Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 01:35 am BST

PDB ID	:	4PXI
Title	:	Elucidation of the Structural and Functional Mechanism of Action of the TetR Family Protein, CprB from S. coelicolor A3(2)
Authors	:	Hussain, B.; Ruchika, B.; Aruna, B.; Ruchi, A.
Deposited on	:	2014-03-24
Resolution	:	3.20 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:

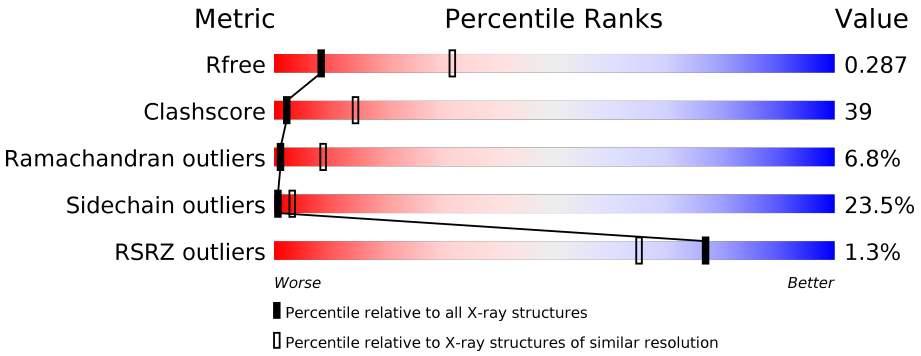
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	215	38% 35% 14% • 10%
1	B	215	% 38% 48% 7% • 5%
1	C	215	36% 42% 14% • 7%
1	D	215	% 36% 43% 9% • 10%
2	E	22	18% 41% 32% 9%
3	F	22	14% 5% 23% 73%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6886 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 CprB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1480	930	276	269	5			
1	B	204	Total	C	N	O	S	0	0	0
			1518	950	277	285	6			
1	C	200	Total	C	N	O	S	0	0	0
			1535	961	295	274	5			
1	D	193	Total	C	N	O	S	0	0	0
			1497	939	279	273	6			

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*CP*AP*TP*AP*CP*GP*GP*GP*AP*CP*GP*CP*CP*CP*CP*GP*TP*TP*TP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	20	Total	C	N	O	P	0	0	0
			405	194	73	119	19			

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

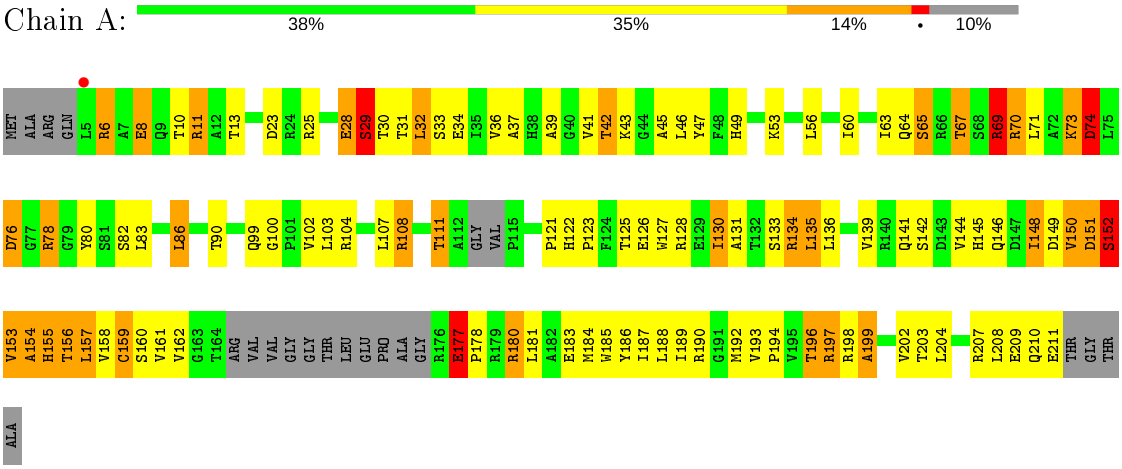
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	22	Total	C	N	O	P	0	0	0
			451	215	85	130	21			

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.

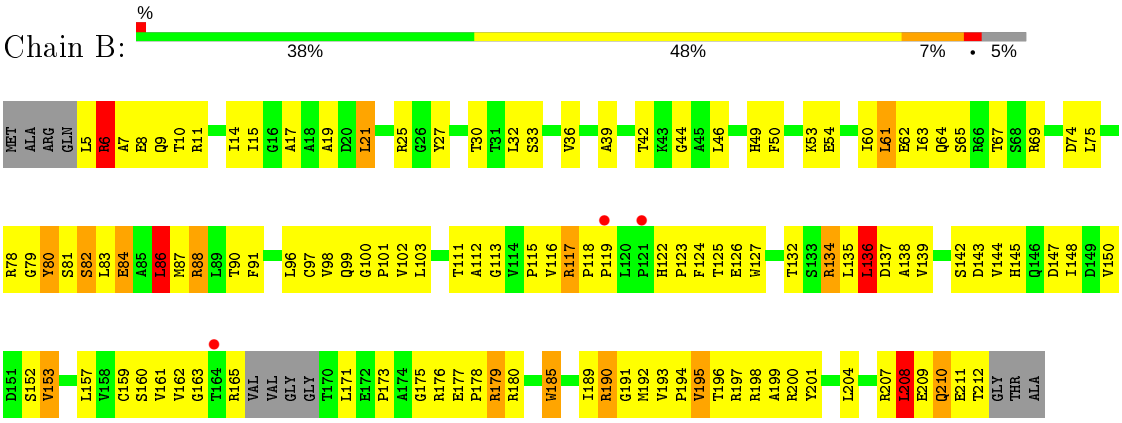
- Molecule 1: CprB

Chain A:



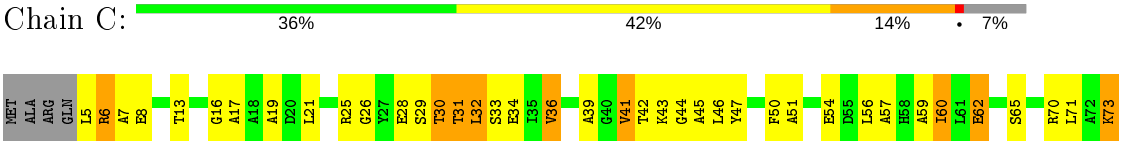
- Molecule 1: CprB

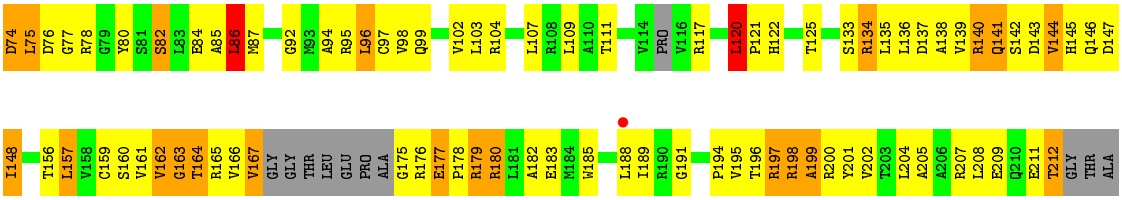
Chain B:



- Molecule 1: CprB

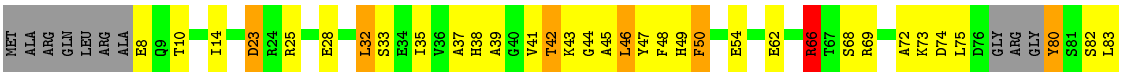
Chain C:

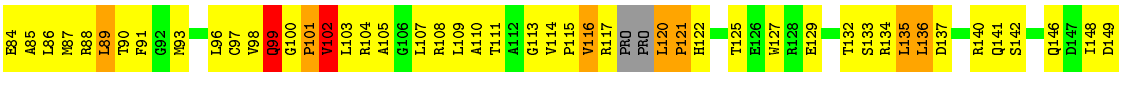


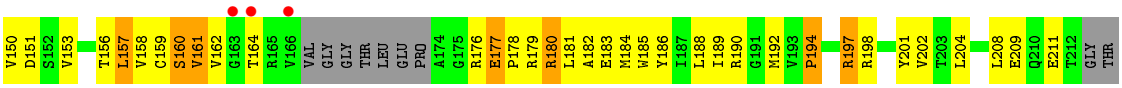


• Molecule 1: CprB

Chain D:

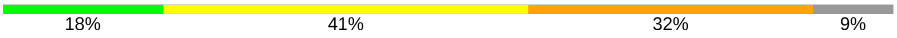






• Molecule 2: DNA (5'-D(*AP*CP*AP*TP*AP*CP*GP*GP*GP*AP*CP*GP*CP*CP*CP*CP *GP*TP*TP*TP*AP*T)-3')

Chain E:



• Molecule 3: DNA (5'-D(*AP*TP*AP*AP*AP*CP*GP*GP*GP*GP*CP*GP*TP*CP*CP*CP *GP*TP*AP*TP*GP*T)-3')

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	149.06Å 149.06Å 69.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.90 – 3.20 60.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (60.90-3.20) 99.6 (60.90-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.220 , 0.294 0.218 , 0.287	Depositor DCC
R_{free} test set	1163 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å^2)	74.4	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l 0.428 for h,-h-k,-l 0.035 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6886	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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	0.66	1/1505 (0.1%)	0.84	0/2043
1	B	0.64	1/1545 (0.1%)	0.86	1/2104 (0.0%)
1	C	0.60	0/1559	0.86	1/2111 (0.0%)
1	D	0.62	1/1519 (0.1%)	0.80	1/2056 (0.0%)
2	E	0.75	1/453 (0.2%)	1.54	10/697 (1.4%)
3	F	0.72	1/506 (0.2%)	1.61	21/780 (2.7%)
All	All	0.65	5/7087 (0.1%)	0.99	34/9791 (0.3%)

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
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5	DA	O3'-P	-5.96	1.53	1.61
2	E	20	DT	O3'-P	5.54	1.67	1.61
1	B	185	TRP	CD2-CE2	5.43	1.47	1.41
1	A	127	TRP	CD2-CE2	5.23	1.47	1.41
1	D	127	TRP	CD2-CE2	5.08	1.47	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3	DA	P-O3'-C3'	15.72	138.56	119.70
3	F	3	DA	P-O3'-C3'	13.69	136.13	119.70
3	F	21	DG	P-O3'-C3'	11.49	133.49	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4	DT	P-O3'-C3'	9.52	131.12	119.70
2	E	20	DT	P-O3'-C3'	9.50	131.10	119.70
3	F	10	DG	P-O3'-C3'	-8.77	109.17	119.70
3	F	18	DT	P-O3'-C3'	8.67	130.10	119.70
3	F	1	DA	O3'-P-O5'	8.54	120.22	104.00
3	F	13	DT	P-O3'-C3'	8.37	129.74	119.70
2	E	12	DG	P-O3'-C3'	-7.65	110.52	119.70
3	F	19	DA	P-O3'-C3'	7.63	128.85	119.70
3	F	7	DG	P-O3'-C3'	-7.58	110.60	119.70
2	E	3	DA	C1'-O4'-C4'	-7.05	103.05	110.10
3	F	2	DT	O5'-P-OP2	-6.94	99.45	105.70
2	E	11	DC	P-O3'-C3'	6.61	127.63	119.70
3	F	4	DA	O5'-P-OP1	-6.49	99.86	105.70
2	E	9	DG	P-O3'-C3'	-6.15	112.32	119.70
1	C	120	LEU	CA-CB-CG	5.90	128.87	115.30
3	F	2	DT	P-O3'-C3'	5.83	126.70	119.70
3	F	3	DA	O3'-P-O5'	5.78	114.99	104.00
3	F	11	DC	OP1-P-O3'	5.74	117.84	105.20
3	F	9	DG	O5'-P-OP1	5.66	117.50	110.70
2	E	9	DG	O3'-P-O5'	-5.66	93.25	104.00
2	E	11	DC	OP2-P-O3'	5.66	117.65	105.20
3	F	1	DA	C1'-O4'-C4'	-5.64	104.46	110.10
3	F	16	DC	O5'-P-OP1	-5.62	100.64	105.70
1	D	46	LEU	CA-CB-CG	5.59	128.16	115.30
1	B	86	LEU	CA-CB-CG	5.56	128.09	115.30
3	F	1	DA	C3'-C2'-C1'	-5.55	95.83	102.50
3	F	14	DC	OP2-P-O3'	5.49	117.27	105.20
2	E	16	DC	OP2-P-O3'	5.23	116.71	105.20
3	F	5	DA	P-O3'-C3'	-5.16	113.51	119.70
3	F	8	DG	O3'-P-O5'	-5.14	94.24	104.00
3	F	20	DT	P-O3'-C3'	5.12	125.85	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	SER	Peptide
1	D	125	THR	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	1480	0	1469	116	0
1	B	1518	0	1464	111	0
1	C	1535	0	1542	113	0
1	D	1497	0	1509	114	0
2	E	405	0	227	53	0
3	F	451	0	249	65	0
All	All	6886	0	6460	513	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 39.

All (513) 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:C:144:VAL:HG12	1:C:145:HIS:H	1.16	1.09
1:A:177:GLU:H	1:A:178:PRO:HD2	1.20	1.04
1:A:154:ALA:HA	1:A:157:LEU:HD13	1.40	1.03
1:C:163:GLY:HA3	1:C:166:VAL:HB	1.06	1.02
1:A:151:ASP:HB3	1:A:153:VAL:HG22	1.41	1.02
1:D:42:THR:HG23	1:D:45:ALA:HB2	1.41	1.02
1:B:86:LEU:HB2	1:B:134:ARG:HG2	1.41	1.02
1:D:180:ARG:HH11	1:D:180:ARG:HG3	1.19	1.01
1:C:163:GLY:HA3	1:C:166:VAL:CB	1.91	1.00
1:C:163:GLY:CA	1:C:166:VAL:HB	1.90	0.99
2:E:10:DA:H2"	2:E:11:DC:H5"	1.43	0.99
1:B:80:TYR:HB3	1:B:84:GLU:HB2	1.42	0.99
1:C:33:SER:HA	1:C:36:VAL:CG2	1.94	0.97
1:D:45:ALA:CA	3:F:1:DA:H2'	1.93	0.97
1:D:45:ALA:HA	3:F:1:DA:H2'	1.46	0.95
1:C:142:SER:HB3	1:C:197:ARG:HH21	1.29	0.95
1:C:175:GLY:HA2	1:C:176:ARG:HB3	1.48	0.93
1:C:33:SER:HA	1:C:36:VAL:HG23	1.49	0.92
3:F:9:DG:H4'	3:F:9:DG:OP1	1.66	0.92
1:C:26:GLY:O	1:C:30:THR:HG23	1.70	0.91
1:B:189:ILE:O	1:B:190:ARG:HB2	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:VAL:HG12	1:C:145:HIS:N	1.84	0.89
2:E:21:DA:H2"	2:E:22:DT:O5'	1.72	0.89
3:F:19:DA:H1'	3:F:20:DT:H5'	1.55	0.88
1:A:42:THR:HG23	1:A:45:ALA:HB2	1.56	0.88
1:B:7:ALA:HB2	3:F:4:DA:H5"	1.55	0.87
2:E:17:DG:H1	3:F:6:DC:H42	1.22	0.87
1:B:210:GLN:CD	1:B:210:GLN:H	1.78	0.86
1:A:196:THR:HG22	1:A:197:ARG:N	1.89	0.86
1:A:86:LEU:HD12	1:A:134:ARG:HB3	1.57	0.86
1:A:154:ALA:HA	1:A:157:LEU:CD1	2.06	0.86
3:F:7:DG:H2"	3:F:8:DG:C8	2.13	0.84
3:F:2:DT:H2"	3:F:3:DA:H5'	1.58	0.83
1:B:86:LEU:HD23	1:B:134:ARG:HB3	1.59	0.83
2:E:16:DC:H2"	2:E:17:DG:C8	2.14	0.83
1:B:190:ARG:HE	1:B:198:ARG:HH21	1.23	0.83
1:B:132:THR:O	1:B:136:LEU:HB3	1.79	0.82
1:C:134:ARG:HG3	1:C:134:ARG:HH11	1.42	0.82
1:D:42:THR:HG23	1:D:45:ALA:CB	2.09	0.82
2:E:11:DC:H2"	2:E:12:DG:C8	2.15	0.81
1:B:207:ARG:O	1:B:208:LEU:HB2	1.79	0.81
1:A:180:ARG:HH11	1:A:180:ARG:HB2	1.47	0.80
1:D:69:ARG:NH1	1:D:69:ARG:HB3	1.97	0.80
1:B:159:CYS:O	1:B:162:VAL:HG22	1.80	0.79
1:C:111:THR:HG21	1:D:111:THR:HG21	1.63	0.79
2:E:21:DA:H2"	2:E:22:DT:H3'	1.64	0.79
1:A:42:THR:HG21	2:E:4:DT:OP1	1.82	0.78
1:B:139:VAL:HG22	1:B:144:VAL:HG21	1.66	0.78
1:B:163:GLY:HA3	1:B:180:ARG:NH2	2.00	0.77
2:E:7:DG:N2	3:F:16:DC:N3	2.29	0.77
3:F:6:DC:H2"	3:F:7:DG:C8	2.20	0.77
1:C:96:LEU:HB2	1:C:103:LEU:HD12	1.66	0.76
1:B:96:LEU:HB2	1:B:103:LEU:HD12	1.67	0.76
2:E:6:DC:H2"	2:E:7:DG:C8	2.20	0.76
2:E:7:DG:H1	3:F:16:DC:H42	1.32	0.76
1:C:145:HIS:CD2	1:D:190:ARG:HH12	2.03	0.76
2:E:6:DC:C2'	2:E:7:DG:C8	2.69	0.76
1:A:42:THR:HG23	1:A:45:ALA:CB	2.17	0.75
1:B:204:LEU:O	1:B:208:LEU:HB2	1.86	0.75
1:C:96:LEU:HB2	1:C:103:LEU:CD1	2.16	0.75
1:C:159:CYS:HA	1:C:162:VAL:HB	1.67	0.75
2:E:17:DG:N2	3:F:6:DC:N3	2.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2:DT:H5"	3:F:2:DT:H6	1.53	0.74
1:B:157:LEU:O	1:B:161:VAL:HG23	1.88	0.73
1:B:80:TYR:CB	1:B:84:GLU:HB2	2.18	0.73
1:A:153:VAL:O	1:A:155:HIS:HD2	1.72	0.73
1:A:145:HIS:CE1	1:A:194:PRO:HA	2.22	0.73
1:D:86:LEU:HD21	1:D:135:LEU:HD13	1.70	0.73
1:D:80:TYR:OH	1:D:88:ARG:NH1	2.22	0.73
1:D:69:ARG:HH11	1:D:69:ARG:HB3	1.53	0.73
2:E:17:DG:H1	3:F:6:DC:N4	1.86	0.73
1:A:183:GLU:HA	1:A:186:TYR:HD2	1.53	0.73
1:C:142:SER:HB3	1:C:197:ARG:NH2	2.04	0.73
1:A:25:ARG:HB2	1:A:30:THR:OG1	1.89	0.73
1:D:32:LEU:HA	1:D:35:ILE:HD12	1.71	0.73
2:E:10:DA:C2'	2:E:11:DC:H5"	2.18	0.72
1:C:94:ALA:O	1:C:98:VAL:HG23	1.89	0.72
1:A:86:LEU:HD13	1:A:135:LEU:HD13	1.71	0.72
1:A:177:GLU:H	1:A:178:PRO:CD	2.00	0.71
1:A:189:ILE:HG23	1:A:193:VAL:HG21	1.71	0.71
2:E:9:DG:H2"	2:E:10:DA:C8	2.24	0.71
1:C:47:TYR:CD1	3:F:13:DT:H72	2.25	0.71
1:A:86:LEU:HD13	1:A:135:LEU:CD1	2.21	0.71
1:C:5:LEU:HD13	3:F:21:DG:OP1	1.90	0.71
1:C:117:ARG:O	1:C:120:LEU:HB3	1.91	0.70
1:D:42:THR:HG21	3:F:2:DT:OP2	1.91	0.70
1:B:139:VAL:HG22	1:B:144:VAL:CG2	2.21	0.70
1:A:86:LEU:CD1	1:A:134:ARG:HB3	2.21	0.70
1:B:165:ARG:HA	1:B:171:LEU:HB2	1.73	0.69
1:D:84:GLU:HG3	1:D:204:LEU:HD11	1.74	0.69
3:F:20:DT:H2"	3:F:21:DG:C5	2.28	0.69
1:C:144:VAL:CG1	1:C:145:HIS:H	1.95	0.69
1:C:36:VAL:HG13	1:C:46:LEU:HD12	1.75	0.68
1:B:195:VAL:HA	1:B:198:ARG:HD3	1.74	0.68
1:D:82:SER:H	1:D:141:GLN:HE22	1.40	0.68
1:A:155:HIS:CD2	1:A:155:HIS:H	2.09	0.68
1:D:188:LEU:O	1:D:192:MET:HB2	1.92	0.68
1:C:21:LEU:HD22	1:C:25:ARG:NH1	2.09	0.68
1:A:187:ILE:HG23	1:B:191:GLY:HA3	1.75	0.67
2:E:18:DT:H2'	2:E:19:DT:C7	2.25	0.67
1:D:43:LYS:HD2	2:E:18:DT:H72	1.76	0.67
2:E:17:DG:H2"	2:E:18:DT:H5"	1.76	0.67
1:B:145:HIS:O	1:B:148:ILE:HG13	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:ALA:HB3	1:C:39:ALA:HB2	1.75	0.67
1:A:209:GLU:O	1:A:211:GLU:N	2.24	0.67
1:B:86:LEU:O	1:B:90:THR:HG23	1.96	0.66
1:C:145:HIS:HD2	1:D:190:ARG:HH12	1.43	0.66
1:C:175:GLY:HA2	1:C:176:ARG:CB	2.25	0.66
1:A:196:THR:CG2	1:A:197:ARG:N	2.59	0.66
1:C:76:ASP:C	1:C:78:ARG:H	1.99	0.65
2:E:6:DC:H2"	2:E:7:DG:H8	1.58	0.65
2:E:21:DA:C2'	2:E:22:DT:H3'	2.26	0.65
1:B:211:GLU:O	1:B:211:GLU:HG2	1.94	0.65
1:D:83:LEU:HD13	1:D:83:LEU:O	1.96	0.65
2:E:18:DT:H2'	2:E:19:DT:H72	1.79	0.65
1:A:86:LEU:CD1	1:A:135:LEU:HD13	2.26	0.65
1:D:180:ARG:HG3	1:D:180:ARG:NH1	1.98	0.65
3:F:7:DG:H2"	3:F:8:DG:H8	1.60	0.65
1:C:21:LEU:HD22	1:C:25:ARG:HH11	1.62	0.65
1:C:92:GLY:O	1:C:95:ARG:HB3	1.96	0.65
1:D:186:TYR:CE1	1:D:202:VAL:HG13	2.32	0.65
1:A:209:GLU:C	1:A:211:GLU:H	1.99	0.64
1:B:189:ILE:O	1:B:190:ARG:CB	2.43	0.64
1:B:19:ALA:HB2	1:B:60:ILE:HD11	1.79	0.64
3:F:9:DG:H2"	3:F:10:DG:C8	2.32	0.64
1:A:151:ASP:N	1:A:151:ASP:OD2	2.29	0.64
1:B:82:SER:HB3	1:B:138:ALA:HB2	1.78	0.64
1:B:21:LEU:HD11	1:B:25:ARG:NH2	2.12	0.64
1:A:177:GLU:N	1:A:178:PRO:HD2	2.04	0.64
1:A:183:GLU:O	1:A:187:ILE:HD12	1.97	0.64
1:C:7:ALA:HB2	2:E:6:DC:H5"	1.79	0.64
2:E:11:DC:H2"	2:E:12:DG:N7	2.13	0.64
1:B:6:ARG:N	1:B:6:ARG:HD3	2.13	0.63
1:D:42:THR:CG2	1:D:45:ALA:HB2	2.24	0.63
1:D:197:ARG:HH11	1:D:197:ARG:HG3	1.62	0.63
2:E:18:DT:H2'	2:E:19:DT:C5	2.34	0.63
1:D:25:ARG:HH21	1:D:25:ARG:HG3	1.61	0.63
1:D:101:PRO:HA	1:D:104:ARG:HH21	1.63	0.63
1:A:144:VAL:HG12	1:A:148:ILE:HD11	1.80	0.63
1:D:180:ARG:HH11	1:D:180:ARG:CG	2.05	0.63
1:B:14:ILE:HG21	1:B:50:PHE:HE2	1.63	0.63
1:B:79:GLY:O	1:B:80:TYR:HB2	1.99	0.62
1:C:19:ALA:HB2	1:C:60:ILE:HD11	1.80	0.62
1:D:88:ARG:HG2	1:D:208:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:LEU:CD2	1:D:135:LEU:HD13	2.29	0.62
1:B:64:GLN:O	1:B:67:THR:HG22	1.98	0.62
1:D:113:GLY:O	1:D:115:PRO:HD3	1.98	0.62
1:A:151:ASP:CA	1:A:152:SER:HB3	2.28	0.62
1:C:179:ARG:CZ	1:C:179:ARG:HB3	2.28	0.62
1:B:189:ILE:HA	1:B:193:VAL:HG23	1.81	0.62
1:A:150:VAL:O	1:A:152:SER:HB3	2.00	0.62
1:A:183:GLU:HA	1:A:186:TYR:CD2	2.33	0.62
1:D:185:TRP:O	1:D:189:ILE:HG12	2.01	0.61
1:A:125:THR:HG22	1:A:128:ARG:HH21	1.66	0.61
1:D:83:LEU:HD13	1:D:87:MET:HG3	1.81	0.61
1:A:23:ASP:HA	1:A:108:ARG:HE	1.64	0.61
1:B:42:THR:HG21	3:F:6:DC:H3'	1.83	0.61
1:C:134:ARG:HG3	1:C:134:ARG:NH1	2.14	0.61
1:A:151:ASP:HA	1:A:152:SER:HB3	1.81	0.61
1:D:189:ILE:HG22	1:D:198:ARG:HG3	1.83	0.61
1:D:44:GLY:O	3:F:1:DA:H8	1.84	0.61
1:A:69:ARG:HH11	1:A:69:ARG:HG2	1.66	0.60
1:B:84:GLU:O	1:B:88:ARG:HG2	2.01	0.60
3:F:9:DG:C4'	3:F:9:DG:OP1	2.44	0.60
1:A:157:LEU:H	1:A:157:LEU:HD12	1.66	0.60
1:A:196:THR:HG22	1:A:197:ARG:HD2	1.84	0.60
1:B:210:GLN:N	1:B:210:GLN:CD	2.51	0.60
1:C:145:HIS:HB3	1:C:147:ASP:OD1	2.02	0.60
1:C:42:THR:OG1	2:E:8:DG:OP2	2.18	0.60
1:A:107:LEU:HD11	1:A:162:VAL:HG22	1.84	0.60
1:A:31:THR:HG23	1:A:34:GLU:HG2	1.83	0.60
1:C:144:VAL:CG1	1:C:145:HIS:N	2.56	0.60
1:C:59:ALA:HA	1:C:62:GLU:HB2	1.84	0.60
1:D:120:LEU:HG	1:D:121:PRO:HD2	1.83	0.60
3:F:2:DT:C6	3:F:2:DT:H5"	2.34	0.59
2:E:18:DT:H2'	2:E:19:DT:C6	2.38	0.59
1:A:42:THR:CG2	1:A:45:ALA:HB2	2.29	0.59
1:C:31:THR:HG23	1:C:34:GLU:CB	2.33	0.59
1:C:33:SER:CA	1:C:36:VAL:HG23	2.29	0.59
1:C:139:VAL:HG22	1:C:146:GLN:HG2	1.83	0.59
1:D:96:LEU:O	1:D:98:VAL:N	2.35	0.59
1:A:11:ARG:HB2	1:A:11:ARG:HH11	1.68	0.59
1:B:195:VAL:HG13	1:B:196:THR:H	1.69	0.58
1:D:110:ALA:HA	1:D:114:VAL:CG2	2.33	0.58
1:D:102:VAL:HG23	1:D:103:LEU:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:HG3	1:D:197:ARG:NH1	2.18	0.58
1:A:86:LEU:O	1:A:86:LEU:HD23	2.03	0.58
1:D:86:LEU:CD2	1:D:135:LEU:CD1	2.81	0.58
1:C:164:THR:O	1:C:167:VAL:HG12	2.03	0.58
1:C:163:GLY:O	1:C:167:VAL:HB	2.04	0.58
1:C:96:LEU:CB	1:C:103:LEU:HD12	2.33	0.58
1:B:14:ILE:HG21	1:B:50:PHE:CE2	2.39	0.58
3:F:16:DC:H2'	3:F:17:DG:C8	2.39	0.57
1:A:104:ARG:HG3	1:A:104:ARG:HH11	1.69	0.57
1:A:209:GLU:C	1:A:211:GLU:N	2.57	0.57
1:B:46:LEU:HD23	1:B:46:LEU:O	2.03	0.57
1:C:32:LEU:O	1:C:36:VAL:HG22	2.04	0.57
1:D:87:MET:O	1:D:90:THR:HB	2.05	0.57
1:A:188:LEU:O	1:A:192:MET:HG2	2.05	0.57
1:C:191:GLY:HA2	1:D:190:ARG:HD3	1.86	0.57
1:B:64:GLN:HA	1:B:67:THR:HG22	1.87	0.57
1:C:137:ASP:O	1:C:140:ARG:HB2	2.03	0.57
1:B:86:LEU:HB2	1:B:134:ARG:CG	2.27	0.56
1:C:159:CYS:O	1:C:160:SER:C	2.43	0.56
1:C:87:MET:HE3	1:C:205:ALA:HB2	1.86	0.56
1:A:151:ASP:HA	1:A:152:SER:CB	2.35	0.56
1:A:159:CYS:O	1:A:161:VAL:N	2.38	0.56
1:D:45:ALA:CB	3:F:1:DA:H2'	2.35	0.56
1:A:156:THR:HB	1:A:157:LEU:HG	1.87	0.56
1:C:198:ARG:O	1:C:202:VAL:HG23	2.05	0.56
1:B:204:LEU:O	1:B:208:LEU:CB	2.54	0.55
1:D:183:GLU:HA	1:D:186:TYR:CD2	2.40	0.55
1:B:7:ALA:CB	3:F:4:DA:H5"	2.34	0.55
1:B:62:GLU:C	1:B:64:GLN:H	2.10	0.55
1:A:69:ARG:HG2	1:A:69:ARG:NH1	2.22	0.55
1:A:34:GLU:HA	1:A:37:ALA:HB3	1.89	0.55
1:A:204:LEU:HD12	1:A:204:LEU:O	2.07	0.55
1:A:183:GLU:O	1:A:186:TYR:HB2	2.07	0.55
1:A:83:LEU:O	1:A:83:LEU:HD23	2.07	0.55
1:A:100:GLY:HA3	1:A:103:LEU:HD12	1.88	0.55
1:A:153:VAL:O	1:A:156:THR:OG1	2.23	0.55
1:D:101:PRO:HG2	1:D:102:VAL:H	1.72	0.55
1:C:36:VAL:HG12	1:C:41:VAL:HG23	1.88	0.54
1:D:98:VAL:O	1:D:100:GLY:N	2.40	0.54
1:D:68:SER:HA	1:D:93:MET:HE1	1.88	0.54
1:D:132:THR:HG23	1:D:136:LEU:HD23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLY:H	1:B:177:GLU:HG3	1.72	0.54
1:C:139:VAL:HG23	1:C:144:VAL:HB	1.89	0.54
1:D:45:ALA:N	3:F:1:DA:H2'	2.23	0.54
1:A:31:THR:CG2	1:A:34:GLU:HG2	2.38	0.54
1:A:6:ARG:H	1:A:6:ARG:NE	2.06	0.54
1:B:5:LEU:C	1:B:7:ALA:H	2.11	0.54
1:B:61:LEU:O	1:B:64:GLN:HB3	2.08	0.54
1:C:175:GLY:CA	1:C:176:ARG:HB3	2.29	0.54
1:C:208:LEU:O	1:C:212:THR:HB	2.08	0.54
3:F:9:DG:H2"	3:F:10:DG:H8	1.71	0.53
2:E:21:DA:N1	3:F:2:DT:O4	2.41	0.53
1:B:19:ALA:HB1	1:B:102:VAL:HA	1.90	0.53
2:E:16:DC:H2"	2:E:17:DG:N7	2.24	0.53
1:B:163:GLY:HA3	1:B:180:ARG:CZ	2.38	0.53
1:D:86:LEU:HD13	1:D:134:ARG:HG3	1.91	0.53
1:A:128:ARG:HG3	1:A:153:VAL:HG21	1.91	0.53
2:E:20:DT:H2"	2:E:21:DA:C8	2.44	0.53
1:B:21:LEU:CD1	1:B:25:ARG:NH2	2.72	0.52
2:E:9:DG:H2"	2:E:10:DA:H8	1.74	0.52
1:B:136:LEU:O	1:B:136:LEU:HG	2.10	0.52
1:D:90:THR:HG22	1:D:91:PHE:N	2.25	0.52
1:D:96:LEU:C	1:D:98:VAL:N	2.63	0.52
1:A:28:GLU:C	1:A:30:THR:N	2.62	0.52
1:B:30:THR:O	1:B:53:LYS:NZ	2.43	0.52
1:D:96:LEU:C	1:D:98:VAL:H	2.12	0.52
2:E:8:DG:H2"	2:E:9:DG:C8	2.45	0.52
1:A:158:VAL:O	1:A:162:VAL:HG23	2.10	0.52
1:A:28:GLU:HA	1:A:53:LYS:NZ	2.25	0.52
1:C:86:LEU:HD21	1:C:185:TRP:HH2	1.74	0.52
1:D:32:LEU:HD12	1:D:35:ILE:HD12	1.92	0.52
1:D:44:GLY:C	3:F:1:DA:H8	2.11	0.52
1:A:64:GLN:O	1:A:67:THR:N	2.43	0.52
1:C:95:ARG:HH11	1:C:96:LEU:HD11	1.75	0.52
1:B:139:VAL:HA	1:B:144:VAL:HG22	1.92	0.51
1:B:80:TYR:CG	1:B:84:GLU:HB2	2.44	0.51
2:E:19:DT:H2'	2:E:20:DT:H71	1.92	0.51
2:E:4:DT:C6	2:E:4:DT:H5'	2.45	0.51
1:D:157:LEU:O	1:D:161:VAL:HG12	2.10	0.51
1:D:43:LYS:O	1:D:46:LEU:HB3	2.10	0.51
2:E:6:DC:H2'	2:E:7:DG:C8	2.45	0.51
3:F:14:DC:OP2	3:F:14:DC:H2'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:DT:O4	3:F:19:DA:N1	2.44	0.51
1:A:36:VAL:HB	1:A:41:VAL:O	2.10	0.51
1:B:189:ILE:HG23	1:B:193:VAL:HG21	1.92	0.51
3:F:2:DT:H2"	3:F:3:DA:C8	2.45	0.51
1:A:185:TRP:O	1:A:189:ILE:HG13	2.10	0.51
1:A:67:THR:HA	1:A:70:ARG:HB3	1.91	0.51
1:B:153:VAL:HG11	1:B:192:MET:SD	2.51	0.51
1:C:177:GLU:N	1:C:178:PRO:HD2	2.26	0.51
1:D:50:PHE:N	1:D:50:PHE:CD2	2.78	0.51
1:A:41:VAL:CG1	1:A:45:ALA:HB3	2.40	0.51
1:C:5:LEU:CD1	3:F:21:DG:OP1	2.59	0.51
1:C:47:TYR:CD1	3:F:13:DT:C7	2.93	0.51
1:C:164:THR:HG21	1:D:158:VAL:HG12	1.92	0.51
1:D:188:LEU:HB3	1:D:192:MET:CE	2.41	0.51
3:F:2:DT:C2'	3:F:3:DA:H5'	2.34	0.51
1:B:86:LEU:HD12	1:B:185:TRP:CH2	2.46	0.51
1:A:45:ALA:HA	2:E:3:DA:H3'	1.93	0.51
1:B:80:TYR:CG	1:B:84:GLU:CB	2.94	0.50
1:C:144:VAL:O	1:C:194:PRO:HD3	2.11	0.50
1:D:23:ASP:HB2	1:D:108:ARG:HG3	1.92	0.50
2:E:21:DA:C5	2:E:22:DT:H2'	2.45	0.50
1:C:76:ASP:C	1:C:78:ARG:N	2.63	0.50
2:E:7:DG:H1	3:F:16:DC:N4	2.04	0.50
2:E:17:DG:N2	3:F:6:DC:C2	2.72	0.50
1:A:71:LEU:HA	1:A:74:ASP:OD1	2.12	0.50
1:C:70:ARG:NH1	1:C:71:LEU:CD1	2.74	0.50
1:D:41:VAL:HG23	1:D:42:THR:O	2.11	0.50
1:D:45:ALA:HB2	3:F:1:DA:C2'	2.42	0.50
1:D:47:TYR:OH	2:E:17:DG:H2"	2.12	0.50
2:E:7:DG:N2	3:F:16:DC:C2	2.77	0.50
1:D:10:THR:O	1:D:14:ILE:HG13	2.12	0.49
1:D:181:LEU:O	1:D:182:ALA:C	2.49	0.49
1:C:135:LEU:O	1:C:138:ALA:N	2.45	0.49
1:D:45:ALA:HB2	3:F:1:DA:C3'	2.42	0.49
3:F:2:DT:OP1	3:F:2:DT:H4'	2.12	0.49
1:A:139:VAL:CG2	1:A:144:VAL:HB	2.42	0.49
1:C:5:LEU:N	1:C:8:GLU:H	2.10	0.49
1:C:65:SER:OG	1:C:121:PRO:HB3	2.13	0.49
1:A:186:TYR:CD1	1:A:202:VAL:HG13	2.48	0.48
3:F:1:DA:H1'	3:F:2:DT:P	2.52	0.48
1:B:81:SER:O	1:B:82:SER:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:DC:C2'	2:E:7:DG:H8	2.19	0.48
1:C:103:LEU:O	1:C:104:ARG:C	2.52	0.48
1:D:117:ARG:HE	1:D:120:LEU:N	2.10	0.48
1:D:25:ARG:NH2	1:D:25:ARG:HG3	2.28	0.48
1:D:141:GLN:O	1:D:142:SER:HB2	2.12	0.48
1:A:151:ASP:HB3	1:A:153:VAL:CG2	2.30	0.48
1:A:153:VAL:C	1:A:155:HIS:HD2	2.15	0.48
1:A:196:THR:CG2	1:A:197:ARG:HD2	2.43	0.48
1:B:139:VAL:CG2	1:B:144:VAL:HG21	2.39	0.48
1:B:175:GLY:N	1:B:177:GLU:OE1	2.43	0.48
1:D:86:LEU:HD21	1:D:135:LEU:CD1	2.38	0.48
1:B:32:LEU:HD21	1:B:53:LYS:HB2	1.96	0.48
1:B:49:HIS:NE2	3:F:5:DA:OP2	2.38	0.48
1:A:190:ARG:NH2	1:B:145:HIS:CD2	2.82	0.47
1:A:65:SER:O	1:A:69:ARG:HG3	2.14	0.47
1:C:92:GLY:O	1:C:96:LEU:HD22	2.14	0.47
1:A:6:ARG:H	1:A:6:ARG:CZ	2.27	0.47
1:C:176:ARG:O	1:C:179:ARG:HB2	2.14	0.47
1:A:47:TYR:OH	3:F:16:DC:OP2	2.21	0.47
3:F:9:DG:H8	3:F:9:DG:H5"	1.79	0.47
1:A:198:ARG:O	1:A:199:ALA:C	2.52	0.47
1:B:195:VAL:HG13	1:B:196:THR:N	2.30	0.47
1:B:33:SER:HA	1:B:36:VAL:HG22	1.97	0.47
1:D:189:ILE:HD12	1:D:201:TYR:HB3	1.97	0.47
1:D:72:ALA:O	1:D:75:LEU:HG	2.14	0.47
1:D:42:THR:CG2	3:F:2:DT:OP2	2.61	0.47
1:A:121:PRO:O	1:A:122:HIS:C	2.52	0.47
1:A:36:VAL:HG23	1:A:37:ALA:N	2.29	0.47
1:A:78:ARG:HD2	1:A:80:TYR:CE2	2.50	0.47
1:C:180:ARG:HA	1:C:183:GLU:OE2	2.14	0.47
2:E:18:DT:C2'	2:E:19:DT:C6	2.97	0.47
1:D:105:ALA:O	1:D:109:LEU:HG	2.15	0.47
1:D:137:ASP:CG	1:D:140:ARG:HH11	2.18	0.47
1:C:6:ARG:NH2	2:E:6:DC:H4'	2.29	0.47
1:D:194:PRO:O	1:D:198:ARG:HB2	2.15	0.47
1:A:159:CYS:HA	1:A:162:VAL:HB	1.97	0.47
1:B:163:GLY:HA3	1:B:180:ARG:HH22	1.78	0.47
1:B:199:ALA:O	1:B:201:TYR:N	2.48	0.47
1:A:202:VAL:O	1:A:203:THR:C	2.53	0.46
1:B:190:ARG:HE	1:B:198:ARG:NH2	2.03	0.46
1:D:32:LEU:O	1:D:33:SER:C	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ARG:O	1:B:171:LEU:N	2.42	0.46
1:B:44:GLY:HA3	3:F:7:DG:O6	2.15	0.46
1:C:157:LEU:O	1:C:161:VAL:HG23	2.16	0.46
1:C:47:TYR:CE1	1:C:51:ALA:HA	2.50	0.46
1:B:124:PHE:C	1:B:126:GLU:N	2.69	0.46
1:C:156:THR:HG22	1:C:160:SER:OG	2.16	0.46
1:C:56:LEU:O	1:C:57:ALA:C	2.54	0.46
1:C:76:ASP:O	1:C:78:ARG:N	2.49	0.46
1:B:201:TYR:HA	1:B:204:LEU:HB3	1.97	0.46
1:C:189:ILE:HD13	1:C:201:TYR:HB3	1.98	0.46
1:C:117:ARG:H	1:C:120:LEU:HD13	1.81	0.46
1:D:101:PRO:O	1:D:102:VAL:C	2.54	0.46
1:D:69:ARG:HH11	1:D:69:ARG:CB	2.27	0.46
1:B:116:VAL:O	1:B:117:ARG:CB	2.64	0.46
1:D:44:GLY:O	3:F:1:DA:C8	2.66	0.46
1:C:109:LEU:HA	1:C:109:LEU:HD23	1.75	0.45
2:E:21:DA:C4	2:E:22:DT:H2'	2.52	0.45
1:C:148:ILE:HA	1:C:148:ILE:HD13	1.77	0.45
1:D:148:ILE:HG21	1:D:192:MET:HG2	1.98	0.45
1:A:107:LEU:O	1:A:111:THR:HG23	2.15	0.45
1:A:8:GLU:CD	1:A:8:GLU:C	2.75	0.45
1:C:82:SER:HB2	1:C:141:GLN:NE2	2.31	0.45
1:C:78:ARG:HD2	1:C:80:TYR:HE2	1.81	0.45
1:D:136:LEU:HD21	1:D:150:VAL:HG21	1.98	0.45
1:A:86:LEU:CD1	1:A:135:LEU:CD1	2.91	0.45
2:E:21:DA:C8	2:E:22:DT:H2'	2.51	0.45
3:F:14:DC:H2"	3:F:15:DC:C6	2.51	0.45
1:A:159:CYS:O	1:A:162:VAL:N	2.50	0.45
1:B:19:ALA:CB	1:B:60:ILE:HD11	2.46	0.45
1:C:96:LEU:O	1:C:97:CYS:C	2.52	0.45
1:D:197:ARG:HH11	1:D:197:ARG:CG	2.29	0.45
1:A:28:GLU:O	1:A:30:THR:N	2.50	0.45
1:D:96:LEU:O	1:D:99:GLN:N	2.50	0.45
1:A:28:GLU:C	1:A:30:THR:H	2.20	0.45
1:D:42:THR:CB	3:F:2:DT:OP2	2.65	0.45
1:D:84:GLU:O	1:D:88:ARG:HG3	2.17	0.45
1:B:179:ARG:NH2	1:B:179:ARG:HB3	2.32	0.45
1:D:159:CYS:O	1:D:161:VAL:N	2.50	0.45
1:B:100:GLY:HA2	1:B:101:PRO:HD2	1.84	0.44
1:D:149:ASP:O	1:D:153:VAL:HG23	2.17	0.44
1:D:62:GLU:O	1:D:66:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:C	1:A:152:SER:HB3	2.36	0.44
1:B:135:LEU:C	1:B:137:ASP:H	2.21	0.44
1:C:46:LEU:HD23	1:C:50:PHE:HB2	1.99	0.44
1:C:179:ARG:O	1:C:182:ALA:HB3	2.17	0.44
1:C:70:ARG:NH1	1:C:71:LEU:HD11	2.32	0.44
1:C:17:ALA:CB	1:C:39:ALA:HB2	2.46	0.44
1:D:42:THR:HG21	3:F:1:DA:C3'	2.47	0.44
1:D:45:ALA:HB2	3:F:1:DA:H3'	1.98	0.44
1:B:62:GLU:O	1:B:64:GLN:N	2.51	0.44
1:A:104:ARG:NH1	1:A:104:ARG:HG3	2.32	0.44
1:A:71:LEU:HG	1:A:71:LEU:O	2.17	0.44
1:A:73:LYS:HA	1:A:73:LYS:HD3	1.61	0.44
1:A:8:GLU:O	1:A:11:ARG:N	2.51	0.44
1:B:17:ALA:CB	1:B:39:ALA:HB2	2.48	0.44
1:B:201:TYR:O	1:B:204:LEU:N	2.51	0.44
1:C:6:ARG:HE	1:C:6:ARG:HB3	1.62	0.44
1:A:123:PRO:O	1:A:126:GLU:HB3	2.18	0.44
1:A:10:THR:O	1:A:13:THR:N	2.51	0.44
1:A:41:VAL:HG12	1:A:42:THR:O	2.17	0.44
1:C:139:VAL:HG13	1:C:140:ARG:HH22	1.83	0.43
1:C:33:SER:HB3	1:C:43:LYS:HE2	1.98	0.43
1:B:124:PHE:O	1:B:127:TRP:N	2.50	0.43
1:D:177:GLU:HB2	1:D:178:PRO:CD	2.47	0.43
1:D:48:PHE:HD2	1:D:49:HIS:HD2	1.65	0.43
1:B:10:THR:O	1:B:11:ARG:C	2.57	0.43
1:D:48:PHE:CD2	1:D:49:HIS:HD2	2.36	0.43
1:A:190:ARG:HH22	1:B:145:HIS:CD2	2.36	0.43
1:B:44:GLY:CA	3:F:7:DG:O6	2.66	0.43
1:C:138:ALA:O	1:C:142:SER:O	2.35	0.43
1:D:41:VAL:HG23	1:D:45:ALA:HB3	2.00	0.43
1:C:141:GLN:HG2	1:C:141:GLN:H	1.47	0.43
1:C:82:SER:HB3	1:C:138:ALA:HB2	1.99	0.43
1:A:23:ASP:HA	1:A:108:ARG:NE	2.33	0.43
1:A:73:LYS:HD3	1:A:76:ASP:OD2	2.18	0.43
1:A:139:VAL:HG23	1:A:144:VAL:HB	1.99	0.43
1:A:159:CYS:C	1:A:161:VAL:N	2.73	0.43
3:F:22:DT:O4'	3:F:22:DT:O2	2.34	0.43
1:B:32:LEU:HD21	1:B:53:LYS:CB	2.49	0.42
1:C:139:VAL:HG12	1:C:140:ARG:HH12	1.84	0.42
1:D:160:SER:C	1:D:162:VAL:H	2.23	0.42
3:F:15:DC:H2"	3:F:16:DC:OP2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:O	1:A:151:ASP:N	2.52	0.42
1:A:36:VAL:HG11	1:A:43:LYS:HA	1.99	0.42
1:A:41:VAL:HG13	1:A:45:ALA:HB3	2.00	0.42
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.60	0.42
1:B:27:TYR:OH	1:B:53:LYS:HG3	2.19	0.42
1:D:10:THR:OG1	1:D:49:HIS:CE1	2.72	0.42
2:E:7:DG:H2"	2:E:8:DG:OP2	2.20	0.42
1:A:28:GLU:H	1:A:28:GLU:CD	2.19	0.42
1:B:113:GLY:O	1:B:115:PRO:HD3	2.19	0.42
1:B:177:GLU:HB2	1:B:178:PRO:HD3	2.02	0.42
1:A:32:LEU:O	1:A:36:VAL:HG22	2.20	0.42
1:C:96:LEU:HA	1:C:99:GLN:HG2	2.01	0.42
1:D:10:THR:OG1	1:D:49:HIS:HE1	2.03	0.42
1:B:145:HIS:CE1	1:B:194:PRO:HD3	2.55	0.42
1:B:81:SER:O	1:B:84:GLU:OE2	2.37	0.42
1:D:116:VAL:HG22	1:D:120:LEU:HB3	2.00	0.42
1:A:125:THR:HG22	1:A:128:ARG:NH2	2.33	0.42
1:B:83:LEU:O	1:B:87:MET:HB2	2.19	0.42
3:F:2:DT:C2'	3:F:3:DA:C8	3.02	0.42
1:A:82:SER:H	1:A:141:GLN:HE22	1.67	0.42
1:A:28:GLU:O	1:A:29:SER:C	2.58	0.42
1:D:47:TYR:CE1	2:E:18:DT:H5'	2.54	0.42
1:A:185:TRP:O	1:A:186:TYR:C	2.58	0.42
1:B:14:ILE:CG2	1:B:50:PHE:HE2	2.30	0.42
1:C:19:ALA:CB	1:C:60:ILE:HD11	2.50	0.42
1:B:143:ASP:O	1:B:194:PRO:HD2	2.20	0.42
1:C:163:GLY:C	1:C:166:VAL:HB	2.40	0.42
1:C:84:GLU:HG3	1:C:204:LEU:CD2	2.50	0.42
1:D:45:ALA:HB2	3:F:1:DA:H2'	2.01	0.42
1:D:14:ILE:HD13	1:D:46:LEU:HA	2.02	0.42
1:D:83:LEU:HD12	1:D:201:TYR:CD1	2.55	0.42
1:D:85:ALA:O	1:D:89:LEU:N	2.49	0.41
1:A:158:VAL:HG12	1:A:159:CYS:N	2.35	0.41
1:C:199:ALA:O	1:C:200:ARG:C	2.59	0.41
1:B:91:PHE:HE2	1:B:185:TRP:CD1	2.39	0.41
1:B:118:PRO:HA	1:B:119:PRO:HA	1.82	0.41
1:C:44:GLY:HA3	2:E:9:DG:O6	2.21	0.41
1:D:178:PRO:HB2	1:D:209:GLU:HA	2.03	0.41
2:E:11:DC:C2'	2:E:12:DG:N7	2.82	0.41
1:A:60:ILE:HA	1:A:63:ILE:HD12	2.03	0.41
1:C:13:THR:HG22	1:C:39:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:LYS:O	1:C:75:LEU:N	2.54	0.41
1:C:96:LEU:N	1:C:96:LEU:HD13	2.34	0.41
3:F:16:DC:H2'	3:F:17:DG:N7	2.36	0.41
3:F:9:DG:C8	3:F:9:DG:H5"	2.56	0.41
1:B:54:GLU:CG	1:B:115:PRO:HB2	2.50	0.41
1:C:32:LEU:HB2	3:F:11:DC:OP2	2.20	0.41
1:B:145:HIS:HB2	1:B:148:ILE:HG23	2.02	0.41
3:F:21:DG:N2	3:F:22:DT:O4	2.54	0.41
1:B:138:ALA:HB1	1:B:143:ASP:HB2	2.03	0.41
1:B:139:VAL:CA	1:B:144:VAL:HG22	2.50	0.41
1:B:179:ARG:NH1	1:B:209:GLU:OE1	2.54	0.41
1:B:96:LEU:O	1:B:97:CYS:C	2.59	0.41
1:C:19:ALA:HB1	1:C:102:VAL:HA	2.03	0.41
1:D:180:ARG:CG	1:D:180:ARG:NH1	2.72	0.41
1:C:6:ARG:HD2	2:E:7:DG:H5'	2.03	0.41
3:F:1:DA:H2"	3:F:2:DT:OP2	2.10	0.41
1:A:130:ILE:CG2	1:A:131:ALA:N	2.84	0.41
1:C:208:LEU:HD23	1:C:208:LEU:HA	1.79	0.41
1:C:42:THR:O	1:C:45:ALA:N	2.54	0.41
1:D:101:PRO:O	1:D:104:ARG:N	2.54	0.41
1:C:28:GLU:CG	1:D:28:GLU:HB3	2.50	0.41
1:B:175:GLY:H	1:B:177:GLU:CG	2.33	0.40
1:B:176:ARG:NH1	1:B:179:ARG:HD3	2.36	0.40
1:B:189:ILE:HG23	1:B:193:VAL:CG2	2.50	0.40
1:D:66:ARG:O	1:D:69:ARG:HG2	2.21	0.40
1:B:210:GLN:H	1:B:210:GLN:NE2	2.18	0.40
1:D:37:ALA:C	1:D:39:ALA:H	2.25	0.40
1:A:150:VAL:HG23	1:A:151:ASP:OD2	2.22	0.40
1:B:21:LEU:HD11	1:B:25:ARG:HH21	1.84	0.40
1:B:62:GLU:C	1:B:64:GLN:N	2.74	0.40
1:C:165:ARG:O	1:C:165:ARG:HG2	2.20	0.40
1:C:73:LYS:HD3	1:C:74:ASP:N	2.36	0.40
1:B:122:HIS:HA	1:B:123:PRO:HD3	1.86	0.40
1:B:204:LEU:O	1:B:208:LEU:HD12	2.22	0.40
1:B:80:TYR:CG	1:B:84:GLU:HB3	2.57	0.40
1:C:5:LEU:HB3	3:F:21:DG:H5'	2.03	0.40
1:D:136:LEU:HD13	1:D:136:LEU:HA	1.50	0.40
1:D:178:PRO:C	1:D:180:ARG:H	2.24	0.40
1:D:32:LEU:HD12	1:D:32:LEU:HA	1.90	0.40
1:D:47:TYR:HH	2:E:17:DG:H2"	1.87	0.40
1:C:6:ARG:CZ	2:E:6:DC:H4'	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	188/215 (87%)	154 (82%)	19 (10%)	15 (8%)	1 6
1	B	200/215 (93%)	145 (72%)	41 (20%)	14 (7%)	1 8
1	C	194/215 (90%)	136 (70%)	45 (23%)	13 (7%)	1 9
1	D	185/215 (86%)	145 (78%)	30 (16%)	10 (5%)	2 14
All	All	767/860 (89%)	580 (76%)	135 (18%)	52 (7%)	1 9

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	153	VAL
1	A	160	SER
1	A	177	GLU
1	A	210	GLN
1	B	78	ARG
1	B	80	TYR
1	B	117	ARG
1	B	142	SER
1	B	190	ARG
1	C	162	VAL
1	D	99	GLN
1	D	102	VAL
1	D	121	PRO
1	A	29	SER
1	A	74	ASP
1	A	152	SER
1	A	154	ALA
1	B	6	ARG
1	B	208	LEU

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Mol	Chain	Res	Type
1	C	77	GLY
1	C	198	ARG
1	D	97	CYS
1	A	39	ALA
1	A	90	THR
1	A	199	ALA
1	B	9	GLN
1	B	82	SER
1	B	136	LEU
1	B	200	ARG
1	C	85	ALA
1	C	86	LEU
1	C	144	VAL
1	C	199	ALA
1	D	101	PRO
1	D	161	VAL
1	D	177	GLU
1	B	63	ILE
1	C	136	LEU
1	D	38	HIS
1	A	69	ARG
1	A	78	ARG
1	B	112	ALA
1	B	173	PRO
1	C	74	ASP
1	C	122	HIS
1	D	66	ARG
1	D	160	SER
1	A	150	VAL
1	C	16	GLY
1	C	41	VAL
1	C	163	GLY

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	148/171 (86%)	105 (71%)	43 (29%)	0 1
1	B	148/171 (86%)	119 (80%)	29 (20%)	1 7
1	C	153/171 (90%)	116 (76%)	37 (24%)	0 2
1	D	154/171 (90%)	121 (79%)	33 (21%)	1 5
All	All	603/684 (88%)	461 (76%)	142 (24%)	1 3

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	8	GLU
1	A	11	ARG
1	A	28	GLU
1	A	29	SER
1	A	32	LEU
1	A	33	SER
1	A	42	THR
1	A	46	LEU
1	A	49	HIS
1	A	56	LEU
1	A	65	SER
1	A	67	THR
1	A	69	ARG
1	A	73	LYS
1	A	74	ASP
1	A	76	ASP
1	A	86	LEU
1	A	99	GLN
1	A	102	VAL
1	A	108	ARG
1	A	111	THR
1	A	130	ILE
1	A	133	SER
1	A	134	ARG
1	A	135	LEU
1	A	136	LEU
1	A	142	SER
1	A	146	GLN
1	A	148	ILE
1	A	151	ASP
1	A	155	HIS
1	A	156	THR

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Mol	Chain	Res	Type
1	A	157	LEU
1	A	159	CYS
1	A	177	GLU
1	A	180	ARG
1	A	181	LEU
1	A	184	MET
1	A	196	THR
1	A	197	ARG
1	A	207	ARG
1	A	208	LEU
1	B	6	ARG
1	B	8	GLU
1	B	15	ILE
1	B	21	LEU
1	B	61	LEU
1	B	65	SER
1	B	69	ARG
1	B	74	ASP
1	B	75	LEU
1	B	84	GLU
1	B	86	LEU
1	B	88	ARG
1	B	98	VAL
1	B	99	GLN
1	B	111	THR
1	B	125	THR
1	B	134	ARG
1	B	136	LEU
1	B	147	ASP
1	B	150	VAL
1	B	152	SER
1	B	153	VAL
1	B	160	SER
1	B	179	ARG
1	B	195	VAL
1	B	197	ARG
1	B	208	LEU
1	B	210	GLN
1	B	212	THR
1	C	6	ARG
1	C	29	SER
1	C	30	THR

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Mol	Chain	Res	Type
1	C	31	THR
1	C	32	LEU
1	C	36	VAL
1	C	54	GLU
1	C	60	ILE
1	C	62	GLU
1	C	73	LYS
1	C	75	LEU
1	C	82	SER
1	C	86	LEU
1	C	96	LEU
1	C	107	LEU
1	C	120	LEU
1	C	125	THR
1	C	133	SER
1	C	134	ARG
1	C	140	ARG
1	C	141	GLN
1	C	143	ASP
1	C	148	ILE
1	C	157	LEU
1	C	164	THR
1	C	167	VAL
1	C	177	GLU
1	C	179	ARG
1	C	180	ARG
1	C	188	LEU
1	C	195	VAL
1	C	196	THR
1	C	197	ARG
1	C	207	ARG
1	C	209	GLU
1	C	211	GLU
1	C	212	THR
1	D	8	GLU
1	D	23	ASP
1	D	32	LEU
1	D	42	THR
1	D	50	PHE
1	D	54	GLU
1	D	66	ARG
1	D	73	LYS

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Mol	Chain	Res	Type
1	D	74	ASP
1	D	80	TYR
1	D	89	LEU
1	D	99	GLN
1	D	102	VAL
1	D	107	LEU
1	D	116	VAL
1	D	120	LEU
1	D	122	HIS
1	D	129	GLU
1	D	133	SER
1	D	135	LEU
1	D	136	LEU
1	D	146	GLN
1	D	151	ASP
1	D	156	THR
1	D	157	LEU
1	D	164	THR
1	D	176	ARG
1	D	179	ARG
1	D	180	ARG
1	D	184	MET
1	D	194	PRO
1	D	197	ARG
1	D	211	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	146	GLN
1	A	155	HIS
1	B	122	HIS
1	B	141	GLN
1	B	145	HIS
1	C	38	HIS
1	C	58	HIS
1	C	64	GLN
1	C	145	HIS
1	D	49	HIS
1	D	64	GLN
1	D	141	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	194/215 (90%)	-0.10	1 (0%) 91 86	51, 83, 130, 148	1 (0%)
1	B	204/215 (94%)	-0.10	3 (1%) 73 61	51, 89, 143, 199	0
1	C	200/215 (93%)	-0.10	1 (0%) 91 86	47, 89, 149, 186	1 (0%)
1	D	193/215 (89%)	-0.00	3 (1%) 72 59	52, 82, 131, 169	0
2	E	20/22 (90%)	0.36	0 100 100	52, 65, 102, 112	1 (5%)
3	F	22/22 (100%)	0.60	3 (13%) 3 2	53, 64, 132, 152	3 (13%)
All	All	833/904 (92%)	-0.05	11 (1%) 77 65	47, 85, 138, 199	6 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	164	THR	7.3
1	B	121	PRO	4.3
3	F	22	DT	3.1
3	F	20	DT	2.8
1	D	166	VAL	2.8
3	F	21	DG	2.7
1	C	188	LEU	2.5
1	B	119	PRO	2.4
1	B	164	THR	2.1
1	D	163	GLY	2.1
1	A	5	LEU	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.