	0.40
1:I:204:ILE:HG23	1:J:100:LEU:HD21	2.04	0.40
1:I:187:LEU:HD21	1:I:224:LYS:HA	2.02	0.40
1:K:98:LYS:HE2	1:K:200:TYR:OH	2.22	0.40
3:O:11:DG:H2"	3:O:12:DC:O5'	2.21	0.40
1:I:275:GLY:C	1:I:277:ILE:H	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:TYR:OH	4:H:2:DT:OP1[2_846]	2.16	0.04

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	
1	A	265/305 (87%)	256 (97%)	9 (3%)	0	100	100
1	B	275/305 (90%)	260 (94%)	14 (5%)	1 (0%)	34	69
1	C	276/305 (90%)	261 (95%)	11 (4%)	4 (1%)	11	40
1	D	249/305 (82%)	238 (96%)	10 (4%)	1 (0%)	34	69
1	I	265/305 (87%)	256 (97%)	9 (3%)	0	100	100
1	J	278/305 (91%)	268 (96%)	8 (3%)	2 (1%)	22	57
1	K	276/305 (90%)	267 (97%)	7 (2%)	2 (1%)	22	57
1	L	265/305 (87%)	256 (97%)	8 (3%)	1 (0%)	34	69
2	E	91/94 (97%)	89 (98%)	2 (2%)	0	100	100
2	F	91/94 (97%)	86 (94%)	4 (4%)	1 (1%)	14	46
2	M	90/94 (96%)	86 (96%)	4 (4%)	0	100	100
2	N	90/94 (96%)	87 (97%)	3 (3%)	0	100	100
All	All	2511/2816 (89%)	2410 (96%)	89 (4%)	12 (0%)	29	64

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	131	ARG
1	C	276	GLU
1	B	259	LYS
1	L	259	LYS
1	K	246	GLU
1	K	247	VAL
1	J	259	LYS
1	J	276	GLU
2	F	92	LEU
1	C	90	GLN
1	C	259	LYS
1	C	21	GLN

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
1	A	207/245 (84%)	204 (99%)	3 (1%)	67 86
1	B	218/245 (89%)	214 (98%)	4 (2%)	59 82
1	C	211/245 (86%)	205 (97%)	6 (3%)	43 73
1	D	196/245 (80%)	191 (97%)	5 (3%)	46 74
1	I	206/245 (84%)	202 (98%)	4 (2%)	57 81
1	J	216/245 (88%)	211 (98%)	5 (2%)	50 77
1	K	216/245 (88%)	213 (99%)	3 (1%)	67 86
1	L	199/245 (81%)	195 (98%)	4 (2%)	55 80
2	E	78/79 (99%)	78 (100%)	0	100 100
2	F	78/79 (99%)	78 (100%)	0	100 100
2	M	73/79 (92%)	73 (100%)	0	100 100
2	N	76/79 (96%)	76 (100%)	0	100 100
All	All	1974/2276 (87%)	1940 (98%)	34 (2%)	60 83

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	29	ASP
1	D	114	LYS
1	D	121	GLU
1	D	138	ARG
1	D	252	ARG
1	C	80	GLU
1	C	85	VAL
1	C	133	SER
1	C	224	LYS
1	C	242	GLU
1	C	276	GLU
1	A	95	ARG
1	A	107	LEU
1	A	229	VAL

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Mol	Chain	Res	Type
1	B	172	LYS
1	B	174	ASP
1	B	228	VAL
1	B	256	ARG
1	L	46	VAL
1	L	117	ARG
1	L	141	GLU
1	L	259	LYS
1	K	104	LYS
1	K	170	TRP
1	K	257	SER
1	I	138	ARG
1	I	164	ARG
1	I	206	PHE
1	I	211	LYS
1	J	90	GLN
1	J	97	ASP
1	J	108	ASP
1	J	178	GLN
1	J	238	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	B	70	GLN
1	B	178	GLN
1	K	178	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	267/305 (87%)	0.82	44 (16%) 1 1	63, 109, 167, 194	0
1	B	279/305 (91%)	0.87	44 (15%) 2 1	61, 98, 160, 201	0
1	C	278/305 (91%)	0.81	38 (13%) 3 1	67, 101, 159, 203	0
1	D	255/305 (83%)	0.93	48 (18%) 1 0	64, 111, 161, 208	0
1	I	267/305 (87%)	1.09	61 (22%) 0 0	64, 108, 167, 209	0
1	J	280/305 (91%)	0.84	39 (13%) 2 1	63, 100, 153, 176	0
1	K	278/305 (91%)	0.88	44 (15%) 2 1	66, 100, 157, 194	0
1	L	267/305 (87%)	0.95	50 (18%) 1 0	64, 113, 159, 187	0
2	E	93/94 (98%)	0.42	2 (2%) 62 41	70, 92, 120, 148	0
2	F	93/94 (98%)	0.74	10 (10%) 5 2	67, 91, 129, 168	0
2	M	92/94 (97%)	0.78	11 (11%) 4 2	62, 91, 127, 166	0
2	N	92/94 (97%)	0.88	12 (13%) 3 1	64, 92, 128, 135	0
3	G	33/34 (97%)	1.13	7 (21%) 0 0	88, 116, 153, 155	0
3	O	33/34 (97%)	0.49	1 (3%) 50 27	91, 118, 151, 166	0
4	H	33/33 (100%)	0.69	2 (6%) 21 9	81, 115, 149, 153	0
4	P	33/33 (100%)	1.17	6 (18%) 1 0	87, 116, 147, 161	0
All	All	2673/2950 (90%)	0.87	419 (15%) 2 1	61, 104, 159, 209	0

All (419) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	82	GLY	9.3
1	B	163	ARG	8.8
1	J	81	ALA	8.2
1	D	149	TYR	8.0
1	C	81	ALA	7.8

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Mol	Chain	Res	Type	RSRZ
1	A	204	ILE	7.8
2	N	57	VAL	7.7
1	K	29	ASP	7.6
1	I	167	PRO	7.2
1	B	177	ASN	7.2
1	I	188	TYR	7.1
1	K	241	GLY	7.0
1	I	225	PHE	6.8
1	J	244	ASP	6.7
1	D	83	VAL	6.7
1	K	179	CYS	6.6
1	L	129	PRO	6.6
1	K	16	SER	6.6
1	D	82	GLY	6.5
1	L	179	CYS	6.5
1	I	185	SER	6.3
1	C	149	TYR	6.2
1	A	170	TRP	6.1
1	C	172	LYS	6.1
1	L	225	PHE	6.1
1	L	141	GLU	6.1
1	I	131	ARG	6.1
1	C	169	ASP	6.0
1	I	109	GLU	6.0
1	I	271	VAL	5.9
1	I	275	GLY	5.9
1	D	128	ALA	5.8
1	K	219	ILE	5.7
1	A	119	MET	5.5
1	I	187	LEU	5.5
1	C	171	GLU	5.4
1	D	21	GLN	5.4
1	C	251	CYS	5.4
1	L	182	ALA	5.2
1	I	22	TYR	5.2
1	J	137	LEU	5.1
1	J	243	PRO	5.0
2	M	8	THR	5.0
1	D	206	PHE	5.0
1	L	183	ALA	5.0
1	C	192	GLU	4.9
1	B	179	CYS	4.9

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Mol	Chain	Res	Type	RSRZ
2	M	14	ARG	4.9
1	A	221	ASP	4.9
1	L	271	VAL	4.9
2	M	9	GLU	4.9
1	K	81	ALA	4.9
1	I	268	ILE	4.8
1	A	76	VAL	4.8
1	A	149	TYR	4.8
1	B	81	ALA	4.8
1	L	208	HIS	4.8
1	D	32	PHE	4.7
1	B	170	TRP	4.7
1	L	80	GLU	4.7
1	C	271	VAL	4.7
1	J	102	GLN	4.7
1	I	176	ILE	4.7
3	G	2	DT	4.7
1	C	264	LEU	4.6
1	J	165	TYR	4.6
1	J	82	GLY	4.6
1	C	92	GLY	4.5
1	C	228	VAL	4.5
1	I	120	PHE	4.5
1	J	206	PHE	4.4
1	L	176	ILE	4.4
1	B	171	GLU	4.4
1	J	2	THR	4.4
4	P	33	DT	4.3
1	A	224	LYS	4.3
1	A	233	PHE	4.3
1	L	204	ILE	4.3
1	J	184	THR	4.3
1	I	274	ALA	4.3
1	B	46	VAL	4.3
1	B	233	PHE	4.3
1	C	19	PHE	4.3
1	L	50	ALA	4.3
1	A	213	LEU	4.2
1	L	246	GLU	4.2
1	B	261	LEU	4.1
1	L	241	GLY	4.1
1	D	207	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	105	LEU	4.1
1	L	122	LEU	4.1
1	A	94	ALA	4.1
1	A	99	LEU	4.1
2	N	15	LEU	4.0
2	F	11	VAL	4.0
4	P	32	DT	4.0
1	I	206	PHE	3.9
1	D	222	ILE	3.9
1	I	272	LEU	3.9
2	M	86	LEU	3.9
1	C	272	LEU	3.9
4	P	18	DA	3.9
1	J	188	TYR	3.9
1	I	174	ASP	3.9
1	B	269	GLU	3.8
1	D	58	THR	3.8
1	I	134	VAL	3.8
1	K	15	VAL	3.8
1	L	128	ALA	3.8
1	L	217	TYR	3.8
1	D	219	ILE	3.7
1	J	227	THR	3.7
1	L	107	LEU	3.7
1	J	80	GLU	3.7
2	F	84	ASP	3.7
2	N	65	GLU	3.7
1	D	220	ALA	3.7
1	K	172	LYS	3.7
1	L	181	SER	3.7
1	J	251	CYS	3.7
1	I	106	ALA	3.7
1	A	205	GLY	3.7
1	I	184	THR	3.7
1	D	228	VAL	3.7
3	G	5	DT	3.6
2	F	50	LEU	3.6
1	K	99	LEU	3.6
1	D	140	ILE	3.6
1	B	225	PHE	3.6
1	B	4	LEU	3.6
1	A	228	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	143	SER	3.6
1	L	73	THR	3.6
1	I	177	ASN	3.5
1	C	11	LEU	3.5
1	J	152	LEU	3.5
1	D	77	TRP	3.5
1	B	221	ASP	3.5
1	I	201	ALA	3.5
1	I	149	TYR	3.5
1	J	163	ARG	3.5
1	L	49	VAL	3.5
1	J	215	PHE	3.5
1	I	60	VAL	3.5
1	I	267	LEU	3.4
1	B	178	GLN	3.4
1	C	248	ARG	3.4
1	L	140	ILE	3.4
1	B	267	LEU	3.4
1	D	81	ALA	3.4
1	I	219	ILE	3.4
1	L	149	TYR	3.4
1	K	185	SER	3.4
1	A	206	PHE	3.3
1	L	177	ASN	3.3
1	C	224	LYS	3.3
1	J	122	LEU	3.3
1	D	141	GLU	3.3
1	K	239	ASN	3.3
1	D	158	VAL	3.3
1	I	102	GLN	3.2
1	C	2	THR	3.2
1	C	99	LEU	3.2
1	J	233	PHE	3.2
4	P	19	DC	3.2
1	D	203	ALA	3.2
1	K	105	LEU	3.2
1	D	156	TYR	3.1
1	I	99	LEU	3.1
1	A	80	GLU	3.1
1	C	217	TYR	3.1
1	D	107	LEU	3.1
3	G	15	DA	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	180	ILE	3.1
1	J	204	ILE	3.1
1	I	146	ARG	3.1
1	I	100	LEU	3.1
1	I	152	LEU	3.1
1	D	20	LEU	3.1
1	L	118	LYS	3.1
1	J	175	THR	3.1
1	L	243	PRO	3.1
1	J	223	ILE	3.1
1	I	65	VAL	3.1
1	K	84	ARG	3.0
1	J	178	GLN	3.0
1	I	251	CYS	3.0
1	K	178	GLN	3.0
1	B	235	ILE	3.0
1	C	94	ALA	3.0
1	K	9	ILE	3.0
1	D	183	ALA	3.0
1	D	46	VAL	3.0
1	J	18	ILE	3.0
1	C	160	TRP	3.0
1	I	141	GLU	3.0
1	K	221	ASP	3.0
2	N	25	GLU	3.0
1	A	180	ILE	2.9
1	I	18	ILE	2.9
2	E	47	ILE	2.9
1	B	48	SER	2.9
1	A	184	THR	2.9
1	L	145	VAL	2.9
1	L	201	ALA	2.9
2	N	5	VAL	2.9
2	N	7	VAL	2.9
1	K	17	MET	2.9
1	J	267	LEU	2.9
1	I	186	CYS	2.9
1	C	204	ILE	2.8
1	L	264	LEU	2.8
1	K	264	LEU	2.8
1	L	24	GLN	2.8
1	D	67	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	45	PRO	2.8
1	L	186	CYS	2.8
1	L	233	PHE	2.8
1	D	121	GLU	2.8
1	L	180	ILE	2.8
3	G	32	DT	2.8
1	K	261	LEU	2.8
1	L	146	ARG	2.8
1	A	33	VAL	2.8
1	L	23	GLY	2.8
1	K	70	GLN	2.7
1	D	233	PHE	2.7
1	A	165	TYR	2.7
1	K	149	TYR	2.7
1	D	188	TYR	2.7
1	J	219	ILE	2.7
2	M	82	ASP	2.7
1	B	183	ALA	2.7
1	B	100	LEU	2.7
1	K	20	LEU	2.7
1	A	15	VAL	2.7
1	J	256	ARG	2.7
1	I	227	THR	2.7
1	A	163	ARG	2.7
2	N	56	VAL	2.7
1	C	200	TYR	2.7
1	I	163	ARG	2.7
2	M	1	MET	2.7
1	L	55	GLU	2.7
1	K	50	ALA	2.7
1	D	270	ASP	2.7
2	M	85	GLY	2.7
1	L	247	VAL	2.6
1	B	243	PRO	2.6
2	F	16	ARG	2.6
1	A	200	TYR	2.6
1	K	192	GLU	2.6
2	M	39	ILE	2.6
1	J	225	PHE	2.6
1	L	174	ASP	2.6
1	C	65	VAL	2.6
1	I	80	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	61	ALA	2.6
1	D	85	VAL	2.6
2	F	3	MET	2.6
1	K	86	TYR	2.6
1	B	264	LEU	2.6
1	D	137	LEU	2.6
1	D	264	LEU	2.6
1	A	179	CYS	2.6
1	K	75	LEU	2.5
1	I	46	VAL	2.5
1	I	229	VAL	2.5
1	I	124	PHE	2.5
1	J	195	ILE	2.5
1	K	190	VAL	2.5
1	I	233	PHE	2.5
1	A	81	ALA	2.5
1	D	131	ARG	2.5
2	M	7	VAL	2.5
1	I	215	PHE	2.5
2	E	58	MET	2.5
1	B	16	SER	2.5
1	A	152	LEU	2.5
1	B	184	THR	2.5
1	A	218	ASP	2.5
1	L	56	PRO	2.5
2	M	13	PRO	2.5
1	B	228	VAL	2.5
1	D	204	ILE	2.5
1	B	176	ILE	2.5
2	F	58	MET	2.5
1	J	247	VAL	2.5
1	D	117	ARG	2.5
1	D	123	ARG	2.5
1	K	201	ALA	2.5
1	A	19	PHE	2.5
1	A	171	GLU	2.5
1	K	252	ARG	2.5
1	I	228	VAL	2.4
1	A	183	ALA	2.4
1	C	62	HIS	2.4
1	J	119	MET	2.4
1	B	193	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	77	TRP	2.4
1	C	50	ALA	2.4
1	A	203	ALA	2.4
1	J	101	TYR	2.4
1	A	102	GLN	2.4
1	L	92	GLY	2.4
1	L	216	VAL	2.4
1	A	248	ARG	2.4
1	A	272	LEU	2.4
1	L	163	ARG	2.4
1	C	221	ASP	2.4
1	D	104	LYS	2.4
1	B	136	GLN	2.4
1	C	83	VAL	2.4
1	D	215	PHE	2.4
1	D	229	VAL	2.4
1	K	122	LEU	2.4
1	I	20	LEU	2.4
1	A	46	VAL	2.4
1	I	255	PHE	2.4
1	B	149	TYR	2.4
2	N	6	VAL	2.3
1	B	180	ILE	2.3
1	B	279	PRO	2.3
1	A	82	GLY	2.3
1	I	148	THR	2.3
1	D	80	GLU	2.3
3	G	14	DG	2.3
1	J	222	ILE	2.3
3	G	9	DT	2.3
1	C	206	PHE	2.3
1	J	255	PHE	2.3
1	K	228	VAL	2.3
1	C	135	GLU	2.3
2	N	24	LEU	2.3
1	K	271	VAL	2.3
1	J	120	PHE	2.3
1	B	270	ASP	2.3
1	K	107	LEU	2.3
1	I	49	VAL	2.3
1	K	118	LYS	2.3
1	A	151	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	P	31	DT	2.3
1	D	247	VAL	2.3
1	B	186	CYS	2.3
1	A	235	ILE	2.3
1	D	252	ARG	2.3
1	L	117	ARG	2.3
2	N	59	ALA	2.3
1	L	105	LEU	2.3
1	K	103	ALA	2.3
1	D	187	LEU	2.3
1	L	116	VAL	2.3
2	N	22	TRP	2.2
1	B	265	ILE	2.2
2	F	86	LEU	2.2
1	C	247	VAL	2.2
1	I	191	THR	2.2
1	B	195	ILE	2.2
1	D	22	TYR	2.2
1	B	200	TYR	2.2
1	A	217	TYR	2.2
1	B	141	GLU	2.2
1	B	168	LYS	2.2
3	G	19	DG	2.2
1	K	223	ILE	2.2
1	I	235	ILE	2.2
4	H	20	DT	2.2
1	L	215	PHE	2.2
2	F	70	PHE	2.2
1	L	115	VAL	2.2
1	I	88	SER	2.2
1	I	122	LEU	2.2
4	P	1	DT	2.2
1	I	204	ILE	2.2
1	I	139	GLY	2.2
1	L	255	PHE	2.2
1	B	162	GLY	2.2
1	A	75	LEU	2.1
1	B	11	LEU	2.1
1	L	229	VAL	2.1
1	K	244	ASP	2.1
1	C	125	GLY	2.1
1	K	82	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	187	LEU	2.1
3	O	2	DT	2.1
1	A	57	GLY	2.1
2	M	89	VAL	2.1
2	N	3	MET	2.1
1	A	108	ASP	2.1
1	C	268	ILE	2.1
1	J	134	VAL	2.1
1	J	171	GLU	2.1
1	B	99	LEU	2.1
1	I	137	LEU	2.1
2	F	77	ARG	2.1
1	D	192	GLU	2.1
1	I	87	ALA	2.1
1	B	190	VAL	2.1
1	I	116	VAL	2.1
1	I	158	VAL	2.1
1	L	138	ARG	2.1
1	A	144	ARG	2.0
1	K	225	PHE	2.0
1	A	83	VAL	2.0
4	H	26	DA	2.0
1	I	170	TRP	2.0
1	C	229	VAL	2.0
1	I	128	ALA	2.0
1	D	159	THR	2.0
1	D	116	VAL	2.0
1	C	183	ALA	2.0
1	K	156	TYR	2.0
1	K	18	ILE	2.0
1	K	277	ILE	2.0
1	J	100	LEU	2.0
1	J	176	ILE	2.0
1	K	141	GLU	2.0
1	B	104	LYS	2.0
1	A	267	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.