Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:55 PM GMT

PDB ID	:	1D5Y
Title	:	CRYSTAL STRUCTURE OF THE E. COLI ROB TRANSCRIPTION FACTOR IN COMPLEX WITH DNA
Authors	:	Kwon, H.J.; Bennik, M.H.J.; Demple, B.; Ellenberger, T.
Deposited on	:	1999-10-12
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

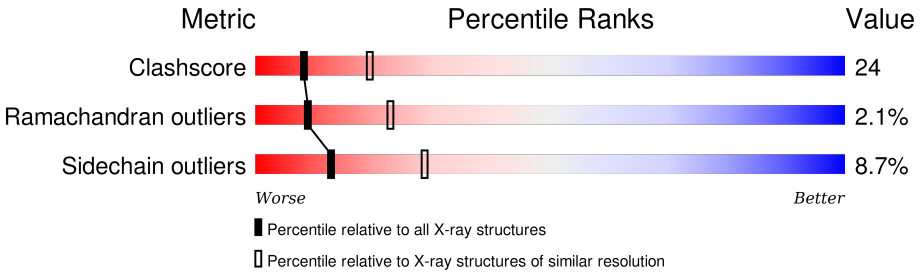
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	M	21	86% 14%
1	O	21	86% 14%
2	N	21	57% 43%
2	P	21	38% 62%
3	A	292	58% 35% 5% •
3	B	292	57% 37% 5% •
3	C	292	57% 36% 6% •

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Mol	Chain	Length	Quality of chain
3	D	292	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10986 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called DNA (5'-D(*TP*GP*AP*CP*AP*GP*CP*AP*CP*TP*GP*AP*AP*TP*GP*TP*CP*AP*AP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	21	Total	C	N	O	P	0	0	0
			431	206	85	120	20			
1	O	21	Total	C	N	O	P	0	0	0
			431	206	85	120	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	21	Total	C	N	O	P	0	0	0
			424	205	71	128	20			
2	P	21	Total	C	N	O	P	0	0	0
			424	205	71	128	20			

- Molecule 3 is a protein called ROB TRANSCRIPTION FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	288	Total	C	N	O	S	0	0	0
			2331	1490	408	423	10			
3	D	288	Total	C	N	O	S	0	0	0
			2307	1471	405	421	10			
3	C	288	Total	C	N	O	S	0	0	0
			2331	1490	408	423	10			
3	B	288	Total	C	N	O	S	0	0	0
			2307	1471	405	421	10			

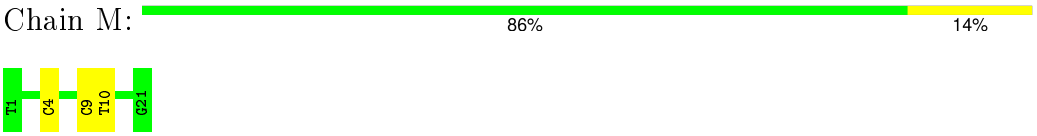
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

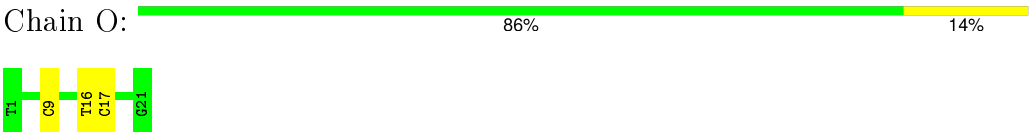
• Molecule 1: DNA (5'-D(*TP*GP*AP*CP*AP*GP*CP*AP*CP*TP*GP*AP*AP*TP*GP*TP*CP*AP*AP*AP*G)-3')

Chain M:



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

Chain O:



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

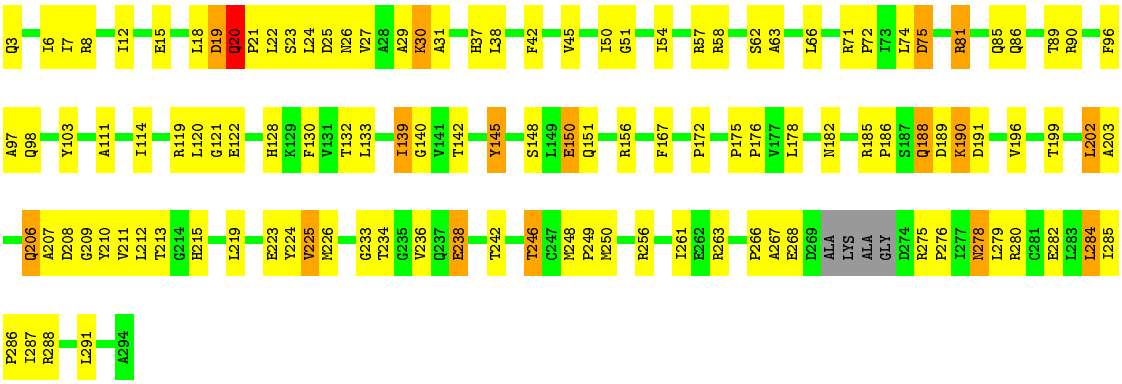
Chain N:

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

Chain P:

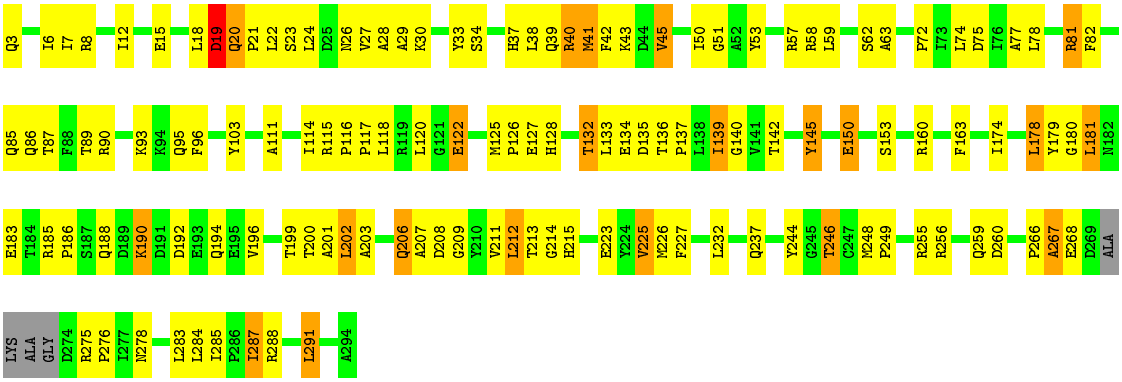
• Molecule 3: ROB TRANSCRIPTION FACTOR

Chain A:



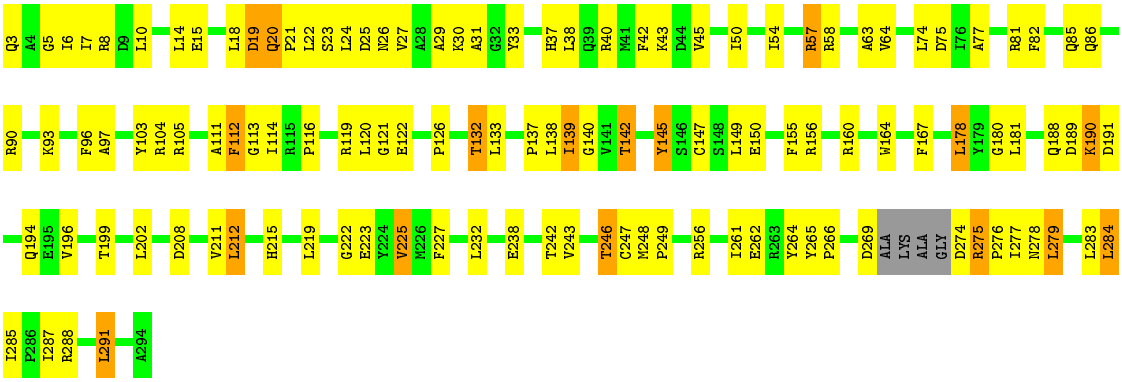
• Molecule 3: ROB TRANSCRIPTION FACTOR

Chain D:



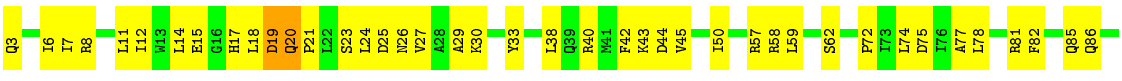
• Molecule 3: ROB TRANSCRIPTION FACTOR

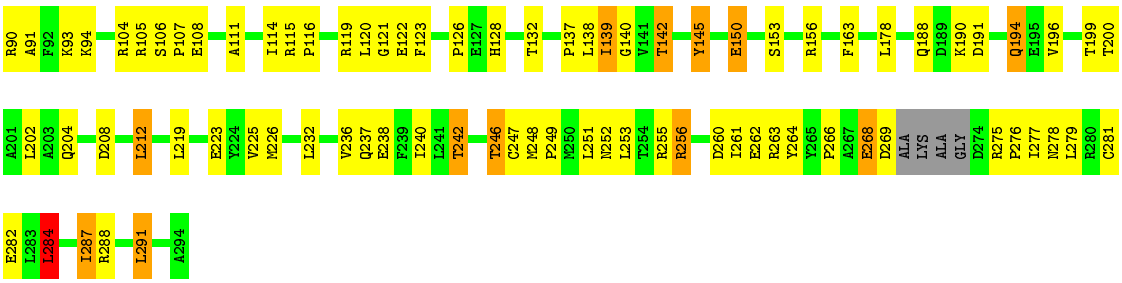
Chain C:



• Molecule 3: ROB TRANSCRIPTION FACTOR

Chain B:




R90 A91 F92 K93 K94 R104 R105 S106 P107 E108 A111 I114 R115 P116 R119 L120 G121 E122 F123 P126 E127 H128 T132 P137 L138 I139 G140 V141 T142 Y145 E150 S153 R156 F163 L178 Q188 D189 K190 D191 Q194 E195 V196 T199 T200
A201 L202 A203 Q204 D208 L212 L219 E223 Y224 V225 M226 L232 V236 Q237 E238 F239 I240 L241 T242 T246 C247 M248 P249 M250 L251 M252 L253 T254 R255 R256 D260 I261 E262 R263 Y264 Y265 P266 A267 E268 D269 ALA LYS ALA GLY D274 R275 P276 I277 M278 L279 R280 C281
E282 L283 K284 I287 R288 L291 A294

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.38Å 208.01Å 67.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	95.1 (30.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10986	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

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	M	0.38	0/485	0.67	0/747
1	O	0.38	0/485	0.67	0/747
2	N	0.38	0/473	0.71	0/728
2	P	0.38	0/473	0.69	0/728
3	A	0.42	0/2389	0.70	0/3237
3	B	0.44	0/2362	0.69	1/3201 (0.0%)
3	C	0.43	0/2389	0.69	0/3237
3	D	0.43	0/2362	0.69	0/3201
All	All	0.42	0/11418	0.69	1/15826 (0.0%)

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
3	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	284	LEU	CA-CB-CG	5.98	129.05	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	145	TYR	Sidechain

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	M	431	0	237	2	0
1	O	431	0	237	2	0
2	N	424	0	241	5	0
2	P	424	0	241	12	0
3	A	2331	0	2304	124	0
3	B	2307	0	2272	106	0
3	C	2331	0	2304	132	0
3	D	2307	0	2272	137	0
All	All	10986	0	10108	515	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 24.

All (515) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:291:LEU:H	3:C:291:LEU:HD12	1.33	0.94
3:B:269:ASP:HB3	3:B:277:ILE:HD12	1.50	0.93
3:A:20:GLN:HB2	3:A:21:PRO:HD3	1.47	0.93
3:A:190:LYS:H	3:A:190:LYS:HZ2	1.16	0.93
3:A:7:ILE:HD12	3:A:45:VAL:HB	1.53	0.90
3:D:291:LEU:HD12	3:D:291:LEU:H	1.36	0.90
3:A:8:ARG:HA	3:A:120:LEU:HD12	1.56	0.88
3:C:20:GLN:HB2	3:C:21:PRO:HD3	1.55	0.87
3:C:139:ILE:HG21	3:C:212:LEU:HD13	1.57	0.86
3:C:37:HIS:HA	3:C:40:ARG:HH12	1.43	0.84
3:A:238:GLU:O	3:A:242:THR:HG23	1.77	0.84
3:A:71:ARG:HH21	3:A:75:ASP:HB3	1.43	0.84
3:B:20:GLN:HB2	3:B:21:PRO:HD3	1.60	0.82
3:C:190:LYS:H	3:C:190:LYS:HZ2	1.27	0.82
3:A:256:ARG:HD3	3:A:287:ILE:O	1.80	0.81
3:A:142:THR:HG22	3:A:199:THR:HG23	1.63	0.81
3:B:291:LEU:HD12	3:B:291:LEU:H	1.48	0.79
3:D:133:LEU:HD11	3:D:284:LEU:HD12	1.64	0.78
3:D:132:THR:HB	3:D:223:GLU:OE2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:ARG:HH11	3:C:40:ARG:HB2	1.49	0.78
3:A:71:ARG:NH2	3:A:75:ASP:HB3	1.99	0.78
3:D:212:LEU:O	3:D:213:THR:HG22	1.84	0.78
3:D:27:VAL:HG22	3:D:30:LYS:NZ	1.98	0.77
3:B:111:ALA:HA	3:B:114:ILE:HD13	1.66	0.77
3:C:3:GLN:HG2	3:C:6:ILE:HG13	1.66	0.77
3:A:96:PHE:HE2	3:A:114:ILE:HD12	1.50	0.77
2:P:18:DT:OP1	3:D:24:LEU:HD12	1.87	0.75
3:D:27:VAL:HA	3:D:30:LYS:HE3	1.69	0.74
3:A:7:ILE:HD12	3:A:45:VAL:CB	2.17	0.74
3:D:275:ARG:HB3	3:D:276:PRO:HD2	1.66	0.74
3:C:8:ARG:HA	3:C:120:LEU:HD12	1.68	0.74
3:B:104:ARG:HD3	3:B:194:GLN:HB3	1.70	0.73
3:C:269:ASP:HB3	3:C:277:ILE:HD12	1.70	0.73
3:D:20:GLN:H	3:D:20:GLN:NE2	1.87	0.73
3:C:3:GLN:HE21	3:C:5:GLY:HA3	1.52	0.73
3:A:7:ILE:CD1	3:A:42:PHE:HA	2.19	0.73
3:A:20:GLN:NE2	3:A:20:GLN:H	1.87	0.72
3:A:212:LEU:O	3:A:213:THR:HG22	1.88	0.72
3:A:29:ALA:C	3:A:31:ALA:H	1.93	0.72
3:A:111:ALA:HA	3:A:114:ILE:HD13	1.70	0.72
3:C:119:ARG:HH21	3:C:246:THR:HG21	1.52	0.71
3:B:3:GLN:HG2	3:B:6:ILE:HG13	1.70	0.71
3:D:59:LEU:HD12	3:D:95:GLN:OE1	1.91	0.71
3:D:22:LEU:HD13	3:D:81:ARG:HB3	1.73	0.71
3:C:24:LEU:CD2	3:C:27:VAL:HG23	2.21	0.71
3:C:291:LEU:HD12	3:C:291:LEU:N	2.06	0.70
3:C:111:ALA:HA	3:C:114:ILE:HD13	1.72	0.70
3:A:27:VAL:HG13	3:A:30:LYS:HZ1	1.56	0.70
3:C:3:GLN:HG3	3:C:5:GLY:H	1.54	0.70
3:D:266:PRO:C	3:D:268:GLU:H	1.95	0.70
3:A:203:ALA:HB3	3:A:206:GLN:HG2	1.73	0.70
3:A:188:GLN:HE21	3:A:188:GLN:HA	1.57	0.69
3:B:18:LEU:HD13	3:B:57:ARG:HB3	1.73	0.69
3:A:139:ILE:HG21	3:A:207:ALA:HB3	1.75	0.69
3:D:248:MET:HB2	3:D:249:PRO:HD3	1.75	0.68
3:A:27:VAL:HG13	3:A:30:LYS:NZ	2.08	0.68
3:A:8:ARG:HE	3:A:120:LEU:CB	2.06	0.68
3:D:19:ASP:HB2	3:D:20:GLN:NE2	2.09	0.68
3:C:119:ARG:NH2	3:C:246:THR:HG21	2.07	0.68
3:D:188:GLN:HA	3:D:188:GLN:HE21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:GLN:O	3:C:90:ARG:HG3	1.94	0.67
3:D:266:PRO:O	3:D:268:GLU:N	2.27	0.67
3:D:29:ALA:HA	3:D:38:LEU:HD12	1.75	0.67
3:D:207:ALA:HB1	3:D:211:VAL:HG23	1.76	0.67
3:B:27:VAL:HA	3:B:30:LYS:HE3	1.76	0.67
3:C:24:LEU:HD23	3:C:27:VAL:HG23	1.75	0.67
3:C:43:LYS:HD3	3:C:43:LYS:O	1.95	0.66
3:C:248:MET:HB2	3:C:249:PRO:HD3	1.76	0.66
3:D:15:GLU:OE2	3:D:57:ARG:NH1	2.28	0.66
3:C:142:THR:HG22	3:C:215:HIS:NE2	2.10	0.66
3:D:150:GLU:CD	3:D:150:GLU:H	1.99	0.66
3:B:291:LEU:HD12	3:B:291:LEU:N	2.10	0.66
3:A:266:PRO:C	3:A:268:GLU:H	1.99	0.66
3:A:20:GLN:HB2	3:A:21:PRO:CD	2.24	0.66
3:D:188:GLN:HA	3:D:188:GLN:NE2	2.11	0.65
3:A:24:LEU:HD11	3:A:26:ASN:HD22	1.60	0.65
2:P:14:DG:H4'	2:P:15:DT:OP1	1.96	0.65
3:B:15:GLU:OE2	3:B:57:ARG:HD3	1.96	0.65
3:D:20:GLN:HB2	3:D:21:PRO:HD3	1.78	0.65
3:C:29:ALA:C	3:C:31:ALA:H	1.99	0.65
3:A:7:ILE:CD1	3:A:45:VAL:HB	2.26	0.64
3:B:8:ARG:HE	3:B:120:LEU:CB	2.10	0.64
3:D:40:ARG:NH1	3:D:40:ARG:HB2	2.13	0.64
1:O:16:DT:H2"	1:O:17:DC:C6	2.31	0.64
3:C:50:ILE:O	3:C:54:ILE:HG13	1.97	0.64
3:A:74:LEU:HD13	3:A:85:GLN:HG3	1.78	0.64
3:D:203:ALA:HB3	3:D:206:GLN:HG2	1.80	0.64
3:A:8:ARG:HE	3:A:120:LEU:HB2	1.63	0.63
3:C:111:ALA:CB	3:C:249:PRO:HG3	2.28	0.63
3:A:50:ILE:HG12	3:A:54:ILE:HD11	1.81	0.63
3:A:15:GLU:OE2	3:A:57:ARG:NH1	2.31	0.63
1:M:4:DC:H2'	3:A:37:HIS:CD2	2.33	0.63
3:C:105:ARG:CZ	3:C:191:ASP:HB3	2.28	0.63
3:A:7:ILE:HD13	3:A:42:PHE:HA	1.80	0.62
3:A:27:VAL:HA	3:A:30:LYS:HE3	1.81	0.62
3:C:238:GLU:O	3:C:242:THR:HG23	1.99	0.62
3:A:142:THR:HG23	3:A:215:HIS:CE1	2.34	0.62
3:D:27:VAL:HG22	3:D:30:LYS:HZ2	1.65	0.62
3:C:7:ILE:CD1	3:C:42:PHE:HA	2.30	0.62
3:C:180:GLY:O	3:C:181:LEU:HD23	2.00	0.62
3:A:86:GLN:O	3:A:90:ARG:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:163:PHE:CD2	3:D:200:THR:HG22	2.35	0.62
3:A:248:MET:HB2	3:A:249:PRO:HD3	1.81	0.61
3:A:207:ALA:HB1	3:A:211:VAL:HG23	1.82	0.61
3:C:275:ARG:HB3	3:C:276:PRO:HD2	1.82	0.61
3:A:266:PRO:O	3:A:268:GLU:N	2.32	0.61
3:D:122:GLU:CD	3:D:122:GLU:H	2.02	0.61
3:B:15:GLU:OE2	3:B:57:ARG:NH1	2.24	0.61
3:D:8:ARG:HG2	3:D:8:ARG:HH11	1.66	0.61
3:C:74:LEU:HD13	3:C:85:GLN:HG3	1.82	0.61
3:B:3:GLN:HG2	3:B:6:ILE:CG1	2.31	0.60
3:C:7:ILE:HD12	3:C:45:VAL:HG21	1.83	0.60
3:B:248:MET:HB2	3:B:249:PRO:HD3	1.82	0.60
3:B:132:THR:HB	3:B:223:GLU:OE1	2.00	0.60
3:D:244:TYR:OH	3:D:260:ASP:OD1	2.12	0.60
3:C:40:ARG:NH1	3:C:40:ARG:HB2	2.16	0.60
3:C:22:LEU:HD13	3:C:81:ARG:HB3	1.82	0.60
3:A:7:ILE:HD11	3:A:42:PHE:HA	1.83	0.60
3:D:142:THR:HG22	3:D:199:THR:OG1	2.02	0.60
3:A:223:GLU:O	3:A:256:ARG:NH1	2.35	0.59
3:A:208:ASP:CG	3:A:209:GLY:H	2.06	0.59
3:C:181:LEU:HD22	3:C:261:ILE:HG12	1.84	0.59
3:D:72:PRO:HG2	3:D:75:ASP:OD1	2.03	0.59
3:D:24:LEU:H	3:D:24:LEU:HD23	1.67	0.59
3:D:27:VAL:HG22	3:D:30:LYS:HZ1	1.68	0.59
3:A:145:TYR:CE2	3:A:196:VAL:HG12	2.38	0.59
2:P:7:DA:H2"	2:P:8:DC:O5'	2.02	0.59
3:B:20:GLN:O	3:B:81:ARG:NE	2.35	0.59
3:D:59:LEU:O	3:D:62:SER:HB2	2.03	0.59
3:D:3:GLN:CG	3:D:6:ILE:HG13	2.32	0.59
3:D:24:LEU:HD23	3:D:27:VAL:H	1.68	0.59
3:D:208:ASP:CG	3:D:209:GLY:H	2.05	0.59
2:P:17:DC:C6	2:P:18:DT:H72	2.38	0.59
3:C:111:ALA:HB1	3:C:249:PRO:HG3	1.84	0.59
3:D:43:LYS:C	3:D:43:LYS:HD3	2.23	0.59
3:D:128:HIS:HA	3:D:226:MET:O	2.03	0.58
3:D:283:LEU:C	3:D:284:LEU:HD23	2.24	0.58
3:A:119:ARG:NH2	3:A:246:THR:HG21	2.18	0.58
3:A:23:SER:HA	3:A:27:VAL:HB	1.85	0.58
3:B:139:ILE:HD13	3:B:140:GLY:N	2.18	0.58
3:B:8:ARG:HE	3:B:120:LEU:HB3	1.69	0.58
3:B:256:ARG:HD3	3:B:287:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:140:GLY:HA3	3:D:201:ALA:HB2	1.84	0.58
3:D:58:ARG:NH2	3:D:81:ARG:HG3	2.18	0.58
3:A:8:ARG:HH11	3:A:8:ARG:HG2	1.68	0.58
3:B:20:GLN:NE2	3:B:20:GLN:H	2.01	0.57
3:B:7:ILE:HD13	3:B:42:PHE:HA	1.86	0.57
3:B:279:LEU:C	3:B:279:LEU:HD12	2.25	0.57
3:D:24:LEU:CD2	3:D:27:VAL:HG23	2.35	0.57
3:C:26:ASN:O	3:C:29:ALA:HB3	2.05	0.57
3:C:188:GLN:NE2	3:C:188:GLN:HA	2.20	0.57
2:N:8:DC:H2"	2:N:9:DA:OP2	2.04	0.57
3:A:24:LEU:CD2	3:A:27:VAL:HG23	2.35	0.57
3:A:24:LEU:HD23	3:A:24:LEU:H	1.70	0.56
3:A:275:ARG:HB3	3:A:276:PRO:HD2	1.86	0.56
3:C:3:GLN:CG	3:C:6:ILE:HG13	2.36	0.56
3:D:8:ARG:HA	3:D:120:LEU:HD12	1.87	0.56
3:D:43:LYS:HD3	3:D:43:LYS:O	2.05	0.56
3:C:269:ASP:HB3	3:C:277:ILE:CD1	2.34	0.56
3:A:148:SER:OG	3:A:151:GLN:HG3	2.05	0.56
3:A:190:LYS:H	3:A:190:LYS:NZ	1.96	0.56
3:C:7:ILE:HD13	3:C:42:PHE:HA	1.86	0.56
3:C:20:GLN:HB2	3:C:21:PRO:CD	2.31	0.56
3:D:225:VAL:CG2	3:D:287:ILE:HD13	2.36	0.56
3:B:3:GLN:CG	3:B:6:ILE:HG13	2.34	0.56
3:B:190:LYS:NZ	3:B:190:LYS:HB2	2.21	0.56
3:D:96:PHE:HE2	3:D:114:ILE:HD12	1.70	0.56
3:A:212:LEU:O	3:A:213:THR:CG2	2.53	0.56
3:A:142:THR:HG22	3:A:199:THR:CG2	2.33	0.55
3:D:139:ILE:HG21	3:D:207:ALA:HB3	1.86	0.55
3:D:8:ARG:O	3:D:12:ILE:HG12	2.06	0.55
3:C:139:ILE:HD13	3:C:139:ILE:C	2.26	0.55
3:A:29:ALA:O	3:A:31:ALA:N	2.39	0.55
3:A:7:ILE:HD12	3:A:45:VAL:CG2	2.36	0.55
3:C:139:ILE:CG2	3:C:212:LEU:HD22	2.37	0.55
3:A:63:ALA:HB1	3:A:103:TYR:OH	2.06	0.55
3:D:202:LEU:HD23	3:D:207:ALA:HB2	1.89	0.55
3:D:114:ILE:O	3:D:116:PRO:HD3	2.07	0.55
3:A:190:LYS:N	3:A:190:LYS:HZ2	1.95	0.55
3:C:3:GLN:HG3	3:C:5:GLY:N	2.19	0.55
3:C:181:LEU:HB2	3:C:199:THR:HB	1.89	0.55
1:O:9:DC:OP1	3:D:87:THR:HG23	2.07	0.55
3:A:202:LEU:HD23	3:A:207:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3:GLN:HG3	3:D:6:ILE:HG13	1.89	0.55
3:A:22:LEU:O	3:A:27:VAL:HG11	2.06	0.54
3:D:190:LYS:H	3:D:190:LYS:HZ2	1.55	0.54
3:C:188:GLN:HE21	3:C:188:GLN:HA	1.72	0.54
3:B:226:MET:HE1	3:B:282:GLU:OE1	2.08	0.54
3:B:226:MET:HE3	3:B:284:LEU:HD11	1.89	0.54
3:B:91:ALA:O	3:B:94:LYS:HB2	2.07	0.54
3:C:284:LEU:N	3:C:284:LEU:HD23	2.23	0.54
3:B:248:MET:CE	3:B:287:ILE:HD11	2.37	0.54
3:B:58:ARG:NH1	3:B:81:ARG:HB2	2.23	0.53
3:D:180:GLY:C	3:D:181:LEU:HD23	2.29	0.53
3:D:50:ILE:HG23	3:D:51:GLY:N	2.23	0.53
3:D:232:LEU:HD22	3:D:276:PRO:HB2	1.91	0.53
3:C:139:ILE:HG23	3:C:212:LEU:HD22	1.90	0.53
3:B:77:ALA:O	3:B:82:PHE:HB2	2.09	0.53
3:A:111:ALA:CB	3:A:249:PRO:HA	2.39	0.53
3:D:266:PRO:C	3:D:268:GLU:N	2.61	0.53
3:B:226:MET:HB2	3:B:284:LEU:HD13	1.91	0.53
2:P:11:DT:H2"	2:P:12:DC:C6	2.43	0.53
3:A:150:GLU:H	3:A:150:GLU:CD	2.11	0.53
3:D:139:ILE:HD13	3:D:140:GLY:N	2.24	0.53
3:D:179:TYR:HB3	3:D:181:LEU:HD21	1.91	0.53
3:B:126:PRO:HD2	3:B:247:CYS:SG	2.49	0.53
3:A:15:GLU:OE2	3:A:57:ARG:HD3	2.09	0.53
3:C:133:LEU:HD11	3:C:284:LEU:HD12	1.91	0.53
3:C:156:ARG:NH1	3:C:262:GLU:OE1	2.42	0.53
3:A:156:ARG:HH21	3:A:182:ASN:CG	2.12	0.53
3:C:137:PRO:O	3:C:138:LEU:HD23	2.09	0.53
3:C:40:ARG:HH11	3:C:40:ARG:CB	2.21	0.52
3:C:24:LEU:H	3:C:27:VAL:HB	1.74	0.52
3:A:188:GLN:NE2	3:A:188:GLN:HA	2.24	0.52
3:C:15:GLU:OE2	3:C:57:ARG:NH1	2.29	0.52
3:D:20:GLN:HE21	3:D:21:PRO:HD3	1.74	0.52
3:C:139:ILE:HD12	3:C:212:LEU:HB3	1.91	0.52
3:A:18:LEU:HD11	3:A:57:ARG:HB3	1.91	0.52
3:A:29:ALA:C	3:A:31:ALA:N	2.63	0.52
3:D:7:ILE:HD12	3:D:45:VAL:HG11	1.92	0.52
3:B:291:LEU:H	3:B:291:LEU:CD1	2.22	0.52
2:P:17:DC:H2"	2:P:18:DT:C6	2.45	0.52
3:C:232:LEU:HD12	3:C:278:ASN:ND2	2.25	0.52
3:C:139:ILE:HD13	3:C:140:GLY:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:ARG:HH22	3:D:81:ARG:HG3	1.74	0.51
3:C:111:ALA:CA	3:C:114:ILE:HD13	2.38	0.51
3:B:108:GLU:CD	3:B:288:ARG:HH22	2.14	0.51
3:C:7:ILE:HG22	3:C:120:LEU:HD11	1.92	0.51
3:B:105:ARG:NH2	3:B:191:ASP:HB3	2.25	0.51
3:C:24:LEU:H	3:C:24:LEU:HD23	1.75	0.51
3:A:188:GLN:HE21	3:A:188:GLN:CA	2.19	0.51
3:B:119:ARG:HD2	3:B:123:PHE:HB2	1.92	0.51
3:D:142:THR:HG23	3:D:215:HIS:CE1	2.46	0.51
3:A:19:ASP:HB2	3:A:20:GLN:NE2	2.25	0.51
3:C:20:GLN:NE2	3:C:20:GLN:H	2.08	0.51
3:C:132:THR:HB	3:C:223:GLU:OE2	2.10	0.51
3:D:27:VAL:HA	3:D:30:LYS:CE	2.37	0.51
3:B:105:ARG:CZ	3:B:191:ASP:HB3	2.41	0.51
3:A:42:PHE:CE2	3:A:50:ILE:HA	2.46	0.51
3:A:24:LEU:CD1	3:A:26:ASN:HD22	2.23	0.51
3:C:114:ILE:N	3:C:114:ILE:HD12	2.26	0.51
3:B:8:ARG:HE	3:B:120:LEU:HB2	1.74	0.51
3:A:142:THR:HG23	3:A:215:HIS:HE1	1.76	0.51
3:D:57:ARG:HD2	3:D:117:PRO:HA	1.93	0.51
3:C:180:GLY:C	3:C:181:LEU:HD23	2.31	0.51
3:B:188:GLN:HA	3:B:188:GLN:HE21	1.76	0.51
3:A:20:GLN:H	3:A:20:GLN:CD	2.15	0.50
3:D:37:HIS:ND1	3:D:40:ARG:HD3	2.25	0.50
3:C:18:LEU:O	3:C:19:ASP:O	2.29	0.50
3:B:86:GLN:O	3:B:90:ARG:HG3	2.11	0.50
3:D:212:LEU:O	3:D:213:THR:CG2	2.57	0.50
3:A:58:ARG:NH2	3:A:81:ARG:HG3	2.26	0.50
3:B:3:GLN:N	3:B:6:ILE:HD12	2.26	0.50
3:A:130:PHE:CE2	3:A:225:VAL:HG13	2.46	0.50
2:P:1:DA:H2"	2:P:2:DC:O5'	2.09	0.50
3:A:8:ARG:HE	3:A:120:LEU:HB3	1.76	0.50
3:B:24:LEU:CD2	3:B:27:VAL:HG23	2.41	0.50
3:A:266:PRO:C	3:A:268:GLU:N	2.64	0.50
3:C:283:LEU:C	3:C:284:LEU:HD23	2.31	0.50
3:A:190:LYS:NZ	3:A:190:LYS:HB2	2.27	0.50
3:A:286:PRO:O	3:A:287:ILE:HD12	2.12	0.50
3:B:114:ILE:O	3:B:116:PRO:HD3	2.11	0.50
3:C:264:TYR:C	3:C:266:PRO:HD3	2.32	0.50
3:D:181:LEU:HD23	3:D:181:LEU:N	2.27	0.50
3:D:111:ALA:CB	3:D:249:PRO:HA	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:24:LEU:HD23	3:A:27:VAL:HG23	1.94	0.50
3:B:8:ARG:HG2	3:B:8:ARG:HH11	1.76	0.50
3:B:253:LEU:HD13	3:B:287:ILE:HG12	1.93	0.50
3:C:22:LEU:HB2	3:C:81:ARG:HD2	1.93	0.50
3:D:3:GLN:HG2	3:D:6:ILE:HG13	1.94	0.50
3:D:41:MET:O	3:D:45:VAL:HG23	2.12	0.50
3:A:62:SER:O	3:A:66:LEU:HG	2.12	0.50
3:C:142:THR:CG2	3:C:215:HIS:NE2	2.75	0.49
3:A:246:THR:O	3:A:250:MET:HB2	2.12	0.49
3:A:167:PHE:CE1	3:A:207:ALA:HA	2.47	0.49
3:B:188:GLN:HA	3:B:188:GLN:NE2	2.27	0.49
3:C:265:TYR:CD1	3:C:265:TYR:N	2.81	0.49
3:B:20:GLN:HB2	3:B:21:PRO:CD	2.39	0.49
3:C:114:ILE:O	3:C:116:PRO:HD3	2.13	0.49
3:A:261:ILE:HB	3:A:284:LEU:HB2	1.94	0.49
3:B:219:LEU:HD23	3:B:219:LEU:C	2.32	0.49
3:B:114:ILE:HD12	3:B:114:ILE:N	2.26	0.49
3:A:111:ALA:HB3	3:A:249:PRO:HA	1.95	0.49
3:B:24:LEU:HD23	3:B:27:VAL:H	1.77	0.49
3:D:115:ARG:NH2	3:D:116:PRO:HD2	2.28	0.49
3:B:212:LEU:HD12	3:B:212:LEU:N	2.27	0.49
3:D:145:TYR:CE2	3:D:196:VAL:HG12	2.47	0.49
3:D:34:SER:O	3:D:38:LEU:HB2	2.13	0.49
3:D:174:ILE:HG21	3:D:267:ALA:HB2	1.95	0.49
3:B:153:SER:HB3	3:B:237:GLN:OE1	2.13	0.49
3:B:15:GLU:OE2	3:B:18:LEU:HD11	2.13	0.49
3:D:39:GLN:O	3:D:43:LYS:N	2.44	0.49
3:D:89:THR:O	3:D:93:LYS:HG3	2.13	0.49
3:D:24:LEU:HG	3:D:26:ASN:H	1.78	0.48
3:D:86:GLN:O	3:D:90:ARG:HG3	2.13	0.48
3:C:24:LEU:HG	3:C:26:ASN:H	1.78	0.48
3:B:23:SER:HA	3:B:27:VAL:HB	1.96	0.48
3:B:72:PRO:HG2	3:B:75:ASP:OD1	2.13	0.48
3:C:139:ILE:HG23	3:C:139:ILE:O	2.12	0.48
3:D:63:ALA:HB1	3:D:103:TYR:OH	2.13	0.48
3:D:188:GLN:CA	3:D:188:GLN:HE21	2.20	0.48
3:A:275:ARG:HH12	3:C:291:LEU:HD21	1.79	0.48
3:A:96:PHE:CE2	3:A:114:ILE:HD12	2.41	0.48
3:B:212:LEU:H	3:B:212:LEU:HD12	1.79	0.48
3:D:24:LEU:CD2	3:D:27:VAL:H	2.27	0.48
3:D:7:ILE:HD11	3:D:42:PHE:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:128:HIS:HA	3:B:226:MET:O	2.14	0.48
2:N:2:DC:H2"	2:N:3:DT:OP2	2.14	0.48
3:A:139:ILE:CG2	3:A:207:ALA:HB3	2.42	0.48
3:A:278:ASN:HA	3:A:278:ASN:HD22	1.54	0.48
3:C:77:ALA:O	3:C:82:PHE:HB2	2.13	0.48
2:N:17:DC:H2"	2:N:18:DT:OP2	2.14	0.48
3:C:63:ALA:HB1	3:C:103:TYR:OH	2.15	0.47
3:A:7:ILE:HG22	3:A:120:LEU:HD11	1.95	0.47
3:A:27:VAL:HG13	3:A:30:LYS:CE	2.44	0.47
3:C:24:LEU:HD23	3:C:27:VAL:CG2	2.42	0.47
3:A:139:ILE:HG21	3:A:207:ALA:CB	2.44	0.47
3:B:142:THR:HB	3:B:199:THR:OG1	2.15	0.47
3:C:37:HIS:HA	3:C:40:ARG:NH1	2.22	0.47
2:N:1:DA:H2"	2:N:2:DC:O5'	2.13	0.47
3:C:43:LYS:C	3:C:43:LYS:HD3	2.35	0.47
3:B:40:ARG:HH11	3:B:44:ASP:HB2	1.80	0.47
3:A:233:GLY:O	3:A:236:VAL:HG23	2.14	0.47
3:C:6:ILE:HD13	3:C:33:TYR:OH	2.14	0.47
3:B:139:ILE:HG23	3:B:212:LEU:HD22	1.96	0.47
3:D:256:ARG:HD3	3:D:287:ILE:O	2.15	0.47
3:A:24:LEU:O	3:A:25:ASP:C	2.53	0.47
3:B:248:MET:HE1	3:B:287:ILE:HD11	1.95	0.47
3:C:211:VAL:O	3:C:211:VAL:HG22	2.14	0.47
3:C:104:ARG:HD3	3:C:194:GLN:HB3	1.97	0.47
3:A:50:ILE:HG23	3:A:51:GLY:N	2.29	0.47
3:D:153:SER:OG	3:D:237:GLN:HB2	2.15	0.47
3:A:22:LEU:HD13	3:A:81:ARG:HB3	1.96	0.47
3:D:40:ARG:HH11	3:D:40:ARG:HB2	1.78	0.47
3:D:190:LYS:NZ	3:D:190:LYS:HB2	2.29	0.47
3:A:63:ALA:HB1	3:A:103:TYR:CE2	2.50	0.46
3:B:261:ILE:HB	3:B:284:LEU:HB2	1.98	0.46
3:C:22:LEU:HD12	3:C:23:SER:H	1.81	0.46
3:C:147:CYS:HB3	3:C:155:PHE:CE2	2.50	0.46
3:D:226:MET:HE2	3:D:284:LEU:HD21	1.97	0.46
3:C:24:LEU:HD21	3:C:27:VAL:HG23	1.98	0.46
3:D:24:LEU:HD23	3:D:24:LEU:N	2.29	0.46
3:C:160:ARG:HG2	3:C:178:LEU:HD11	1.97	0.46
3:B:137:PRO:O	3:B:138:LEU:HD23	2.16	0.46
3:D:7:ILE:CD1	3:D:42:PHE:HA	2.46	0.46
2:P:15:DT:H2"	2:P:16:DG:OP2	2.15	0.46
3:D:183:GLU:HG2	3:D:259:GLN:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:175:PRO:HA	3:A:176:PRO:HD3	1.79	0.46
3:A:119:ARG:HH21	3:A:246:THR:HG21	1.79	0.46
3:B:29:ALA:HA	3:B:38:LEU:HD12	1.97	0.46
3:A:133:LEU:HD12	3:A:224:TYR:CE1	2.51	0.46
3:A:285:ILE:HG23	3:A:286:PRO:HD2	1.98	0.46
3:C:269:ASP:CB	3:C:277:ILE:HD12	2.43	0.46
3:D:160:ARG:HG3	3:D:178:LEU:HD13	1.98	0.46
3:D:15:GLU:OE2	3:D:18:LEU:HD11	2.16	0.46
3:B:242:THR:HA	3:B:246:THR:HG23	1.97	0.46
3:C:242:THR:HA	3:C:246:THR:HG23	1.97	0.46
3:A:63:ALA:HB1	3:A:103:TYR:CZ	2.51	0.46
3:B:232:LEU:HD12	3:B:278:ASN:ND2	2.31	0.46
3:A:279:LEU:C	3:A:279:LEU:HD12	2.37	0.46
3:C:145:TYR:CE2	3:C:196:VAL:HG12	2.51	0.46
3:D:226:MET:CE	3:D:284:LEU:HD21	2.46	0.45
3:C:27:VAL:HG13	3:C:30:LYS:CE	2.45	0.45
3:C:29:ALA:C	3:C:31:ALA:N	2.67	0.45
3:C:22:LEU:HB2	3:C:81:ARG:CD	2.46	0.45
3:B:275:ARG:HB3	3:B:276:PRO:HD2	1.98	0.45
3:A:172:PRO:HD2	3:A:210:TYR:CE1	2.51	0.45
3:B:150:GLU:CD	3:B:150:GLU:H	2.18	0.45
3:D:255:ARG:HH11	3:D:255:ARG:HG2	1.80	0.45
3:D:284:LEU:N	3:D:284:LEU:HD23	2.31	0.45
3:D:223:GLU:O	3:D:256:ARG:NH1	2.50	0.45
3:D:178:LEU:HD23	3:D:202:LEU:CD1	2.47	0.45
3:B:8:ARG:O	3:B:12:ILE:HG12	2.17	0.45
3:B:251:LEU:O	3:B:252:ASN:C	2.54	0.45
3:C:126:PRO:HD2	3:C:247:CYS:SG	2.56	0.45
3:B:27:VAL:HA	3:B:30:LYS:CE	2.45	0.45
3:B:59:LEU:O	3:B:62:SER:HB2	2.17	0.45
3:D:256:ARG:HG2	3:D:288:ARG:HB2	1.99	0.45
3:C:96:PHE:HE2	3:C:114:ILE:HD12	1.82	0.45
3:B:139:ILE:C	3:B:139:ILE:HD13	2.36	0.45
3:C:188:GLN:CA	3:C:188:GLN:HE21	2.28	0.45
3:B:40:ARG:NH1	3:B:44:ASP:HB2	2.32	0.45
3:C:225:VAL:HG23	3:C:287:ILE:HD13	1.98	0.45
3:D:139:ILE:HG23	3:D:139:ILE:O	2.16	0.45
3:B:7:ILE:CD1	3:B:42:PHE:HA	2.47	0.45
3:D:134:GLU:O	3:D:135:ASP:C	2.56	0.45
3:B:268:GLU:OE1	3:B:268:GLU:O	2.35	0.45
3:B:105:ARG:HG3	3:B:191:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:139:ILE:HD13	3:A:140:GLY:N	2.33	0.44
3:B:238:GLU:O	3:B:242:THR:CG2	2.66	0.44
3:D:63:ALA:HB1	3:D:103:TYR:CZ	2.52	0.44
3:D:225:VAL:HG23	3:D:287:ILE:HD13	1.98	0.44
3:A:8:ARG:NE	3:A:120:LEU:HB2	2.31	0.44
3:A:8:ARG:O	3:A:12:ILE:HG12	2.17	0.44
3:C:190:LYS:NZ	3:C:190:LYS:HB2	2.32	0.44
3:C:8:ARG:HG2	3:C:8:ARG:HH11	1.83	0.44
3:A:18:LEU:CD1	3:A:57:ARG:HB3	2.47	0.44
3:B:266:PRO:C	3:B:268:GLU:H	2.19	0.44
3:C:20:GLN:HE21	3:C:21:PRO:HD3	1.83	0.44
3:C:58:ARG:CZ	3:C:81:ARG:HB2	2.48	0.44
3:D:248:MET:HE1	3:D:287:ILE:HD11	2.00	0.44
3:D:23:SER:HA	3:D:27:VAL:HB	1.98	0.44
3:D:77:ALA:O	3:D:82:PHE:HB2	2.17	0.44
3:B:246:THR:C	3:B:249:PRO:HD2	2.37	0.44
3:C:15:GLU:OE2	3:C:57:ARG:HD3	2.18	0.44
3:B:3:GLN:HG2	3:B:6:ILE:CD1	2.48	0.44
3:D:116:PRO:HB3	3:D:246:THR:HB	1.99	0.44
3:A:97:ALA:O	3:A:98:GLN:HB2	2.16	0.43
3:A:285:ILE:HG22	3:A:287:ILE:CD1	2.48	0.43
3:D:136:THR:HA	3:D:137:PRO:HD3	1.89	0.43
3:C:219:LEU:HD23	3:C:219:LEU:C	2.38	0.43
3:B:74:LEU:O	3:B:78:LEU:HG	2.19	0.43
3:B:106:SER:HA	3:B:107:PRO:HD3	1.84	0.43
3:C:227:PHE:HE1	3:C:285:ILE:HD12	1.83	0.43
3:B:266:PRO:C	3:B:268:GLU:N	2.72	0.43
3:D:248:MET:HE1	3:D:285:ILE:HG21	1.99	0.43
3:D:12:ILE:N	3:D:12:ILE:HD13	2.33	0.43
3:D:7:ILE:HD12	3:D:45:VAL:HG21	2.01	0.43
3:B:24:LEU:HG	3:B:26:ASN:H	1.83	0.43
2:P:10:DT:H2"	2:P:11:DT:OP2	2.18	0.43
3:A:22:LEU:HD13	3:A:81:ARG:HD3	2.00	0.43
3:D:139:ILE:CG2	3:D:207:ALA:HB3	2.49	0.43
3:C:243:VAL:O	3:C:248:MET:HG2	2.19	0.43
3:A:219:LEU:HD23	3:A:219:LEU:C	2.39	0.43
3:A:185:ARG:HA	3:A:186:PRO:HD3	1.84	0.43
3:D:226:MET:HE3	3:D:226:MET:HB2	1.87	0.43
3:C:164:TRP:O	3:C:167:PHE:HB3	2.19	0.43
3:C:112:PHE:CD2	3:C:113:GLY:N	2.87	0.43
3:D:275:ARG:HB3	3:D:276:PRO:CD	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:43:LYS:O	3:B:43:LYS:HD3	2.19	0.43
3:A:22:LEU:HD12	3:A:23:SER:H	1.83	0.42
3:C:111:ALA:C	3:C:114:ILE:HD13	2.39	0.42
3:D:38:LEU:O	3:D:41:MET:HB3	2.19	0.42
3:C:291:LEU:H	3:C:291:LEU:CD1	2.13	0.42
3:B:119:ARG:HH21	3:B:246:THR:HG21	1.83	0.42
3:B:17:HIS:C	3:B:19:ASP:N	2.69	0.42
3:C:18:LEU:HD13	3:C:57:ARG:HB3	2.01	0.42
3:D:259:GLN:HB3	3:D:259:GLN:HE21	1.66	0.42
3:A:3:GLN:CG	3:A:6:ILE:HG13	2.49	0.42
3:C:279:LEU:HD12	3:C:279:LEU:C	2.39	0.42
3:A:263:ARG:HD2	3:A:282:GLU:OE1	2.19	0.42
3:B:248:MET:N	3:B:249:PRO:CD	2.82	0.42
3:B:145:TYR:CE2	3:B:196:VAL:HG12	2.54	0.42
3:B:226:MET:CE	3:B:284:LEU:HD11	2.50	0.42
3:B:264:TYR:CD2	3:B:281:CYS:HB3	2.54	0.42
3:A:275:ARG:O	3:A:276:PRO:C	2.57	0.42
3:D:139:ILE:HD11	3:D:214:GLY:HA3	2.01	0.42
3:B:93:LYS:HB3	3:B:93:LYS:HE2	1.75	0.42
3:C:139:ILE:HG21	3:C:212:LEU:CD1	2.38	0.42
3:A:287:ILE:HG23	3:A:288:ARG:N	2.34	0.42
3:D:127:GLU:O	3:D:227:PHE:HA	2.20	0.42
2:N:11:DT:H2"	2:N:12:DC:C6	2.55	0.42
3:A:72:PRO:HG2	3:A:75:ASP:OD1	2.20	0.42
3:C:274:ASP:O	3:C:274:ASP:CG	2.58	0.42
3:C:7:ILE:HD12	3:C:45:VAL:CG2	2.49	0.42
3:D:7:ILE:CD1	3:D:45:VAL:HG21	2.50	0.42
3:B:247:CYS:O	3:B:251:LEU:HG	2.19	0.42
3:B:78:LEU:O	3:B:81:ARG:N	2.52	0.41
3:C:63:ALA:HB1	3:C:103:TYR:CE2	2.55	0.41
3:B:266:PRO:HA	3:B:269:ASP:OD2	2.19	0.41
3:D:226:MET:HB2	3:D:284:LEU:HD22	2.01	0.41
3:A:128:HIS:HA	3:A:226:MET:O	2.20	0.41
3:C:291:LEU:N	3:C:291:LEU:CD1	2.76	0.41
3:D:24:LEU:HD21	3:D:27:VAL:HG23	2.01	0.41
3:D:139:ILE:O	3:D:139:ILE:CG2	2.68	0.41
2:P:15:DT:H1'	2:P:16:DG:H5'	2.02	0.41
3:B:42:PHE:CD2	3:B:50:ILE:HB	2.55	0.41
3:C:18:LEU:CD1	3:C:57:ARG:HB3	2.50	0.41
3:D:185:ARG:HA	3:D:186:PRO:HD3	1.92	0.41
3:A:26:ASN:O	3:A:29:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:208:ASP:CG	3:A:209:GLY:N	2.73	0.41
3:C:266:PRO:HA	3:C:269:ASP:OD2	2.21	0.41
3:D:28:ALA:O	3:D:38:LEU:HD11	2.20	0.41
3:B:190:LYS:HZ3	3:B:190:LYS:HB2	1.84	0.41
3:B:163:PHE:HB3	3:B:200:THR:HG21	2.02	0.41
3:A:50:ILE:CG1	3:A:54:ILE:HD11	2.50	0.41
3:A:89:THR:O	3:A:90:ARG:C	2.59	0.41
2:P:8:DC:H2"	2:P:9:DA:OP2	2.21	0.41
3:B:226:MET:HE1	3:B:263:ARG:NH1	2.35	0.41
3:B:156:ARG:NH1	3:B:262:GLU:OE1	2.53	0.41
3:A:114:ILE:HG21	3:A:249:PRO:HG2	2.03	0.41
3:C:27:VAL:HA	3:C:30:LYS:HE3	2.02	0.41
3:C:64:VAL:HG12	3:C:149:LEU:HD11	2.02	0.41
3:C:96:PHE:O	3:C:97:ALA:HB3	2.21	0.41
3:D:7:ILE:HD12	3:D:45:VAL:CB	2.51	0.41
3:C:132:THR:HA	3:C:222:GLY:O	2.20	0.41
3:D:125:MET:O	3:D:126:PRO:C	2.59	0.41
3:C:8:ARG:HA	3:C:120:LEU:CD1	2.46	0.41
3:C:242:THR:O	3:C:246:THR:HG23	2.21	0.41
3:D:178:LEU:HD23	3:D:178:LEU:HA	1.95	0.41
3:C:14:LEU:O	3:C:18:LEU:HG	2.21	0.41
3:C:63:ALA:HB1	3:C:103:TYR:CZ	2.56	0.41
3:D:190:LYS:HB3	3:D:192:ASP:OD1	2.20	0.41
1:M:9:DC:H2"	1:M:10:DT:OP2	2.21	0.41
3:B:236:VAL:O	3:B:240:ILE:HG13	2.21	0.41
3:D:74:LEU:O	3:D:78:LEU:HG	2.21	0.41
3:D:256:ARG:CG	3:D:288:ARG:HB2	2.50	0.40
3:C:287:ILE:HG23	3:C:288:ARG:N	2.36	0.40
3:D:59:LEU:HD21	3:D:82:PHE:CZ	2.56	0.40
3:D:188:GLN:CA	3:D:188:GLN:NE2	2.78	0.40
3:D:37:HIS:O	3:D:38:LEU:C	2.59	0.40
3:B:24:LEU:HD21	3:B:26:ASN:HB2	2.03	0.40
3:C:188:GLN:CA	3:C:188:GLN:NE2	2.83	0.40
3:B:11:LEU:HD23	3:B:14:LEU:HD12	2.03	0.40
2:P:17:DC:H2"	2:P:18:DT:H6	1.85	0.40
3:C:7:ILE:HD11	3:C:42:PHE:HA	2.01	0.40
3:B:255:ARG:NH2	3:B:260:ASP:OD2	2.50	0.40
3:D:53:TYR:CE1	3:D:118:LEU:HG	2.57	0.40
3:D:22:LEU:HB2	3:D:81:ARG:HD2	2.04	0.40
3:D:139:ILE:HD13	3:D:139:ILE:C	2.42	0.40
3:C:232:LEU:HD12	3:C:278:ASN:HD21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:232:LEU:CD1	3:C:278:ASN:HD21	2.35	0.40
3:A:275:ARG:NH1	3:C:291:LEU:HD21	2.36	0.40
3:C:8:ARG:C	3:C:10:LEU:H	2.25	0.40
3:B:7:ILE:HD12	3:B:45:VAL:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	284/292 (97%)	256 (90%)	20 (7%)	8 (3%)	6 15
3	B	284/292 (97%)	239 (84%)	41 (14%)	4 (1%)	14 35
3	C	284/292 (97%)	252 (89%)	27 (10%)	5 (2%)	11 27
3	D	284/292 (97%)	252 (89%)	25 (9%)	7 (2%)	7 18
All	All	1136/1168 (97%)	999 (88%)	113 (10%)	24 (2%)	9 23

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	19	ASP
3	A	267	ALA
3	D	19	ASP
3	D	33	TYR
3	D	267	ALA
3	C	19	ASP
3	C	112	PHE
3	C	189	ASP
3	C	208	ASP
3	B	19	ASP
3	B	208	ASP

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Mol	Chain	Res	Type
3	A	30	LYS
3	A	81	ARG
3	A	206	GLN
3	D	45	VAL
3	D	206	GLN
3	C	121	GLY
3	B	121	GLY
3	A	189	ASP
3	A	20	GLN
3	D	41	MET
3	D	81	ARG
3	B	33	TYR
3	A	121	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	
3	A	246/247 (100%)	225 (92%)	21 (8%)	13	30
3	B	242/247 (98%)	221 (91%)	21 (9%)	13	29
3	C	246/247 (100%)	223 (91%)	23 (9%)	11	25
3	D	242/247 (98%)	222 (92%)	20 (8%)	14	31
All	All	976/988 (99%)	891 (91%)	85 (9%)	13	29

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	20	GLN
3	A	38	LEU
3	A	75	ASP
3	A	122	GLU
3	A	132	THR
3	A	139	ILE
3	A	145	TYR
3	A	150	GLU

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Mol	Chain	Res	Type
3	A	178	LEU
3	A	188	GLN
3	A	190	LYS
3	A	191	ASP
3	A	202	LEU
3	A	225	VAL
3	A	234	THR
3	A	238	GLU
3	A	246	THR
3	A	278	ASN
3	A	280	ARG
3	A	284	LEU
3	A	291	LEU
3	D	19	ASP
3	D	20	GLN
3	D	40	ARG
3	D	85	GLN
3	D	122	GLU
3	D	132	THR
3	D	139	ILE
3	D	145	TYR
3	D	150	GLU
3	D	178	LEU
3	D	181	LEU
3	D	190	LYS
3	D	194	GLN
3	D	202	LEU
3	D	212	LEU
3	D	225	VAL
3	D	246	THR
3	D	278	ASN
3	D	287	ILE
3	D	291	LEU
3	C	20	GLN
3	C	25	ASP
3	C	38	LEU
3	C	57	ARG
3	C	75	ASP
3	C	93	LYS
3	C	122	GLU
3	C	132	THR
3	C	139	ILE

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Mol	Chain	Res	Type
3	C	142	THR
3	C	145	TYR
3	C	150	GLU
3	C	178	LEU
3	C	190	LYS
3	C	202	LEU
3	C	212	LEU
3	C	225	VAL
3	C	246	THR
3	C	256	ARG
3	C	275	ARG
3	C	279	LEU
3	C	284	LEU
3	C	291	LEU
3	B	20	GLN
3	B	25	ASP
3	B	85	GLN
3	B	115	ARG
3	B	122	GLU
3	B	139	ILE
3	B	142	THR
3	B	150	GLU
3	B	178	LEU
3	B	194	GLN
3	B	202	LEU
3	B	204	GLN
3	B	212	LEU
3	B	225	VAL
3	B	242	THR
3	B	246	THR
3	B	256	ARG
3	B	268	GLU
3	B	284	LEU
3	B	287	ILE
3	B	291	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	17	HIS
3	A	20	GLN
3	A	26	ASN

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Mol	Chain	Res	Type
3	A	37	HIS
3	A	188	GLN
3	A	215	HIS
3	A	252	ASN
3	A	278	ASN
3	D	3	GLN
3	D	20	GLN
3	D	26	ASN
3	D	98	GLN
3	D	188	GLN
3	D	215	HIS
3	D	252	ASN
3	D	259	GLN
3	D	278	ASN
3	C	3	GLN
3	C	17	HIS
3	C	20	GLN
3	C	98	GLN
3	C	188	GLN
3	C	204	GLN
3	C	252	ASN
3	C	278	ASN
3	B	17	HIS
3	B	20	GLN
3	B	26	ASN
3	B	79	GLN
3	B	98	GLN
3	B	188	GLN
3	B	278	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

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.