



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:02 PM UTC

PDB ID : 1NGM / pdb_00001ngm
Title : Crystal structure of a yeast Brf1-TBP-DNA ternary complex
Authors : Juo, Z.S.; Kassavetis, G.A.; Wang, J.; Geiduschek, E.P.; Sigler, P.B.
Deposited on : 2002-12-17
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

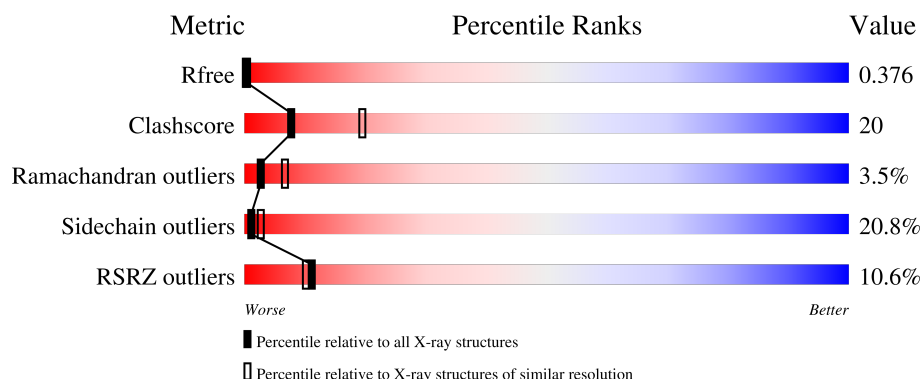
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	19	5% 16% 84%
1	G	19	42% 58%
1	K	19	5% 74% 21% 5%
1	O	19	26% 74%
2	D	19	5% 63% 37%

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Mol	Chain	Length	Quality of chain
2	H	19	 5% 42% 53%
2	L	19	 26% 47% 47% 5%
2	P	19	 16% 47% 53%
3	A	180	 9% 42% 48% 8%
3	E	180	 15% 48% 44% 7%
3	I	180	 14% 45% 42% 13%
3	M	180	 8% 44% 40% 15%
4	B	72	 8% 56% 40%
4	F	72	 7% 51% 36% 10%
4	J	72	 7% 36% 32% 6% 26%
4	N	72	 10% 57% 17% 26%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10800 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called 5'-D(*CP*TP*AP*TP*AP*AP*AP*AP*AP*AP*T
P*GP*TP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	19	Total	C	N	O	P	0	0	0
			386	189	66	113	18			
1	G	19	Total	C	N	O	P	0	0	0
			386	189	66	113	18			
1	K	19	Total	C	N	O	P	0	0	0
			386	189	66	113	18			
1	O	19	Total	C	N	O	P	0	0	0
			386	189	66	113	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	19	Total	C	N	O	P	0	0	0
			387	189	69	111	18			
2	H	19	Total	C	N	O	P	0	0	0
			387	189	69	111	18			
2	L	19	Total	C	N	O	P	0	0	0
			387	189	69	111	18			
2	P	19	Total	C	N	O	P	0	0	0
			387	189	69	111	18			

- Molecule 3 is a protein called Transcription initiation factor TFIID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	180	Total	C	N	O	S	0	0	0
			1416	921	242	247	6			
3	E	180	Total	C	N	O	S	0	0	0
			1416	921	242	247	6			
3	I	180	Total	C	N	O	S	0	0	0
			1416	921	242	247	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	180	Total	C	N	O	S	0	0	0
			1416	921	242	247	6			

- Molecule 4 is a protein called Transcription factor IIIB BRF1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	72	Total	C	N	O	S	0	0	0
			586	363	98	124	1			
4	F	72	Total	C	N	O	S	0	0	0
			586	363	98	124	1			
4	J	53	Total	C	N	O		0	0	0
			436	268	73	95				
4	N	53	Total	C	N	O		0	0	0
			436	268	73	95				

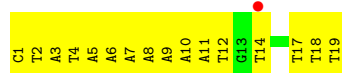
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	435	GLY	-	cloning artifact	UNP P29056
B	436	SER	-	cloning artifact	UNP P29056
F	435	GLY	-	cloning artifact	UNP P29056
F	436	SER	-	cloning artifact	UNP P29056
J	435	GLY	-	cloning artifact	UNP P29056
J	436	SER	-	cloning artifact	UNP P29056
N	435	GLY	-	cloning artifact	UNP P29056
N	436	SER	-	cloning artifact	UNP P29056

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.

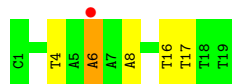
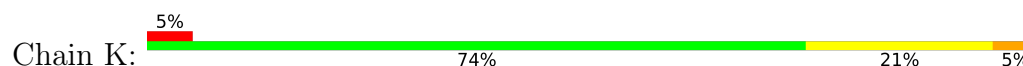
- Molecule 1: 5'-D(*CP*TP*AP*TP*AP*AP*AP*AP*AP*AP*TP*GP*TP*TP*TP*TP*TP*T P*T)-3'



- Molecule 1: 5'-D(*CP*TP*AP*TP*AP*AP*AP*AP*AP*AP*TP*GP*TP*TP*TP*TP*TP*T P*T)-3'



- Molecule 1: 5'-D(*CP*TP*AP*TP*AP*AP*AP*AP*AP*AP*TP*GP*TP*TP*TP*TP*TP*T P*T)-3'

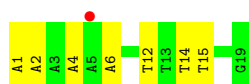


- Molecule 1: 5'-D(*CP*TP*AP*TP*AP*AP*AP*AP*AP*AP*TP*GP*TP*TP*TP*TP*TP*T P*T)-3'

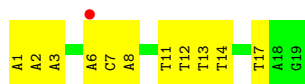
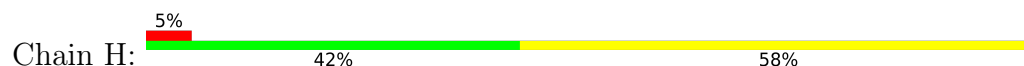


- Molecule 2: 5'-D(*AP*AP*AP*AP*AP*AP*CP*AP*TP*TP*TP*TP*TP*TP*TP*AP*TP*A P*G)-3'

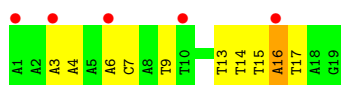




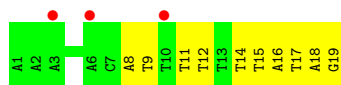
- Molecule 2: 5'-D(*AP*AP*AP*AP*AP*AP*CP*AP*TP*TP*TP*TP*TP*TP*TP*TP*AP*TP*AP*G)-3'



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



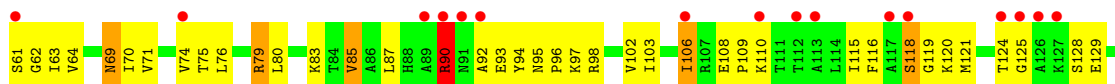
- Molecule 2: 5'-D(*AP*AP*AP*AP*AP*AP*CP*AP*TP*TP*TP*TP*TP*TP*TP*TP*AP*TP*AP*G)-3'

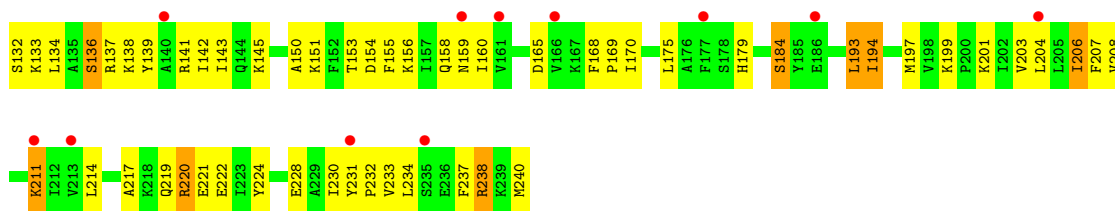


- Molecule 3: Transcription initiation factor TFIID

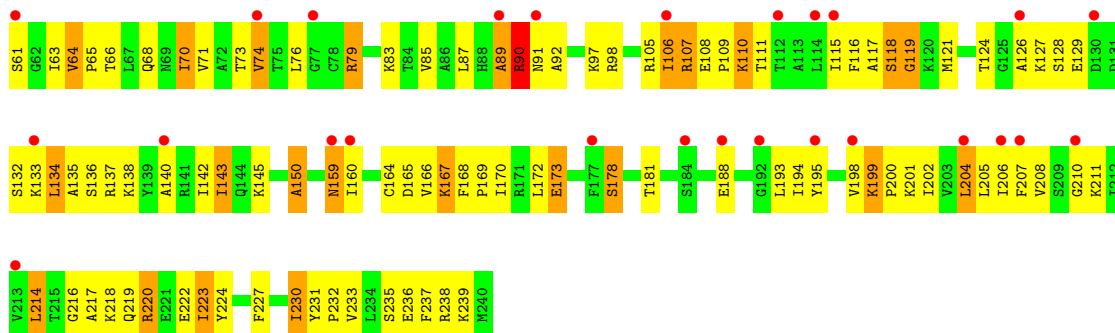
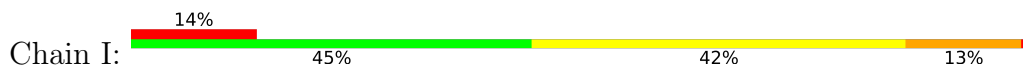


- Molecule 3: Transcription initiation factor TFIID

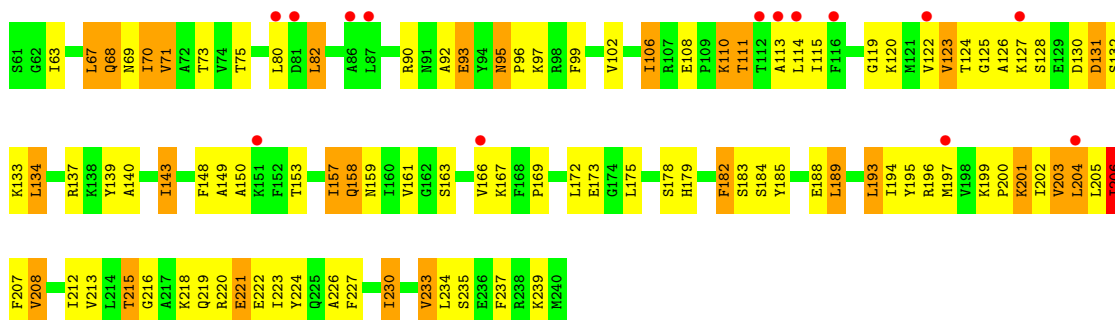
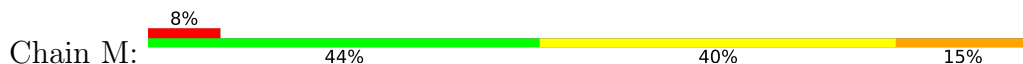




• Molecule 3: Transcription initiation factor TFIID



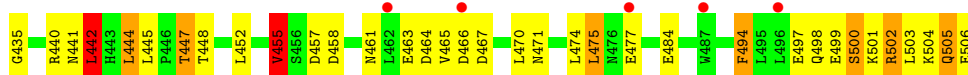
• Molecule 3: Transcription initiation factor TFIID



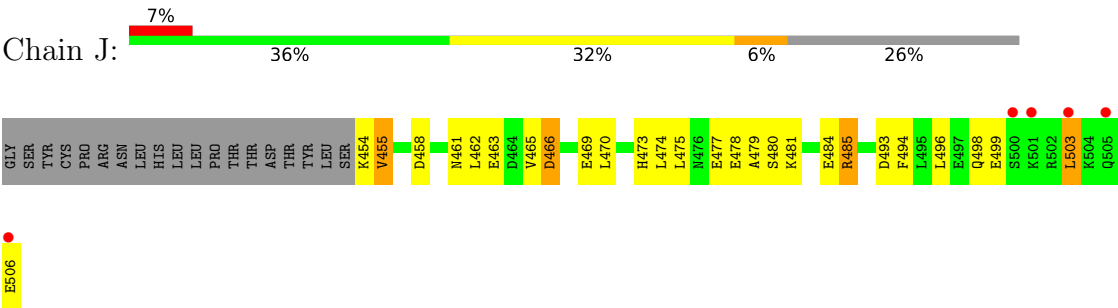
• Molecule 4: Transcription factor IIIB BRF1 subunit



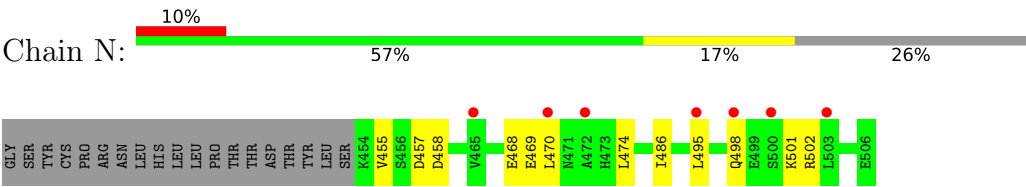
• Molecule 4: Transcription factor IIIB BRF1 subunit



● Molecule 4: Transcription factor IIIB BRF1 subunit



● Molecule 4: Transcription factor IIIB BRF1 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.61Å 152.60Å 256.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.95 50.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.95) 95.3 (50.00-2.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.96Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.276 , 0.308 0.366 , 0.376	Depositor DCC
R_{free} test set	7532 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 12.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	10800	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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 22.23 % 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 5.9524e-03.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.30	0/432	0.93	0/665
1	G	0.43	0/432	1.13	2/665 (0.3%)
1	K	0.41	0/432	1.13	1/665 (0.2%)
1	O	0.34	0/432	1.04	0/665
2	D	0.30	0/434	1.00	0/668
2	H	0.40	0/434	1.07	0/668
2	L	0.49	0/434	1.29	4/668 (0.6%)
2	P	0.34	0/434	0.87	0/668
3	A	0.55	0/1443	0.92	1/1942 (0.1%)
3	E	0.73	1/1443 (0.1%)	1.04	1/1942 (0.1%)
3	I	0.75	0/1443	1.08	0/1942
3	M	0.59	0/1443	0.93	1/1942 (0.1%)
4	B	0.47	0/595	0.90	0/804
4	F	0.67	0/595	1.04	2/804 (0.2%)
4	J	0.60	0/440	0.94	0/590
4	N	0.42	0/440	0.87	0/590
All	All	0.57	1/11306 (0.0%)	1.01	12/15888 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	240	MET	SD-CE	6.08	1.94	1.79

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	16	DA	C4'-C3'-O3'	7.09	120.64	110.00
4	F	444	LEU	N-CA-C	-6.99	105.29	114.31
4	F	455	VAL	N-CA-C	6.64	118.36	108.46
1	K	6	DA	C5'-C4'-C3'	-5.94	105.99	114.90
2	L	16	DA	N9-C1'-C2'	-5.81	104.79	113.50
2	L	16	DA	O4'-C1'-N9	5.53	116.69	108.40
1	G	9	DA	O3'-P-O5'	-5.38	95.93	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	189	LEU	N-CA-C	-5.30	107.46	114.04
2	L	9	DT	C4'-C3'-O3'	-5.29	102.06	110.00
3	A	217	ALA	N-CA-C	5.15	117.33	110.53
1	G	10	DA	C5'-C4'-O4'	5.13	117.10	109.40
3	E	69	ASN	N-CA-C	5.00	116.18	107.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	386	0	220	14	0
1	G	386	0	220	9	0
1	K	386	0	220	5	0
1	O	386	0	220	20	0
2	D	387	0	219	9	0
2	H	387	0	219	15	0
2	L	387	0	219	12	0
2	P	387	0	219	17	0
3	A	1416	0	1493	86	0
3	E	1416	0	1493	70	0
3	I	1416	0	1493	80	0
3	M	1416	0	1493	78	0
4	B	586	0	562	24	0
4	F	586	0	562	33	0
4	J	436	0	417	18	0
4	N	436	0	417	5	0
All	All	10800	0	9686	408	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 20.

All (408) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:111:THR:HG21	3:A:135:ALA:HB1	1.25	1.19
2:L:13:DT:H2''	2:L:14:DT:H5''	1.23	1.12
3:A:111:THR:HG21	3:A:135:ALA:CB	1.82	1.08
3:I:89:ALA:O	4:J:475:LEU:HG	1.62	0.99
3:I:145:LYS:HG2	4:J:474:LEU:HD11	1.45	0.98
1:G:5:DA:H5''	3:E:203:VAL:HG21	1.42	0.98
3:E:129:GLU:HG2	4:F:448:THR:HG23	1.47	0.95
3:E:90:ARG:HG2	3:E:90:ARG:HH11	1.32	0.93
3:A:129:GLU:HB2	4:B:451:TYR:HB3	1.50	0.90
3:E:79:ARG:HA	3:E:118:SER:O	1.73	0.88
3:E:156:LYS:HE3	3:E:158:GLN:HE22	1.41	0.85
4:F:435:GLY:HA2	3:I:128:SER:HB3	1.58	0.84
3:A:71:VAL:HG22	3:A:124:THR:HG22	1.64	0.79
3:M:169:PRO:HB2	3:M:239:LYS:HB3	1.65	0.79
2:L:14:DT:OP1	3:I:105:ARG:NH1	2.16	0.78
3:A:89:ALA:HA	4:B:473:HIS:O	1.82	0.78
3:A:214:LEU:HD21	3:A:226:ALA:HB3	1.64	0.78
2:L:13:DT:H2''	2:L:14:DT:C5'	2.08	0.78
3:A:115:ILE:HD12	3:A:121:MET:HB3	1.67	0.76
3:E:90:ARG:HG2	3:E:90:ARG:NH1	1.98	0.76
3:E:237:PHE:O	3:E:238:ARG:CB	2.33	0.76
3:M:82:LEU:HG	3:M:102:VAL:HG23	1.66	0.75
3:A:106:ILE:HG13	3:A:107:ARG:N	2.00	0.75
3:I:168:PHE:CD1	3:I:238:ARG:HG3	2.22	0.74
1:C:9:DA:H1'	1:C:10:DA:C8	2.23	0.73
3:A:102:VAL:HB	3:A:115:ILE:HG22	1.71	0.73
3:A:202:ILE:HG12	3:A:217:ALA:HB2	1.72	0.71
3:E:64:VAL:HG11	3:I:64:VAL:HG22	1.73	0.71
3:I:204:LEU:HD21	3:I:230:ILE:HG21	1.72	0.71
3:M:182:PHE:HD1	3:M:182:PHE:N	1.89	0.70
3:M:184:SER:HB2	3:M:194:ILE:HB	1.72	0.70
3:E:156:LYS:HE3	3:E:158:GLN:NE2	2.07	0.70
3:I:79:ARG:HA	3:I:118:SER:O	1.91	0.70
4:J:485:ARG:HG3	4:J:485:ARG:HH11	1.57	0.70
2:P:16:DA:C2	3:M:213:VAL:HG11	2.28	0.69
3:I:173:GLU:CD	3:I:173:GLU:H	2.00	0.69
3:M:206:ILE:HD13	3:M:212:ILE:HD12	1.73	0.69
3:A:111:THR:CG2	3:A:135:ALA:HB1	2.15	0.69
3:E:237:PHE:O	3:E:238:ARG:HB3	1.92	0.69
3:M:182:PHE:N	3:M:182:PHE:CD1	2.60	0.68
3:E:95:ASN:C	3:E:95:ASN:HD22	2.00	0.68
3:M:71:VAL:HB	3:M:159:ASN:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:466:ASP:HA	4:B:470:LEU:HD22	1.76	0.68
3:M:68:GLN:HG3	3:M:163:SER:HB3	1.75	0.67
3:M:133:LYS:HD2	4:N:455:VAL:CG1	2.24	0.67
3:M:99:PHE:HE2	3:M:114:LEU:HD22	1.59	0.67
3:M:183:SER:HB3	3:M:193:LEU:HD21	1.77	0.67
3:A:111:THR:CG2	3:A:135:ALA:CB	2.69	0.66
2:D:1:DA:H2''	2:D:2:DA:H5'	1.78	0.66
1:O:4:DT:H3	2:P:16:DA:H61	1.43	0.66
3:A:82:LEU:HG	3:A:117:ALA:HB2	1.78	0.66
2:H:17:DT:H5''	3:E:211:LYS:HZ2	1.61	0.65
3:A:113:ALA:HA	3:A:123:VAL:HA	1.78	0.65
3:M:195:TYR:HB3	3:M:204:LEU:HB2	1.77	0.65
3:I:74:VAL:HG11	3:I:121:MET:HE3	1.79	0.65
3:M:69:ASN:HD21	3:M:125:GLY:H	1.41	0.65
3:M:207:PHE:HE2	3:M:213:VAL:HG23	1.62	0.65
3:M:128:SER:HB3	3:M:131:ASP:HB2	1.80	0.64
1:C:19:DT:H2'	2:H:1:DA:C2	2.33	0.64
2:H:1:DA:H2'	2:H:2:DA:C8	2.32	0.64
2:P:16:DA:H2	3:M:213:VAL:HG11	1.63	0.63
3:E:90:ARG:HH11	3:E:90:ARG:CG	2.10	0.63
3:A:214:LEU:HD21	3:A:226:ALA:CB	2.27	0.63
1:O:6:DA:H2	3:M:71:VAL:HG21	1.63	0.63
1:G:5:DA:C5'	3:E:203:VAL:HG21	2.25	0.63
3:E:90:ARG:HA	4:F:475:LEU:HD21	1.81	0.63
1:G:17:DT:H2'	1:G:18:DT:C6	2.33	0.62
3:M:172:LEU:HG	3:M:208:VAL:HG13	1.79	0.62
3:A:142:ILE:O	3:A:146:ILE:HG13	2.00	0.62
4:F:435:GLY:HA2	3:I:128:SER:CB	2.28	0.62
3:I:76:LEU:HB2	3:I:119:GLY:O	2.00	0.61
3:A:111:THR:HG21	3:A:135:ALA:HB2	1.77	0.61
1:O:4:DT:H2''	1:O:5:DA:H5'	1.82	0.61
3:I:164:CYS:SG	3:I:227:PHE:CE1	2.95	0.60
3:A:91:ASN:HB2	3:A:104:MET:HA	1.83	0.60
4:F:440:ARG:HG3	4:F:440:ARG:HH11	1.65	0.60
3:A:129:GLU:HB2	4:B:451:TYR:CB	2.27	0.60
4:F:448:THR:HG22	4:F:452:LEU:CD1	2.30	0.60
3:E:76:LEU:HA	3:E:151:LYS:O	2.02	0.60
4:J:485:ARG:HG3	4:J:485:ARG:NH1	2.16	0.60
3:I:74:VAL:HG11	3:I:121:MET:CE	2.32	0.60
1:O:3:DA:H2''	1:O:4:DT:H5'	1.83	0.59
3:E:83:LYS:O	3:E:87:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:137:ARG:NH1	4:F:464:ASP:OD1	2.36	0.59
3:I:71:VAL:HG22	3:I:124:THR:HG22	1.84	0.59
2:D:12:DT:H5''	3:A:98:ARG:HD3	1.84	0.59
1:O:7:DA:H2''	1:O:8:DA:O4'	2.03	0.59
4:F:440:ARG:HD3	4:F:445:LEU:HD11	1.85	0.59
2:H:17:DT:H5''	3:E:211:LYS:NZ	2.18	0.59
1:C:7:DA:H2''	1:C:8:DA:H5'	1.84	0.58
3:E:197:MET:HE3	3:E:204:LEU:HD11	1.85	0.58
1:C:4:DT:O2	3:A:215:THR:HG21	2.03	0.58
3:M:133:LYS:HD2	4:N:455:VAL:HG11	1.85	0.58
1:O:11:DA:H61	2:P:9:DT:H3	1.52	0.58
3:M:73:THR:HG22	3:M:158:GLN:NE2	2.18	0.58
3:I:111:THR:HB	3:I:124:THR:O	2.03	0.58
2:P:11:DT:H2'	2:P:12:DT:C6	2.38	0.57
3:E:153:THR:O	3:E:154:ASP:HB2	2.02	0.57
1:K:8:DA:H1'	3:I:116:PHE:CE1	2.39	0.57
3:E:61:SER:O	3:E:63:ILE:N	2.35	0.57
3:E:106:ILE:HG22	3:E:139:TYR:CZ	2.39	0.57
3:E:133:LYS:HD3	4:F:455:VAL:HG22	1.86	0.57
1:O:13:DG:H1'	1:O:14:DT:H5''	1.87	0.57
3:A:205:LEU:HB2	3:A:213:VAL:HB	1.86	0.57
3:I:118:SER:OG	3:I:119:GLY:N	2.37	0.57
3:I:129:GLU:OE1	3:I:220:ARG:NH2	2.32	0.56
3:A:106:ILE:HD12	4:B:473:HIS:NE2	2.20	0.56
3:A:116:PHE:HE1	3:A:122:VAL:HG23	1.70	0.56
3:A:171:ARG:NH1	3:A:174:GLY:HA3	2.21	0.56
3:A:214:LEU:HD22	3:A:223:ILE:HG23	1.88	0.56
3:E:206:ILE:HD12	3:E:234:LEU:HD21	1.88	0.56
3:A:141:ARG:HH21	3:A:145:LYS:HG3	1.69	0.56
3:M:67:LEU:HD21	3:M:220:ARG:HG3	1.87	0.55
2:L:14:DT:H2''	2:L:15:DT:H5'	1.87	0.55
1:O:6:DA:C2	3:M:71:VAL:HG21	2.41	0.55
2:P:14:DT:H2''	2:P:15:DT:H5'	1.88	0.55
3:A:206:ILE:HD13	3:A:212:ILE:HG23	1.87	0.55
2:P:8:DA:H2''	2:P:9:DT:O5'	2.06	0.55
4:J:503:LEU:O	4:J:506:GLU:HB2	2.07	0.55
3:I:90:ARG:HA	4:J:475:LEU:HD21	1.89	0.55
4:J:461:ASN:ND2	4:J:463:GLU:HG3	2.21	0.55
3:E:64:VAL:HG12	3:I:66:THR:HG22	1.89	0.54
3:E:145:LYS:HD2	4:F:474:LEU:HD11	1.88	0.54
3:I:202:ILE:HD11	3:I:217:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:206:ILE:HD12	3:M:234:LEU:HD21	1.89	0.54
3:M:207:PHE:CE2	3:M:213:VAL:HG23	2.41	0.54
1:K:6:DA:C2	3:I:71:VAL:HG21	2.42	0.54
2:D:14:DT:H2''	2:D:15:DT:H5'	1.89	0.54
1:O:2:DT:H2''	1:O:3:DA:H8	1.72	0.54
3:A:70:ILE:HG12	3:A:126:ALA:O	2.07	0.54
3:I:129:GLU:CD	3:I:220:ARG:HH21	2.15	0.54
3:E:175:LEU:HD22	3:E:193:LEU:HD21	1.89	0.54
3:I:74:VAL:HG13	3:I:121:MET:HE2	1.90	0.54
3:A:70:ILE:HG23	3:A:160:ILE:HG12	1.90	0.54
3:A:134:LEU:HA	3:A:137:ARG:HB2	1.89	0.54
2:H:2:DA:H2''	2:H:3:DA:C8	2.43	0.54
3:A:163:SER:HA	3:A:212:ILE:O	2.07	0.54
3:E:74:VAL:HG21	3:E:136:SER:HB3	1.90	0.54
3:E:85:VAL:HG22	3:E:102:VAL:HG11	1.89	0.54
3:A:185:TYR:HB2	3:A:193:LEU:HD12	1.90	0.54
3:A:106:ILE:HG13	3:A:107:ARG:H	1.71	0.53
3:A:195:TYR:HD2	3:A:204:LEU:HD13	1.73	0.53
2:L:16:DA:H4'	3:I:68:GLN:HG3	1.90	0.53
1:C:17:DT:N3	2:D:4:DA:H2	2.06	0.53
3:I:231:TYR:HB3	3:I:232:PRO:HD3	1.90	0.53
2:H:1:DA:H2'	2:H:2:DA:H8	1.72	0.53
4:F:448:THR:HG22	4:F:452:LEU:HD12	1.90	0.53
3:M:71:VAL:HG22	3:M:124:THR:HG22	1.90	0.53
2:L:13:DT:C2'	2:L:14:DT:H5''	2.17	0.53
3:A:137:ARG:HG3	3:A:152:PHE:CE1	2.44	0.52
3:M:178:SER:CB	3:M:237:PHE:HZ	2.22	0.52
3:M:178:SER:HB2	3:M:237:PHE:HZ	1.74	0.52
4:J:470:LEU:O	4:J:473:HIS:HB2	2.10	0.52
1:K:16:DT:H2''	1:K:17:DT:O5'	2.09	0.52
3:A:206:ILE:HG23	3:A:212:ILE:HD12	1.92	0.52
3:M:99:PHE:CE2	3:M:114:LEU:HD22	2.44	0.52
3:M:130:ASP:O	3:M:134:LEU:HB2	2.09	0.52
3:A:166:VAL:HG21	3:A:170:ILE:HD11	1.92	0.52
3:I:109:PRO:O	3:I:111:THR:HG23	2.10	0.52
2:L:15:DT:H2''	2:L:16:DA:C8	2.45	0.52
3:A:95:ASN:HD22	3:A:98:ARG:HB2	1.75	0.52
3:A:106:ILE:HG22	3:A:139:TYR:OH	2.10	0.52
3:I:116:PHE:O	3:I:117:ALA:C	2.52	0.52
3:I:74:VAL:CG1	3:I:121:MET:HE2	2.40	0.51
3:I:129:GLU:O	3:I:132:SER:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:DT:H3	2:D:6:DA:H2	1.58	0.51
1:G:8:DA:H1'	3:E:116:PHE:CE1	2.45	0.51
2:L:17:DT:H1'	3:I:207:PHE:CZ	2.45	0.51
3:E:220:ARG:HG2	3:E:224:TYR:CE2	2.45	0.51
3:I:74:VAL:CG1	3:I:121:MET:CE	2.88	0.51
3:M:73:THR:HG22	3:M:158:GLN:HE21	1.75	0.51
3:A:155:PHE:HE2	4:B:452:LEU:HD21	1.76	0.51
3:M:137:ARG:NH2	4:N:458:ASP:O	2.43	0.51
3:A:99:PHE:CD2	3:A:101:ALA:HB3	2.45	0.51
3:E:74:VAL:HB	3:E:121:MET:HE2	1.91	0.51
3:I:97:LYS:HG3	4:J:494:PHE:HB2	1.92	0.51
3:A:88:HIS:O	3:A:89:ALA:HB2	2.11	0.50
3:E:106:ILE:HG13	3:E:108:GLU:H	1.77	0.50
3:I:87:LEU:HD13	4:J:484:GLU:HB2	1.92	0.50
3:I:204:LEU:HD23	3:I:206:ILE:HD11	1.93	0.50
3:A:140:ALA:HB3	4:B:462:LEU:HD22	1.92	0.50
3:I:235:SER:O	3:I:236:GLU:C	2.52	0.50
3:A:105:ARG:HD3	3:A:112:THR:HG23	1.92	0.50
3:E:75:THR:HG23	3:E:120:LYS:HD3	1.93	0.50
3:E:95:ASN:C	3:E:95:ASN:ND2	2.70	0.50
4:B:441:ASN:HB3	4:B:444:LEU:HD12	1.93	0.50
4:F:440:ARG:HG3	4:F:440:ARG:NH1	2.27	0.50
3:M:221:GLU:O	3:M:224:TYR:N	2.44	0.50
2:P:16:DA:H2	3:M:213:VAL:CG1	2.24	0.50
3:A:129:GLU:OE2	4:B:448:THR:HA	2.12	0.50
3:E:71:VAL:HG13	3:E:124:THR:HG22	1.92	0.50
1:C:17:DT:H2'	1:C:18:DT:C6	2.47	0.50
1:K:6:DA:H2	3:I:71:VAL:HG21	1.77	0.50
3:A:111:THR:CG2	3:A:135:ALA:HB2	2.40	0.50
3:A:137:ARG:HG2	4:B:462:LEU:HD23	1.94	0.49
3:E:133:LYS:HG3	3:E:155:PHE:CE2	2.47	0.49
1:C:5:DA:C6	1:C:6:DA:N6	2.81	0.49
3:I:143:ILE:HG22	3:I:150:ALA:HB2	1.93	0.49
3:M:133:LYS:HD2	4:N:455:VAL:HG13	1.93	0.49
3:A:129:GLU:HG2	4:B:448:THR:HG23	1.94	0.49
3:A:180:GLY:HA2	3:A:183:SER:HB2	1.94	0.49
3:M:215:THR:OG1	3:M:216:GLY:N	2.44	0.49
2:H:6:DA:C2	2:H:7:DC:C2	3.00	0.49
3:I:76:LEU:HD21	3:I:140:ALA:HA	1.94	0.49
3:I:223:ILE:HG22	3:I:224:TYR:N	2.27	0.49
2:D:14:DT:C7	2:D:15:DT:H73	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:133:LYS:HD2	4:F:452:LEU:HD23	1.95	0.49
4:F:458:ASP:OD1	4:F:461:ASN:N	2.41	0.49
4:F:504:LYS:C	4:F:506:GLU:H	2.21	0.49
3:I:61:SER:C	3:I:63:ILE:H	2.20	0.49
3:A:139:TYR:CD1	3:A:139:TYR:N	2.80	0.49
3:E:165:ASP:HB2	3:E:211:LYS:HD2	1.94	0.49
3:E:159:ASN:HA	3:E:217:ALA:O	2.13	0.49
3:A:137:ARG:HH12	4:B:462:LEU:HA	1.78	0.48
4:F:448:THR:HG22	4:F:452:LEU:HD11	1.95	0.48
2:L:16:DA:C4'	3:I:68:GLN:HG3	2.43	0.48
1:O:5:DA:H2''	1:O:6:DA:H5'	1.95	0.48
4:B:470:LEU:HA	4:B:473:HIS:HD2	1.78	0.48
3:E:94:TYR:CZ	3:E:96:PRO:HG3	2.48	0.48
3:M:223:ILE:O	3:M:226:ALA:HB3	2.13	0.48
3:A:121:MET:HG3	3:A:123:VAL:HG23	1.96	0.48
4:F:435:GLY:CA	3:I:128:SER:HB3	2.38	0.48
4:F:441:ASN:OD1	4:F:441:ASN:C	2.56	0.48
3:I:219:GLN:N	3:I:222:GLU:OE1	2.46	0.48
4:J:454:LYS:HD3	4:J:455:VAL:H	1.78	0.48
2:H:7:DC:H2''	2:H:8:DA:C8	2.49	0.48
1:O:10:DA:C2	1:O:11:DA:C6	3.01	0.48
3:A:102:VAL:HB	3:A:115:ILE:CG2	2.42	0.48
3:E:219:GLN:HG2	3:E:222:GLU:OE2	2.14	0.48
2:D:14:DT:H5''	3:A:112:THR:OG1	2.13	0.48
3:E:93:GLU:HG3	3:E:103:ILE:HB	1.95	0.48
3:E:184:SER:HB2	3:E:194:ILE:HD12	1.95	0.48
3:M:203:VAL:O	3:M:204:LEU:HD23	2.14	0.48
2:L:6:DA:C2	2:L:7:DC:C2	3.02	0.48
3:A:86:ALA:C	3:A:88:HIS:H	2.21	0.48
3:E:133:LYS:HG3	3:E:155:PHE:CD2	2.48	0.48
3:E:221:GLU:CG	4:F:447:THR:HG22	2.44	0.48
3:M:75:THR:HG23	3:M:120:LYS:HD3	1.95	0.47
3:A:195:TYR:CD2	3:A:204:LEU:HD13	2.49	0.47
3:E:69:ASN:HD21	3:E:125:GLY:H	1.62	0.47
3:E:90:ARG:HA	3:E:90:ARG:HD3	1.62	0.47
3:I:107:ARG:O	3:I:108:GLU:CG	2.61	0.47
3:M:110:LYS:O	3:M:111:THR:HG23	2.14	0.47
3:A:186:GLU:HB2	3:A:189:LEU:HB3	1.95	0.47
3:M:161:VAL:HG22	3:M:215:THR:HB	1.97	0.47
3:M:206:ILE:HG23	3:M:212:ILE:CD1	2.44	0.47
3:A:88:HIS:HA	4:B:475:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:205:LEU:O	3:A:212:ILE:HA	2.15	0.47
4:B:461:ASN:C	4:B:463:GLU:H	2.22	0.47
4:F:502:ARG:HA	4:F:505:GLN:HB2	1.97	0.47
4:F:470:LEU:C	4:F:470:LEU:HD23	2.40	0.47
3:A:88:HIS:HA	4:B:475:LEU:HD11	1.96	0.47
4:F:441:ASN:O	4:F:442:LEU:C	2.57	0.47
3:M:197:MET:HB3	3:M:202:ILE:H	1.79	0.46
1:O:6:DA:H2''	1:O:7:DA:O5'	2.15	0.46
3:A:159:ASN:HD21	3:A:216:GLY:H	1.63	0.46
3:A:217:ALA:HB3	3:A:223:ILE:HG13	1.97	0.46
1:C:7:DA:C2'	1:C:8:DA:H5'	2.45	0.46
3:A:82:LEU:O	3:A:83:LYS:C	2.58	0.46
3:I:106:ILE:HG12	3:I:108:GLU:H	1.80	0.46
3:I:217:ALA:HB3	3:I:223:ILE:HD12	1.98	0.46
3:I:70:ILE:HG23	3:I:160:ILE:HG12	1.97	0.46
3:I:195:TYR:HB3	3:I:204:LEU:HB2	1.97	0.46
2:H:14:DT:H1'	3:E:69:ASN:OD1	2.16	0.46
4:B:437:TYR:CD2	4:B:438:CYS:N	2.84	0.46
3:E:169:PRO:HA	3:E:208:VAL:O	2.15	0.46
3:E:87:LEU:HD13	4:F:484:GLU:HB2	1.97	0.46
3:M:63:ILE:HD13	3:M:166:VAL:HG12	1.97	0.46
3:E:138:LYS:HG2	4:F:470:LEU:HD12	1.98	0.46
2:H:13:DT:OP1	3:E:98:ARG:NH2	2.42	0.46
3:I:145:LYS:HB3	4:J:474:LEU:HD21	1.97	0.46
1:C:2:DT:O4	1:C:3:DA:N6	2.49	0.46
3:A:70:ILE:HG13	3:A:128:SER:O	2.16	0.46
3:I:90:ARG:HG2	3:I:91:ASN:ND2	2.31	0.46
3:I:199:LYS:HA	3:I:200:PRO:HA	1.79	0.46
3:M:140:ALA:HA	3:M:143:ILE:HD12	1.97	0.46
3:I:115:ILE:HD13	3:I:143:ILE:HD11	1.98	0.45
3:M:182:PHE:CD2	3:M:196:ARG:O	2.69	0.45
3:A:206:ILE:HG23	3:A:212:ILE:CD1	2.46	0.45
3:I:230:ILE:HG13	3:I:230:ILE:O	2.15	0.45
3:M:185:TYR:HB2	3:M:193:LEU:HD23	1.97	0.45
2:P:16:DA:C2	3:M:213:VAL:CG1	2.98	0.45
4:F:441:ASN:OD1	4:F:441:ASN:O	2.33	0.45
3:M:69:ASN:HD21	3:M:125:GLY:N	2.13	0.45
3:M:179:HIS:O	3:M:183:SER:OG	2.24	0.45
3:A:104:MET:O	3:A:112:THR:O	2.34	0.45
3:A:141:ARG:O	3:A:145:LYS:HB2	2.17	0.45
4:B:500:SER:HA	4:B:503:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:115:ILE:HG13	3:E:121:MET:HG3	1.99	0.45
1:O:6:DA:N3	3:M:71:VAL:HG11	2.32	0.45
1:O:8:DA:H61	2:P:12:DT:H3	1.65	0.45
1:O:8:DA:N6	2:P:12:DT:H3	2.14	0.45
3:I:117:ALA:O	3:I:118:SER:C	2.59	0.45
3:I:90:ARG:HB3	4:J:473:HIS:O	2.17	0.45
1:O:2:DT:H2''	1:O:3:DA:O5'	2.17	0.45
2:P:11:DT:C2'	2:P:12:DT:C6	3.00	0.45
1:C:17:DT:N3	2:D:4:DA:C2	2.85	0.44
1:K:4:DT:H5''	3:I:194:ILE:HG12	1.99	0.44
3:I:231:TYR:HB3	3:I:232:PRO:CD	2.47	0.44
4:J:463:GLU:O	4:J:466:ASP:HB2	2.17	0.44
3:A:166:VAL:HG22	3:A:210:GLY:O	2.17	0.44
3:A:199:LYS:HA	3:A:200:PRO:HA	1.75	0.44
3:I:87:LEU:O	4:J:480:SER:OG	2.31	0.44
3:I:134:LEU:O	3:I:138:LYS:HG3	2.16	0.44
3:M:221:GLU:O	3:M:222:GLU:C	2.59	0.44
1:G:13:DG:C2	2:H:8:DA:C2	3.05	0.44
2:H:6:DA:H2''	2:H:7:DC:O5'	2.18	0.44
3:A:141:ARG:HB3	4:B:470:LEU:HD11	1.98	0.44
3:E:214:LEU:HD12	3:E:214:LEU:N	2.33	0.44
3:M:80:LEU:HD12	3:M:119:GLY:HA2	1.99	0.44
1:O:1:DC:H42	2:P:19:DG:H1	1.66	0.44
3:M:197:MET:O	3:M:201:LYS:HA	2.18	0.44
3:I:159:ASN:HD21	3:I:216:GLY:CA	2.30	0.44
2:H:11:DT:C5	2:H:12:DT:H73	2.53	0.44
3:A:152:PHE:HB2	4:B:462:LEU:HD21	2.00	0.44
3:E:133:LYS:HB3	4:F:455:VAL:HG21	2.00	0.44
3:E:141:ARG:NH2	3:E:145:LYS:HE3	2.33	0.44
3:M:106:ILE:HB	3:M:139:TYR:CE1	2.53	0.43
3:A:196:ARG:HD3	3:A:203:VAL:HG22	2.00	0.43
3:E:109:PRO:O	3:E:110:LYS:C	2.61	0.43
3:E:168:PHE:CE1	3:E:238:ARG:HB2	2.53	0.43
3:M:206:ILE:HD12	3:M:234:LEU:CD2	2.48	0.43
3:I:159:ASN:HD21	3:I:216:GLY:H	1.64	0.43
3:I:172:LEU:HD22	3:I:193:LEU:HB2	1.98	0.43
3:E:237:PHE:O	3:E:238:ARG:HB2	2.16	0.43
3:I:70:ILE:HA	3:I:159:ASN:O	2.18	0.43
3:I:165:ASP:OD2	3:I:211:LYS:HE2	2.19	0.43
3:M:70:ILE:N	3:M:126:ALA:O	2.51	0.43
3:M:143:ILE:HG22	3:M:148:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:139:TYR:N	3:A:139:TYR:HD1	2.17	0.43
3:I:138:LYS:HE2	4:J:465:VAL:HB	2.00	0.43
2:P:17:DT:H4'	3:M:207:PHE:CE2	2.54	0.43
4:F:463:GLU:HA	4:F:466:ASP:OD2	2.18	0.43
4:F:466:ASP:O	4:F:467:ASP:HB3	2.18	0.43
1:C:7:DA:O4'	3:A:158:GLN:HG3	2.19	0.43
1:G:6:DA:C2	3:E:71:VAL:HG21	2.54	0.43
2:P:17:DT:H2''	2:P:18:DA:C8	2.54	0.43
3:A:94:TYR:CZ	3:A:96:PRO:HG3	2.54	0.43
3:M:219:GLN:O	3:M:220:ARG:C	2.62	0.43
3:A:113:ALA:HA	3:A:122:VAL:O	2.19	0.42
3:A:219:GLN:O	3:A:222:GLU:HB2	2.19	0.42
3:M:63:ILE:HB	3:M:227:PHE:CE2	2.54	0.42
3:M:230:ILE:HG12	3:M:230:ILE:O	2.18	0.42
1:O:17:DT:H2''	1:O:18:DT:O5'	2.18	0.42
3:I:165:ASP:OD1	3:I:167:LYS:HD2	2.18	0.42
3:A:116:PHE:CE1	3:A:122:VAL:HG23	2.53	0.42
2:H:13:DT:H2''	2:H:14:DT:H5'	2.02	0.42
3:E:70:ILE:HG23	3:E:160:ILE:HG12	2.00	0.42
3:I:64:VAL:HA	3:I:65:PRO:HD3	1.89	0.42
2:L:15:DT:H6	2:L:15:DT:H2'	1.64	0.42
3:A:105:ARG:HA	3:A:112:THR:HA	2.01	0.42
3:E:221:GLU:CD	4:F:447:THR:HG22	2.45	0.42
4:F:494:PHE:CD2	4:F:494:PHE:C	2.97	0.42
1:G:16:DT:H2''	1:G:17:DT:H6	1.84	0.42
4:B:470:LEU:C	4:B:472:ALA:H	2.28	0.42
1:C:11:DA:H2''	1:C:12:DT:C6	2.55	0.42
1:O:5:DA:OP1	3:M:196:ARG:NH1	2.51	0.42
3:I:89:ALA:HB3	3:I:92:ALA:HB2	2.00	0.42
1:G:3:DA:H2''	1:G:4:DT:H5'	2.01	0.42
3:I:166:VAL:HG22	3:I:210:GLY:O	2.20	0.42
3:A:186:GLU:HA	3:A:187:PRO:HD3	1.91	0.41
4:F:444:LEU:HD23	4:F:444:LEU:HA	1.85	0.41
3:M:70:ILE:HG23	3:M:157:ILE:CG2	2.50	0.41
3:M:133:LYS:HB3	4:N:455:VAL:HG21	2.02	0.41
1:O:4:DT:H3	2:P:16:DA:N6	2.14	0.41
3:E:220:ARG:CG	3:E:224:TYR:CE2	3.03	0.41
3:I:207:PHE:O	3:I:208:VAL:C	2.62	0.41
3:I:111:THR:HG22	3:I:126:ALA:N	2.35	0.41
3:M:102:VAL:O	3:M:115:ILE:HD12	2.20	0.41
3:M:161:VAL:HG22	3:M:215:THR:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:475:LEU:HB3	4:J:479:ALA:HB3	2.03	0.41
3:M:92:ALA:O	3:M:93:GLU:C	2.64	0.41
3:A:76:LEU:HB3	3:A:150:ALA:HB1	2.03	0.41
3:A:197:MET:O	3:A:201:LYS:HA	2.20	0.41
4:F:500:SER:O	4:F:503:LEU:HB2	2.20	0.41
3:I:230:ILE:O	3:I:233:VAL:HB	2.20	0.41
3:M:95:ASN:HA	3:M:96:PRO:HD3	1.88	0.41
3:M:199:LYS:HA	3:M:200:PRO:HA	1.84	0.41
3:A:99:PHE:HD2	3:A:101:ALA:HB3	1.84	0.41
3:M:113:ALA:HA	3:M:122:VAL:O	2.21	0.41
4:B:437:TYR:HD2	4:B:438:CYS:H	1.68	0.41
3:I:109:PRO:HD2	3:I:135:ALA:HB2	2.03	0.41
3:M:159:ASN:ND2	3:M:216:GLY:H	2.19	0.41
1:G:5:DA:H8	1:G:5:DA:H2'	1.81	0.41
3:A:155:PHE:CE2	4:B:452:LEU:HD21	2.56	0.41
3:E:211:LYS:H	3:E:211:LYS:HG2	1.70	0.41
4:F:457:ASP:O	4:F:458:ASP:C	2.64	0.41
3:M:123:VAL:HG12	3:M:123:VAL:O	2.21	0.41
3:M:182:PHE:HD1	3:M:182:PHE:H	1.66	0.41
2:L:3:DA:C2	2:L:4:DA:C4	3.09	0.40
2:P:11:DT:C6	2:P:12:DT:H72	2.56	0.40
3:M:205:LEU:HB2	3:M:213:VAL:HB	2.03	0.40
3:M:233:VAL:O	3:M:233:VAL:HG13	2.20	0.40
4:B:470:LEU:HA	4:B:473:HIS:CD2	2.56	0.40
3:E:230:ILE:O	3:E:233:VAL:HB	2.22	0.40
3:E:231:TYR:O	3:E:232:PRO:C	2.65	0.40
3:I:137:ARG:HH22	4:J:458:ASP:HB3	1.86	0.40
3:I:178:SER:HG	3:I:237:PHE:HZ	1.68	0.40
3:I:214:LEU:HD21	3:I:227:PHE:HB2	2.02	0.40
1:C:1:DC:H2'	1:C:2:DT:C6	2.57	0.40
3:I:169:PRO:HG2	3:I:239:LYS:HB3	2.02	0.40
3:M:106:ILE:HD13	3:M:108:GLU:H	1.87	0.40
3:M:178:SER:CB	3:M:237:PHE:CZ	3.03	0.40
2:H:17:DT:H1'	3:E:207:PHE:CE2	2.56	0.40
2:D:1:DA:H2''	2:D:2:DA:C5'	2.50	0.40
3:A:161:VAL:HA	3:A:215:THR:HA	2.03	0.40
3:E:70:ILE:HD12	3:E:128:SER:C	2.46	0.40
3:I:230:ILE:HG13	3:I:233:VAL:HB	2.03	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	178/180 (99%)	140 (79%)	29 (16%)	9 (5%)	1	3
3	E	178/180 (99%)	154 (86%)	15 (8%)	9 (5%)	1	3
3	I	178/180 (99%)	159 (89%)	12 (7%)	7 (4%)	2	5
3	M	178/180 (99%)	154 (86%)	20 (11%)	4 (2%)	5	15
4	B	70/72 (97%)	58 (83%)	11 (16%)	1 (1%)	9	24
4	F	70/72 (97%)	56 (80%)	12 (17%)	2 (3%)	3	10
4	J	51/72 (71%)	46 (90%)	4 (8%)	1 (2%)	6	16
4	N	51/72 (71%)	47 (92%)	4 (8%)	0	100	100
All	All	954/1008 (95%)	814 (85%)	107 (11%)	33 (4%)	3	7

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	106	ILE
3	E	90	ARG
3	E	118	SER
3	E	150	ALA
3	E	238	ARG
4	F	442	LEU
3	I	89	ALA
3	I	118	SER
3	I	150	ALA
3	M	206	ILE
3	A	149	ALA
3	E	62	GLY
3	E	220	ARG
3	I	110	LYS
3	I	201	LYS
4	J	493	ASP
3	M	93	GLU

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Mol	Chain	Res	Type
3	M	150	ALA
3	A	89	ALA
3	A	98	ARG
3	A	110	LYS
3	A	114	LEU
3	A	146	ILE
3	A	150	ALA
3	E	92	ALA
3	M	149	ALA
4	B	476	ASN
3	E	119	GLY
3	I	119	GLY
3	A	87	LEU
3	E	179	HIS
4	F	505	GLN
3	I	90	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	152/152 (100%)	122 (80%)	30 (20%)	1	3
3	E	152/152 (100%)	132 (87%)	20 (13%)	4	12
3	I	152/152 (100%)	118 (78%)	34 (22%)	1	2
3	M	152/152 (100%)	114 (75%)	38 (25%)	0	1
4	B	67/67 (100%)	50 (75%)	17 (25%)	0	1
4	F	67/67 (100%)	53 (79%)	14 (21%)	1	2
4	J	49/67 (73%)	37 (76%)	12 (24%)	1	1
4	N	49/67 (73%)	39 (80%)	10 (20%)	1	3
All	All	840/876 (96%)	665 (79%)	175 (21%)	1	3

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	61	SER
3	A	63	ILE
3	A	64	VAL
3	A	70	ILE
3	A	80	LEU
3	A	90	ARG
3	A	91	ASN
3	A	98	ARG
3	A	106	ILE
3	A	108	GLU
3	A	110	LYS
3	A	120	LYS
3	A	130	ASP
3	A	132	SER
3	A	134	LEU
3	A	136	SER
3	A	143	ILE
3	A	145	LYS
3	A	154	ASP
3	A	175	LEU
3	A	181	THR
3	A	184	SER
3	A	186	GLU
3	A	189	LEU
3	A	193	LEU
3	A	198	VAL
3	A	202	ILE
3	A	214	LEU
3	A	215	THR
3	A	218	LYS
4	B	442	LEU
4	B	448	THR
4	B	449	ASP
4	B	464	ASP
4	B	468	GLU
4	B	470	LEU
4	B	474	LEU
4	B	475	LEU
4	B	478	GLU
4	B	482	LEU
4	B	485	ARG
4	B	488	ILE
4	B	499	GLU

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Mol	Chain	Res	Type
4	B	501	LYS
4	B	502	ARG
4	B	504	LYS
4	B	506	GLU
3	E	79	ARG
3	E	80	LEU
3	E	85	VAL
3	E	90	ARG
3	E	97	LYS
3	E	106	ILE
3	E	132	SER
3	E	134	LEU
3	E	136	SER
3	E	142	ILE
3	E	143	ILE
3	E	170	ILE
3	E	184	SER
3	E	193	LEU
3	E	194	ILE
3	E	199	LYS
3	E	201	LYS
3	E	206	ILE
3	E	211	LYS
3	E	228	GLU
4	F	442	LEU
4	F	447	THR
4	F	455	VAL
4	F	465	VAL
4	F	471	ASN
4	F	475	LEU
4	F	477	GLU
4	F	494	PHE
4	F	497	GLU
4	F	498	GLN
4	F	499	GLU
4	F	500	SER
4	F	501	LYS
4	F	502	ARG
3	I	64	VAL
3	I	70	ILE
3	I	73	THR
3	I	74	VAL

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Mol	Chain	Res	Type
3	I	79	ARG
3	I	83	LYS
3	I	85	VAL
3	I	90	ARG
3	I	98	ARG
3	I	106	ILE
3	I	107	ARG
3	I	110	LYS
3	I	127	LYS
3	I	133	LYS
3	I	134	LEU
3	I	136	SER
3	I	142	ILE
3	I	143	ILE
3	I	159	ASN
3	I	167	LYS
3	I	170	ILE
3	I	173	GLU
3	I	178	SER
3	I	181	THR
3	I	188	GLU
3	I	198	VAL
3	I	199	LYS
3	I	204	LEU
3	I	205	LEU
3	I	214	LEU
3	I	218	LYS
3	I	220	ARG
3	I	223	ILE
3	I	230	ILE
4	J	455	VAL
4	J	462	LEU
4	J	466	ASP
4	J	469	GLU
4	J	477	GLU
4	J	478	GLU
4	J	481	LYS
4	J	485	ARG
4	J	496	LEU
4	J	498	GLN
4	J	499	GLU
4	J	503	LEU

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Mol	Chain	Res	Type
3	M	67	LEU
3	M	68	GLN
3	M	70	ILE
3	M	71	VAL
3	M	82	LEU
3	M	90	ARG
3	M	95	ASN
3	M	97	LYS
3	M	106	ILE
3	M	110	LYS
3	M	111	THR
3	M	123	VAL
3	M	127	LYS
3	M	131	ASP
3	M	132	SER
3	M	134	LEU
3	M	143	ILE
3	M	153	THR
3	M	157	ILE
3	M	158	GLN
3	M	167	LYS
3	M	173	GLU
3	M	175	LEU
3	M	182	PHE
3	M	188	GLU
3	M	189	LEU
3	M	193	LEU
3	M	201	LYS
3	M	203	VAL
3	M	204	LEU
3	M	206	ILE
3	M	208	VAL
3	M	215	THR
3	M	218	LYS
3	M	221	GLU
3	M	230	ILE
3	M	233	VAL
3	M	235	SER
4	N	457	ASP
4	N	468	GLU
4	N	469	GLU
4	N	470	LEU

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Mol	Chain	Res	Type
4	N	474	LEU
4	N	486	ILE
4	N	495	LEU
4	N	498	GLN
4	N	501	LYS
4	N	502	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	95	ASN
3	A	159	ASN
3	E	69	ASN
3	E	95	ASN
3	E	158	GLN
3	E	159	ASN
3	E	179	HIS
3	E	219	GLN
4	F	498	GLN
4	F	505	GLN
3	I	68	GLN
3	I	91	ASN
3	I	159	ASN
3	I	225	GLN
4	J	498	GLN
3	M	68	GLN
3	M	69	ASN
3	M	88	HIS
3	M	159	ASN

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 [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	19/19 (100%)	1.23	1 (5%) 32 27	21, 27, 30, 31	0
1	G	19/19 (100%)	0.67	0 100 100	24, 27, 32, 32	0
1	K	19/19 (100%)	1.05	1 (5%) 32 27	24, 29, 32, 32	0
1	O	19/19 (100%)	0.94	0 100 100	26, 29, 31, 32	0
2	D	19/19 (100%)	1.07	1 (5%) 32 27	25, 28, 30, 30	0
2	H	19/19 (100%)	1.06	1 (5%) 32 27	24, 29, 36, 37	0
2	L	19/19 (100%)	1.50	5 (26%) 1 1	24, 27, 32, 32	0
2	P	19/19 (100%)	1.00	3 (15%) 5 4	25, 27, 30, 32	0
3	A	180/180 (100%)	1.05	17 (9%) 14 12	24, 28, 30, 31	0
3	E	180/180 (100%)	1.20	27 (15%) 5 5	23, 28, 33, 39	0
3	I	180/180 (100%)	1.16	26 (14%) 6 5	22, 28, 33, 39	0
3	M	180/180 (100%)	0.97	14 (7%) 19 17	22, 28, 30, 31	0
4	B	72/72 (100%)	0.82	6 (8%) 17 15	27, 29, 30, 31	0
4	F	72/72 (100%)	0.91	5 (6%) 23 19	23, 29, 33, 34	0
4	J	53/72 (73%)	0.91	5 (9%) 14 12	24, 29, 33, 34	0
4	N	53/72 (73%)	1.03	7 (13%) 7 7	28, 29, 29, 30	0
All	All	1122/1160 (96%)	1.05	119 (10%) 11 10	21, 28, 32, 39	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	113	ALA	4.1
3	E	235	SER	4.0
3	M	87	LEU	4.0
3	A	75	THR	3.7
2	L	1	DA	3.5

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Mol	Chain	Res	Type	RSRZ
4	J	503	LEU	3.5
3	E	74	VAL	3.4
3	E	91	ASN	3.4
3	I	160	ILE	3.3
3	I	206	ILE	3.3
4	J	500	SER	3.3
4	J	506	GLU	3.2
4	N	472	ALA	3.2
3	E	124	THR	3.2
3	I	184	SER	3.1
2	L	3	DA	3.1
3	A	70	ILE	3.1
3	I	115	ILE	3.0
3	E	89	ALA	3.0
3	E	61	SER	3.0
3	E	161	VAL	2.9
3	E	113	ALA	2.9
3	A	115	ILE	2.9
3	E	159	ASN	2.8
2	L	6	DA	2.8
3	M	166	VAL	2.8
3	M	81	ASP	2.8
3	A	194	ILE	2.6
3	E	106	ILE	2.6
3	E	90	ARG	2.6
3	A	113	ALA	2.6
3	E	213	VAL	2.6
3	I	198	VAL	2.6
3	I	126	ALA	2.6
4	J	501	LYS	2.6
3	E	92	ALA	2.6
3	E	125	GLY	2.6
3	E	231	TYR	2.6
3	A	114	LEU	2.6
3	I	112	THR	2.6
3	E	140	ALA	2.6
3	I	177	PHE	2.6
4	N	500	SER	2.5
3	A	77	GLY	2.5
4	B	439	PRO	2.5
3	E	166	VAL	2.5
4	F	477	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
4	J	505	GLN	2.5
3	I	140	ALA	2.5
3	E	110	LYS	2.5
3	E	127	LYS	2.5
3	A	213	VAL	2.5
3	M	122	VAL	2.5
3	E	186	GLU	2.5
3	I	207	PHE	2.5
3	I	204	LEU	2.4
3	E	118	SER	2.4
2	P	3	DA	2.4
4	N	503	LEU	2.4
3	I	188	GLU	2.4
3	E	177	PHE	2.4
3	I	91	ASN	2.4
3	E	211	LYS	2.4
3	M	116	PHE	2.4
3	A	158	GLN	2.3
3	M	112	THR	2.3
3	I	89	ALA	2.3
3	E	112	THR	2.3
3	I	195	TYR	2.3
3	E	126	ALA	2.3
3	M	151	LYS	2.3
2	P	10	DT	2.2
3	A	150	ALA	2.2
3	E	204	LEU	2.2
3	I	133	LYS	2.2
3	I	159	ASN	2.2
3	M	114	LEU	2.2
2	L	16	DA	2.2
4	B	488	ILE	2.2
4	N	498	GLN	2.2
4	F	466	ASP	2.2
2	L	10	DT	2.2
3	I	61	SER	2.2
3	A	76	LEU	2.2
4	B	442	LEU	2.2
4	F	496	LEU	2.2
3	A	122	VAL	2.2
3	I	74	VAL	2.2
4	B	492	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	6	DA	2.2
3	M	197	MET	2.2
4	F	487	TRP	2.2
3	I	106	ILE	2.1
3	I	213	VAL	2.1
3	I	130	ASP	2.1
4	B	495	LEU	2.1
4	F	462	LEU	2.1
3	I	192	GLY	2.1
4	B	503	LEU	2.1
4	N	495	LEU	2.1
3	E	117	ALA	2.1
1	C	14	DT	2.1
3	A	121	MET	2.1
3	A	123	VAL	2.1
3	M	204	LEU	2.1
2	P	6	DA	2.1
3	A	233	VAL	2.1
3	M	80	LEU	2.1
4	N	470	LEU	2.1
3	A	73	THR	2.1
3	A	217	ALA	2.1
3	M	86	ALA	2.1
3	M	127	LYS	2.0
2	D	5	DA	2.0
3	I	77	GLY	2.0
3	I	114	LEU	2.0
3	I	210	GLY	2.0
1	K	6	DA	2.0
4	N	465	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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.