



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:41 PM UTC

PDB ID : 1D5Y / pdb_00001d5y
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

<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

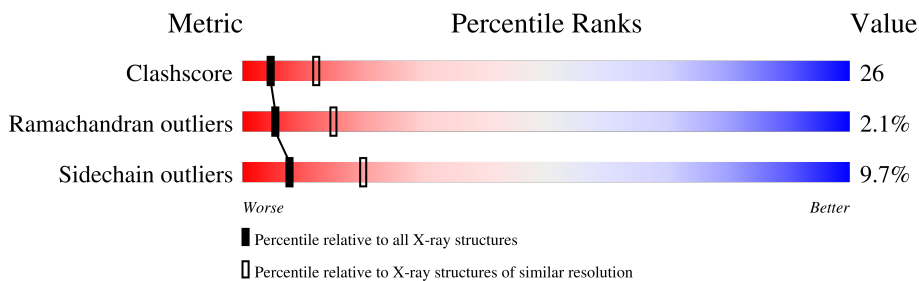
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	M	21	81% 19%
1	O	21	86% 14%
2	N	21	57% 43%
2	P	21	38% 62%
3	A	292	54% 37% 7% ..
3	B	292	52% 39% 7% .
3	C	292	54% 37% 7% ..
3	D	292	50% 38% 9% ..

2 Entry composition

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, 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. 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. 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.

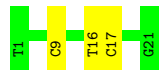
- Molecule 1: DNA (5'-D(*TP*GP*AP*CP*AP*GP*CP*AP*CP*TP*GP*AP*AP*TP*GP*TP*CP*AP*AP*AP*G)-3')

Chain M:  81% 19%



- 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:  86% 14%

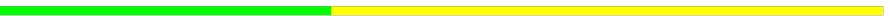


- Molecule 2: DNA (5'-D(*AP*CP*TP*TP*TP*GP*AP*CP*AP*TP*TP*CP*AP*GP*TP*GP*CP*TP*GP*TP*C)-3')

Chain N:  57% 43%



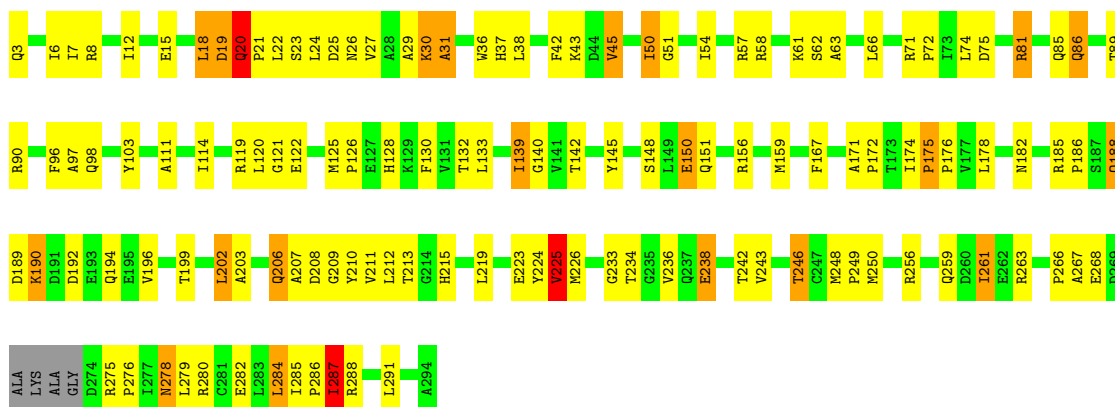
- Molecule 2: DNA (5'-D(*AP*CP*TP*TP*TP*GP*AP*CP*AP*TP*TP*CP*AP*GP*TP*GP*CP*TP*GP*TP*C)-3')

Chain P:  38% 62%

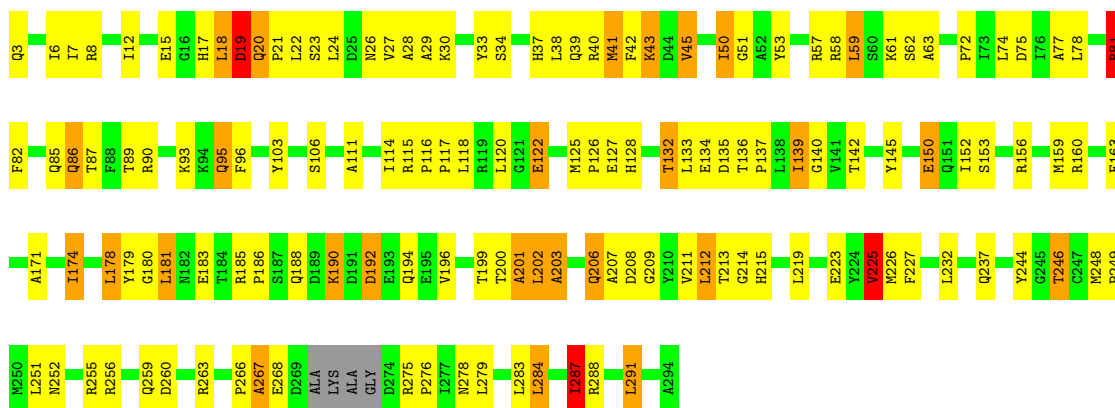


- Molecule 3: ROB TRANSCRIPTION FACTOR

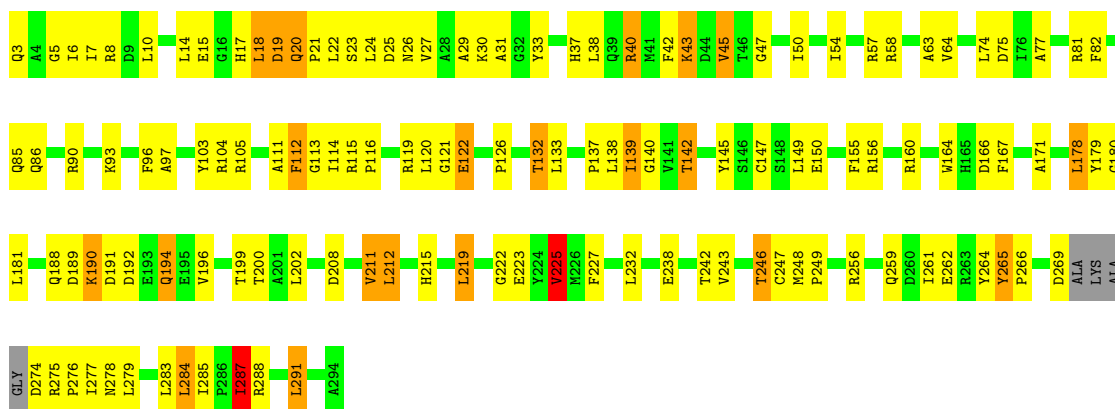
Chain A:  54% 37% 7% ..



• Molecule 3: ROB TRANSCRIPTION FACTOR

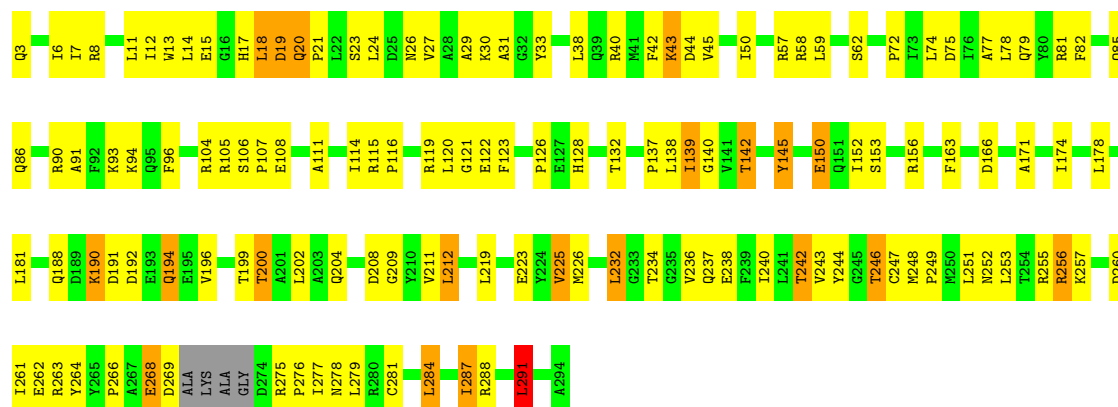


- Molecule 3: ROB TRANSCRIPTION FACTOR



• Molecule 3: ROB TRANSCRIPTION FACTOR





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	0.30	0/485	0.58	0/747
1	O	0.31	0/485	0.58	0/747
2	N	0.31	0/473	0.68	0/728
2	P	0.31	0/473	0.65	0/728
3	A	0.52	0/2389	1.07	15/3237 (0.5%)
3	B	0.54	0/2362	1.05	14/3201 (0.4%)
3	C	0.52	0/2389	1.05	15/3237 (0.5%)
3	D	0.54	0/2362	1.06	20/3201 (0.6%)
All	All	0.50	0/11418	0.99	64/15826 (0.4%)

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 (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	18	LEU	N-CA-C	-9.88	100.35	111.71
3	A	192	ASP	N-CA-C	-9.32	101.16	114.12
3	D	171	ALA	CA-C-N	9.16	128.81	119.56
3	D	171	ALA	C-N-CA	9.16	128.81	119.56
3	D	192	ASP	N-CA-C	-9.11	101.88	113.72
3	B	192	ASP	N-CA-C	-8.73	102.37	113.72
3	B	18	LEU	N-CA-C	-8.22	102.36	112.38
3	A	171	ALA	CA-C-N	7.94	127.58	119.56
3	A	171	ALA	C-N-CA	7.94	127.58	119.56
3	C	192	ASP	N-CA-C	-7.92	104.09	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	171	ALA	N-CA-C	7.37	119.49	109.24
3	B	115	ARG	CA-C-N	7.22	124.93	119.66
3	B	115	ARG	C-N-CA	7.22	124.93	119.66
3	D	174	ILE	N-CA-C	7.05	115.66	107.77
3	A	18	LEU	N-CA-C	-7.00	103.66	111.71
3	D	152	ILE	N-CA-C	6.99	117.50	110.23
3	D	50	ILE	N-CA-C	6.98	117.69	110.36
3	A	287	ILE	N-CA-C	6.82	120.20	108.95
3	D	18	LEU	N-CA-C	-6.69	104.01	111.71
3	B	174	ILE	N-CA-C	6.62	115.18	107.77
3	D	106	SER	CA-C-N	6.32	125.81	119.24
3	D	106	SER	C-N-CA	6.32	125.81	119.24
3	C	265	TYR	CA-C-N	6.27	126.39	119.87
3	C	265	TYR	C-N-CA	6.27	126.39	119.87
3	D	81	ARG	N-CA-C	6.21	120.17	112.47
3	D	203	ALA	N-CA-C	-6.16	100.72	109.96
3	A	45	VAL	N-CA-C	6.14	116.32	110.42
3	C	47	GLY	N-CA-C	-6.13	106.78	115.43
3	D	61	LYS	N-CA-C	-6.08	104.66	111.28
3	D	95	GLN	N-CA-C	5.93	117.54	111.14
3	D	171	ALA	N-CA-C	5.92	118.87	109.64
3	A	50	ILE	N-CA-C	5.91	116.56	110.36
3	A	175	PRO	CA-C-N	5.90	125.44	119.19
3	A	175	PRO	C-N-CA	5.90	125.44	119.19
3	C	45	VAL	N-CA-C	5.78	116.00	110.74
3	B	200	THR	N-CA-C	-5.75	99.81	109.07
3	C	171	ALA	N-CA-C	5.67	118.62	109.15
3	A	31	ALA	N-CA-C	-5.67	106.36	113.72
3	B	152	ILE	N-CA-C	5.64	116.09	110.23
3	D	287	ILE	N-CA-C	5.63	117.53	108.85
3	C	200	THR	N-CA-C	-5.62	100.02	109.07
3	C	179	TYR	N-CA-C	5.51	118.47	109.59
3	C	287	ILE	N-CA-C	5.44	117.62	109.20
3	A	174	ILE	N-CA-C	5.43	113.85	107.77
3	C	225	VAL	N-CA-C	-5.42	100.67	108.53
3	D	225	VAL	N-CA-C	-5.41	100.68	108.53
3	B	209	GLY	N-CA-C	5.39	121.01	112.06
3	B	257	LYS	N-CA-C	-5.35	103.08	110.35
3	C	166	ASP	N-CA-C	-5.28	105.60	111.36
3	A	225	VAL	N-CA-C	-5.23	100.94	108.53
3	B	96	PHE	N-CA-C	5.21	120.49	113.72
3	C	225	VAL	CB-CA-C	-5.20	102.91	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	261	ILE	N-CA-C	5.18	115.31	107.75
3	A	225	VAL	CB-CA-C	-5.17	102.95	110.81
3	D	201	ALA	N-CA-C	5.15	116.64	108.96
3	D	59	LEU	N-CA-C	-5.11	105.61	111.07
3	D	225	VAL	CB-CA-C	-5.08	103.08	110.81
3	D	263	ARG	CB-CG-CD	-5.07	99.63	111.30
3	B	166	ASP	N-CA-C	-5.06	105.76	111.28
3	B	225	VAL	CB-CA-C	-5.02	103.35	110.83
3	A	61	LYS	N-CA-C	-5.01	105.81	111.28
3	C	115	ARG	CA-C-N	5.01	123.27	119.66
3	C	115	ARG	C-N-CA	5.01	123.27	119.66
3	B	291	LEU	N-CA-C	-5.01	101.14	109.46

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 ⓘ

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	3	0
1	O	431	0	237	2	0
2	N	424	0	241	5	0
2	P	424	0	241	14	0
3	A	2331	0	2304	131	0
3	B	2307	0	2272	114	0
3	C	2331	0	2304	140	0
3	D	2307	0	2272	145	0
All	All	10986	0	10108	548	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 26.

All (548) 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:B:248:MET:HE1	3:B:287:ILE:HD11	1.42	1.00
3:A:190:LYS:H	3:A:190:LYS:HZ2	1.15	0.94
3:C:291:LEU:HD12	3:C:291:LEU:H	1.33	0.94
3:A:20:GLN:HB2	3:A:21:PRO:HD3	1.47	0.93
3:B:269:ASP:HB3	3:B:277:ILE:HD12	1.50	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:D:27:VAL:HG22	3:D:30:LYS:HZ2	1.36	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:D:248:MET:HE1	3:D:287:ILE:HD11	1.58	0.84
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:226:MET:HE3	3:B:284:LEU:HD11	1.58	0.83
3:B:20:GLN:HB2	3:B:21:PRO:HD3	1.60	0.82
3:C:190:LYS:H	3:C:190:LYS:HZ2	1.28	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:H	3:B:291:LEU:HD12	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
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:A:29:ALA:C	3:A:31:ALA:H	1.93	0.77
3:C:3:GLN:HG2	3:C:6:ILE:HG13	1.66	0.77
3:B:111:ALA:HA	3:B:114:ILE:HD13	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:266:PRO:C	3:D:268:GLU:H	1.95	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:248:MET:HE1	3:C:287:ILE:HD11	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:7:ILE:CD1	3:A:42:PHE:HA	2.19	0.73
3:A:20:GLN:H	3:A:20:GLN:NE2	1.87	0.72
3:A:212:LEU:O	3:A:213:THR:HG22	1.88	0.72
2:P:17:DC:C2'	2:P:18:DT:H71	2.19	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:150:GLU:CD	3:D:150:GLU:H	1.99	0.71
3:D:226:MET:HE2	3:D:284:LEU:HD21	1.72	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:111:ALA:HA	3:C:114:ILE:HD13	1.72	0.70
3:C:291:LEU:HD12	3:C:291:LEU:N	2.06	0.70
3:A:266:PRO:C	3:A:268:GLU:H	1.99	0.70
3:C:3:GLN:HG3	3:C:5:GLY:H	1.54	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:C:29:ALA:C	3:C:31:ALA:H	1.99	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:A:27:VAL:HG13	3:A:30:LYS:NZ	2.08	0.68
3:D:248:MET:HB2	3:D:249:PRO:HD3	1.75	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:D:188:GLN:HE21	3:D:188:GLN:HA	1.58	0.68
3:C:119:ARG:NH2	3:C:246:THR:HG21	2.07	0.68
3:D:156:ARG:HA	3:D:159:MET:HE3	1.75	0.68
2:P:17:DC:H2''	2:P:18:DT:H71	1.75	0.67
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:O	3:C:43:LYS:HD3	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:B:291:LEU:HD12	3:B:291:LEU:N	2.10	0.66
3:A:20:GLN:HB2	3:A:21:PRO:CD	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:122:GLU:CD	3:D:122:GLU:H	2.02	0.65
3:D:188:GLN:HA	3:D:188:GLN:NE2	2.11	0.65
2:P:14:DG:H4'	2:P:15:DT:OP1	1.96	0.65
3:A:24:LEU:HD11	3:A:26:ASN:HD22	1.60	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:A:7:ILE:CD1	3:A:45:VAL:HB	2.26	0.64
3:A:208:ASP:CG	3:A:209:GLY:H	2.06	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:A:74:LEU:HD13	3:A:85:GLN:HG3	1.78	0.64
3:C:50:ILE:O	3:C:54:ILE:HG13	1.97	0.64
3:D:203:ALA:HB3	3:D:206:GLN:HG2	1.80	0.64
3:D:208:ASP:CG	3:D:209:GLY:H	2.05	0.64
3:D:43:LYS:HD3	3:D:43:LYS:C	2.23	0.63
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:15:GLU:OE2	3:A:57:ARG:NH1	2.31	0.63
3:A:50:ILE:HG12	3:A:54:ILE:HD11	1.81	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:D:283:LEU:C	3:D:284:LEU:HD23	2.24	0.62
3:A:248:MET:HE1	3:A:287:ILE:HD11	1.81	0.62
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:C:7:ILE:CD1	3:C:42:PHE:HA	2.30	0.62
3:A:86:GLN:O	3:A:90:ARG:HG3	1.99	0.62
3:C:180:GLY:O	3:C:181:LEU:HD23	2.00	0.62
3:D:163:PHE:CD2	3:D:200:THR:HG22	2.35	0.62
3:A:207:ALA:HB1	3:A:211:VAL:HG23	1.82	0.61
3:A:248:MET:HB2	3:A:249:PRO:HD3	1.81	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:B:15:GLU:OE2	3:B:57:ARG:NH1	2.24	0.61
3:B:279:LEU:HD12	3:B:279:LEU:C	2.25	0.61
3:D:8:ARG:HH11	3:D:8:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	3:C:40:ARG:NH1	2.16	0.60
3:C:139:ILE:HD13	3:C:139:ILE:C	2.26	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: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
2:P:7:DA:H2''	2:P:8:DC:O5'	2.02	0.59
3:A:145:TYR:CE2	3:A:196:VAL:HG12	2.38	0.59
3:D:24:LEU:H	3:D:24:LEU:HD23	1.67	0.59
3:D:3:GLN:CG	3:D:6:ILE:HG13	2.32	0.59
3:D:59:LEU:O	3:D:62:SER:HB2	2.03	0.59
3:D:190:LYS:HZ2	3:D:190:LYS:HB2	1.67	0.59
3:B:20:GLN:O	3:B:81:ARG:NE	2.35	0.59
3:D:24:LEU:HD23	3:D:27:VAL:H	1.68	0.59
3:C:111:ALA:HB1	3:C:249:PRO:HG3	1.84	0.59
3:D:128:HIS:HA	3:D:226:MET:O	2.03	0.58
3:A:119:ARG:NH2	3:A:246:THR:HG21	2.18	0.58
3:D:180:GLY:C	3:D:181:LEU:HD23	2.29	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
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:HG2	3:A:8:ARG:HH11	1.68	0.58
3:B:7:ILE:HD13	3:B:42:PHE:HA	1.86	0.57
3:B:20:GLN:NE2	3:B:20:GLN:H	2.01	0.57
3:A:150:GLU:CD	3:A:150:GLU:H	2.11	0.57
3:A:156:ARG:HH21	3:A:182:ASN:CG	2.12	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:A:27:VAL:HG13	3:A:30:LYS:HZ1	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:190:LYS:HZ2	3:A:190:LYS:N	1.94	0.56
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: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:3:GLN:CG	3:C:6:ILE:HG13	2.36	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:B:108:GLU:CD	3:B:288:ARG:HH22	2.14	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:96:PHE:HE2	3:D:114:ILE:HD12	1.70	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:HB2	3:B:190:LYS:NZ	2.21	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:8:ARG:O	3:D:12:ILE:HG12	2.06	0.55
3:D:139:ILE:HG21	3:D:207:ALA:HB3	1.86	0.55
3:A:29:ALA:O	3:A:31:ALA:N	2.39	0.55
3:C:180:GLY:C	3:C:181:LEU:HD23	2.31	0.55
3:A:7:ILE:HD12	3:A:45:VAL:CG2	2.36	0.55
3:A:20:GLN:H	3:A:20:GLN:CD	2.15	0.55
3:A:63:ALA:HB1	3:A:103:TYR:OH	2.06	0.55
3:C:139:ILE:CG2	3:C:212:LEU:HD22	2.37	0.55
3:D:114:ILE:O	3:D:116:PRO:HD3	2.07	0.55
3:D:202:LEU:HD23	3:D:207:ALA:HB2	1.89	0.55
3:C:3:GLN:HG3	3:C:5:GLY:N	2.19	0.55
1:O:9:DC:OP1	3:D:87:THR:HG23	2.07	0.55
3:C:181:LEU:HB2	3:C:199:THR:HB	1.89	0.55
3:A:202:LEU:HD23	3:A:207:ALA:HB2	1.89	0.55
3:C:264:TYR:C	3:C:266:PRO:HD3	2.32	0.55
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:C:283:LEU:C	3:C:284:LEU:HD23	2.31	0.54
3:C:188:GLN:HA	3:C:188:GLN:HE21	1.72	0.54
2:P:17:DC:H2'	2:P:18:DT:H71	1.89	0.54
3:B:91:ALA:O	3:B:94:LYS:HB2	2.07	0.54
3:B:219:LEU:C	3:B:219:LEU:HD23	2.32	0.54
3:C:284:LEU:HD23	3:C:284:LEU:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:226:MET:HE3	3:B:284:LEU:CD1	2.32	0.54
3:A:266:PRO:C	3:A:268:GLU:N	2.64	0.54
3:B:58:ARG:NH1	3:B:81:ARG:HB2	2.23	0.53
3:B:226:MET:HE1	3:B:263:ARG:NH1	2.23	0.53
3:D:50:ILE:HG23	3:D:51:GLY:N	2.23	0.53
3:A:156:ARG:HA	3:A:159:MET:HE3	1.91	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
2:P:11:DT:H2''	2:P:12:DC:C6	2.43	0.53
3:A:29:ALA:C	3:A:31:ALA:N	2.63	0.53
3:A:111:ALA:CB	3:A:249:PRO:HA	2.39	0.53
3:B:226:MET:HB2	3:B:284:LEU:HD13	1.91	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:137:PRO:O	3:C:138:LEU:HD23	2.09	0.53
3:C:156:ARG:NH1	3:C:262:GLU:OE1	2.42	0.53
3:A:188:GLN:HA	3:A:188:GLN:NE2	2.24	0.52
3:C:24:LEU:H	3:C:27:VAL:HB	1.74	0.52
3:C:40:ARG:HH11	3:C:40:ARG:CB	2.21	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:A:18:LEU:HD11	3:A:57:ARG:HB3	1.91	0.52
3:C:139:ILE:HD12	3:C:212:LEU:HB3	1.91	0.52
3:D:7:ILE:HD12	3:D:45:VAL:HG11	1.92	0.52
3:C:43:LYS:HD3	3:C:43:LYS:C	2.35	0.52
2:P:17:DC:H2''	2:P:18:DT:C6	2.45	0.52
3:B:291:LEU:H	3:B:291:LEU:CD1	2.22	0.52
3:A:24:LEU:O	3:A:25:ASP:C	2.53	0.52
3:C:232:LEU:HD12	3:C:278:ASN:ND2	2.25	0.52
1:M:7:DC:H41	3:A:36:TRP:CG	2.26	0.51
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:C:139:ILE:HD13	3:C:140:GLY:N	2.25	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:HD23	3:C:24:LEU:H	1.75	0.51
3:A:188:GLN:HE21	3:A:188:GLN:CA	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:142:THR:HG23	3:D:215:HIS:CE1	2.46	0.51
3:B:119:ARG:HD2	3:B:123:PHE:HB2	1.92	0.51
3:A:19:ASP:HB2	3:A:20:GLN:NE2	2.25	0.51
3:C:20:GLN:H	3:C:20:GLN:NE2	2.08	0.51
3:C:29:ALA:C	3:C:31:ALA:N	2.67	0.51
3:C:132:THR:HB	3:C:223:GLU:OE2	2.10	0.51
3:B:139:ILE:HD13	3:B:139:ILE:C	2.36	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:24:LEU:CD1	3:A:26:ASN:HD22	2.23	0.51
3:A:42:PHE:CE2	3:A:50:ILE:HA	2.46	0.51
3:D:266:PRO:C	3:D:268:GLU:N	2.61	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:B:188:GLN:HE21	3:B:188:GLN:HA	1.76	0.51
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:A:279:LEU:C	3:A:279:LEU:HD12	2.37	0.50
2:P:1:DA:H2''	2:P:2:DC:O5'	2.09	0.50
3:A:130:PHE:CE2	3:A:225:VAL:HG13	2.46	0.50
3:B:3:GLN:N	3:B:6:ILE:HD12	2.26	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: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:D:181:LEU:HD23	3:D:181:LEU:N	2.27	0.50
3:B:114:ILE:O	3:B:116:PRO:HD3	2.11	0.50
3:D:111:ALA:CB	3:D:249:PRO:HA	2.40	0.50
3:A:24:LEU:HD23	3:A:27:VAL:HG23	1.94	0.50
3:D:3:GLN:HG2	3:D:6:ILE:HG13	1.94	0.50
3:C:22:LEU:HB2	3:C:81:ARG:HD2	1.93	0.50
3:B:8:ARG:HH11	3:B:8:ARG:HG2	1.76	0.50
3:B:251:LEU:O	3:B:252:ASN:C	2.54	0.50
3:B:253:LEU:HD13	3:B:287:ILE:HG12	1.93	0.50
3:A:62:SER:O	3:A:66:LEU:HG	2.12	0.50
3:D:41:MET:O	3:D:45:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:246:THR:O	3:A:250:MET:HB2	2.12	0.49
3:C:142:THR:CG2	3:C:215:HIS:NE2	2.75	0.49
3:A:167:PHE:CE1	3:A:207:ALA:HA	2.47	0.49
3:C:265:TYR:N	3:C:265:TYR:CD1	2.81	0.49
3:B:188:GLN:HA	3:B:188:GLN:NE2	2.27	0.49
3:A:261:ILE:HB	3:A:284:LEU:HB2	1.94	0.49
3:D:134:GLU:O	3:D:135:ASP:C	2.56	0.49
3:C:114:ILE:O	3:C:116:PRO:HD3	2.13	0.49
3:B:20:GLN:HB2	3:B:21:PRO:CD	2.39	0.49
3:A:111:ALA:HB3	3:A:249:PRO:HA	1.95	0.49
3:B:114:ILE:N	3:B:114:ILE:HD12	2.26	0.49
3:D:115:ARG:NH2	3:D:116:PRO:HD2	2.28	0.49
3:B:24:LEU:HD23	3:B:27:VAL:H	1.77	0.49
3:D:145:TYR:CE2	3:D:196:VAL:HG12	2.47	0.49
3:B:212:LEU:HD12	3:B:212:LEU:N	2.27	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:150:GLU:H	3:B:150:GLU:CD	2.18	0.49
3:B:153:SER:HB3	3:B:237:GLN:OE1	2.13	0.49
3:D:39:GLN:O	3:D:43:LYS:N	2.44	0.49
3:B:15:GLU:OE2	3:B:18:LEU:HD11	2.13	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:B:246:THR:C	3:B:249:PRO:HD2	2.37	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:D:63:ALA:HB1	3:D:103:TYR:OH	2.13	0.48
3:C:139:ILE:HG23	3:C:139:ILE:O	2.12	0.48
3:D:188:GLN:HE21	3:D:188:GLN:CA	2.20	0.48
3:C:219:LEU:C	3:C:219:LEU:HD23	2.38	0.48
3:A:96:PHE:CE2	3:A:114:ILE:HD12	2.41	0.48
3:A:275:ARG:HH12	3:C:291:LEU:HD21	1.79	0.48
3:D:208:ASP:CG	3:D:209:GLY:N	2.72	0.48
3:B:212:LEU:HD12	3:B:212:LEU:H	1.79	0.48
2:N:2:DC:H2"	2:N:3:DT:OP2	2.14	0.48
3:D:7:ILE:HD11	3:D:42:PHE:HA	1.96	0.48
3:D:24:LEU:CD2	3:D:27:VAL:H	2.27	0.48
3:B:128:HIS:HA	3:B:226:MET:O	2.14	0.48
3:B:266:PRO:C	3:B:268:GLU:H	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:17:DC:H2''	2:N:18:DT:OP2	2.14	0.48
3:A:139:ILE:CG2	3:A:207:ALA:HB3	2.42	0.48
3:A:219:LEU:C	3:A:219:LEU:HD23	2.39	0.48
3:A:278:ASN:HD22	3:A:278:ASN:HA	1.54	0.48
3:C:77:ALA:O	3:C:82:PHE:HB2	2.13	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:A:139:ILE:HG21	3:A:207:ALA:CB	2.44	0.47
3:C:24:LEU:HD23	3:C:27:VAL:CG2	2.42	0.47
3:B:142:THR:HB	3:B:199:THR:OG1	2.15	0.47
3:B:266:PRO:C	3:B:268:GLU:N	2.72	0.47
2:N:1:DA:H2''	2:N:2:DC:O5'	2.13	0.47
3:C:37:HIS:HA	3:C:40:ARG:NH1	2.22	0.47
3:C:111:ALA:C	3:C:114:ILE:HD13	2.39	0.47
3:A:233:GLY:O	3:A:236:VAL:HG23	2.14	0.47
3:B:40:ARG:HH11	3:B:44:ASP:HB2	1.80	0.47
3:C:6:ILE:HD13	3:C:33:TYR:OH	2.14	0.47
3:C:279:LEU:HD12	3:C:279:LEU:C	2.39	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:C:104:ARG:HD3	3:C:194:GLN:HB3	1.97	0.47
3:C:211:VAL:O	3:C:211:VAL:HG22	2.14	0.47
3:B:17:HIS:C	3:B:19:ASP:N	2.69	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:275:ARG:O	3:A:276:PRO:C	2.57	0.47
3:A:22:LEU:HD13	3:A:81:ARG:HB3	1.96	0.47
3:D:40:ARG:HB2	3:D:40:ARG:HH11	1.78	0.47
3:D:190:LYS:HB2	3:D:190:LYS:NZ	2.29	0.47
3:A:63:ALA:HB1	3:A:103:TYR:CE2	2.50	0.46
3:C:274:ASP:CG	3:C:274:ASP:O	2.58	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:C:24:LEU:HD21	3:C:27:VAL:HG23	1.98	0.46
3:A:208:ASP:CG	3:A:209:GLY:N	2.73	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
2:P:15:DT:H2''	2:P:16:DG:OP2	2.15	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:D:7:ILE:CD1	3:D:42:PHE:HA	2.46	0.46
3:D:183:GLU:HG2	3:D:259:GLN:HB3	1.98	0.46
3:A:119:ARG:HH21	3:A:246:THR:HG21	1.79	0.46
3:A:133:LEU:HD12	3:A:224:TYR:CE1	2.51	0.46
3:B:29:ALA:HA	3:B:38:LEU:HD12	1.97	0.46
3:A:285:ILE:HG23	3:A:286:PRO:HD2	1.98	0.46
3:D:15:GLU:OE2	3:D:18:LEU:HD11	2.16	0.46
3:D:160:ARG:HG3	3:D:178:LEU:HD13	1.98	0.46
3:C:269:ASP:CB	3:C:277:ILE:HD12	2.43	0.46
3:B:242:THR:HA	3:B:246:THR:HG23	1.97	0.46
3:A:63:ALA:HB1	3:A:103:TYR:CZ	2.51	0.46
3:D:125:MET:O	3:D:126:PRO:C	2.59	0.46
3:C:145:TYR:CE2	3:C:196:VAL:HG12	2.51	0.46
3:C:242:THR:HA	3:C:246:THR:HG23	1.97	0.46
3:B:232:LEU:HD12	3:B:278:ASN:ND2	2.31	0.46
3:A:172:PRO:HD2	3:A:210:TYR:CE1	2.51	0.45
3:D:255:ARG:HG2	3:D:255:ARG:HH11	1.80	0.45
3:C:22:LEU:HB2	3:C:81:ARG:CD	2.46	0.45
3:C:27:VAL:HG13	3:C:30:LYS:CE	2.45	0.45
3:B:275:ARG:HB3	3:B:276:PRO:HD2	1.98	0.45
3:D:284:LEU:HD23	3:D:284:LEU:N	2.31	0.45
3:D:178:LEU:HD23	3:D:202:LEU:CD1	2.47	0.45
3:D:223:GLU:O	3:D:256:ARG:NH1	2.50	0.45
3:C:126:PRO:HD2	3:C:247:CYS:SG	2.56	0.45
3:B:8:ARG:O	3:B:12:ILE:HG12	2.17	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:139:ILE:HD13	3:D:139:ILE:C	2.42	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:C:122:GLU:CD	3:C:122:GLU:N	2.74	0.45
3:C:188:GLN:HE21	3:C:188:GLN:CA	2.28	0.45
3:C:225:VAL:HG23	3:C:287:ILE:HD13	1.98	0.45
3:B:40:ARG:NH1	3:B:44:ASP:HB2	2.32	0.45
3:D:37:HIS:O	3:D:38:LEU:C	2.59	0.45
3:D:139:ILE:O	3:D:139:ILE:HG23	2.16	0.45
3:C:8:ARG:C	3:C:10:LEU:H	2.25	0.45
3:C:122:GLU:CD	3:C:122:GLU:H	2.25	0.45
3:B:7:ILE:CD1	3:B:42:PHE:HA	2.47	0.45
3:A:89:THR:O	3:A:90:ARG:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:105:ARG:HG3	3:B:191:ASP:OD1	2.17	0.45
3:B:268:GLU:O	3:B:268:GLU:OE1	2.35	0.45
3:A:139:ILE:HD13	3:A:140:GLY:N	2.33	0.44
3:D:63:ALA:HB1	3:D:103:TYR:CZ	2.52	0.44
3:B:238:GLU:O	3:B:242:THR:CG2	2.66	0.44
3:D:225:VAL:HG23	3:D:287:ILE:HD13	1.98	0.44
3:A:8:ARG:O	3:A:12:ILE:HG12	2.17	0.44
3:A:8:ARG:NE	3:A:120:LEU:HB2	2.31	0.44
3:A:212:LEU:C	3:A:213:THR:HG22	2.42	0.44
3:C:190:LYS:NZ	3:C:190:LYS:HB2	2.32	0.44
3:B:78:LEU:O	3:B:79:GLN:C	2.59	0.44
3:A:18:LEU:CD1	3:A:57:ARG:HB3	2.47	0.44
3:C:8:ARG:HG2	3:C:8:ARG:HH11	1.83	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: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:C:15:GLU:OE2	3:C:57:ARG:HD3	2.18	0.44
3:D:116:PRO:HB3	3:D:246:THR:HB	1.99	0.44
3:B:3:GLN:HG2	3:B:6:ILE:CD1	2.48	0.44
3:A:97:ALA:O	3:A:98:GLN:HB2	2.16	0.43
3:B:248:MET:HE1	3:B:287:ILE:CD1	2.31	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:D:150:GLU:CD	3:D:150:GLU:N	2.73	0.43
3:C:227:PHE:HE1	3:C:285:ILE:HD12	1.83	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:D:12:ILE:N	3:D:12:ILE:HD13	2.33	0.43
2:P:10:DT:H2"	2:P:11:DT:OP2	2.18	0.43
3:D:7:ILE:HD12	3:D:45:VAL:HG21	2.01	0.43
3:D:219:LEU:C	3:D:219:LEU:HD23	2.43	0.43
3:B:24:LEU:HG	3:B:26:ASN:H	1.83	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:D:226:MET:CE	3:D:284:LEU:HD21	2.46	0.43
3:D:279:LEU:C	3:D:279:LEU:HD12	2.44	0.43
3:C:243:VAL:O	3:C:248:MET:HG2	2.19	0.43
3:A:125:MET:O	3:A:126:PRO:C	2.59	0.43
3:A:185:ARG:HA	3:A:186:PRO:HD3	1.84	0.43
3:C:112:PHE:CD2	3:C:113:GLY:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:TRP:O	3:C:167:PHE:HB3	2.19	0.43
3:B:13:TRP:CD1	3:B:13:TRP:C	2.96	0.43
3:D:275:ARG:HB3	3:D:276:PRO:CD	2.43	0.43
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:D:38:LEU:O	3:D:41:MET:HB3	2.19	0.42
3:C:24:LEU:O	3:C:25:ASP:C	2.62	0.42
3:B:190:LYS:HB2	3:B:190:LYS:HZ3	1.82	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:A:3:GLN:CG	3:A:6:ILE:HG13	2.49	0.42
3:D:259:GLN:HB3	3:D:259:GLN:HE21	1.66	0.42
3:C:18:LEU:HD13	3:C:57:ARG:HB3	2.01	0.42
3:A:263:ARG:HD2	3:A:282:GLU:OE1	2.19	0.42
3:B:132:THR:HB	3:B:223:GLU:CD	2.45	0.42
3:C:139:ILE:C	3:C:139:ILE:CD1	2.93	0.42
3:B:145:TYR:CE2	3:B:196:VAL:HG12	2.54	0.42
3:B:248:MET:N	3:B:249:PRO:CD	2.82	0.42
3:B:264:TYR:CD2	3:B:281:CYS:HB3	2.54	0.42
3:D:139:ILE:HD11	3:D:214:GLY:HA3	2.01	0.42
3:B:93:LYS:HE2	3:B:93:LYS:HB3	1.75	0.42
2:N:11:DT:H2''	2:N:12:DC:C6	2.55	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
3:C:20:GLN:H	3:C:20:GLN:CD	2.28	0.42
3:C:139:ILE:HG21	3:C:212:LEU:CD1	2.38	0.42
3:A:72:PRO:HG2	3:A:75:ASP:OD1	2.20	0.42
3:D:190:LYS:HZ2	3:D:190:LYS:H	1.67	0.42
3:B:40:ARG:HH12	3:B:44:ASP:CG	2.28	0.42
3:B:232:LEU:C	3:B:234:THR:H	2.28	0.42
3:D:7:ILE:CD1	3:D:45:VAL:HG21	2.50	0.42
3:D:17:HIS:C	3:D:19:ASP:N	2.75	0.42
3:C:7:ILE:HD12	3:C:45:VAL:CG2	2.49	0.42
3:B:38:LEU:C	3:B:38:LEU:HD23	2.45	0.42
3:B:247:CYS:O	3:B:251:LEU:HG	2.19	0.42
3:C:63:ALA:HB1	3:C:103:TYR:CE2	2.55	0.41
3:B:78:LEU:O	3:B:81:ARG:N	2.52	0.41
3:A:128:HIS:HA	3:A:226:MET:O	2.20	0.41
3:D:226:MET:HB2	3:D:284:LEU:HD22	2.01	0.41
3:B:266:PRO:HA	3:B:269:ASP:OD2	2.19	0.41
2:P:15:DT:H1'	2:P:16:DG:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:185:ARG:HA	3:D:186:PRO:HD3	1.92	0.41
3:C:18:LEU:CD1	3:C:57:ARG:HB3	2.50	0.41
3:C:291:LEU:N	3:C:291:LEU:CD1	2.76	0.41
3:B:42:PHE:CD2	3:B:50:ILE:HB	2.55	0.41
3:A:26:ASN:O	3:A:29:ALA:HB3	2.20	0.41
3:D:28:ALA:O	3:D:38:LEU:HD11	2.20	0.41
3:D:256:ARG:HD3	3:D:287:ILE:C	2.45	0.41
3:C:266:PRO:HA	3:C:269:ASP:OD2	2.21	0.41
3:B:29:ALA:C	3:B:31:ALA:H	2.29	0.41
3:B:163:PHE:HB3	3:B:200:THR:HG21	2.02	0.41
3:B:279:LEU:C	3:B:279:LEU:CD1	2.91	0.41
2:P:8:DC:H2"	2:P:9:DA:OP2	2.21	0.41
3:A:50:ILE:CG1	3:A:54:ILE:HD11	2.50	0.41
3:D:27:VAL:CG2	3:D:30:LYS:HZ2	2.20	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:D:7:ILE:HD12	3:D:45:VAL:CB	2.51	0.41
3:C:96:PHE:O	3:C:97:ALA:HB3	2.21	0.41
3:C:132:THR:HA	3:C:222:GLY:O	2.20	0.41
3:A:139:ILE:HD13	3:A:139:ILE:C	2.46	0.41
3:A:150:GLU:CD	3:A:150:GLU:N	2.76	0.41
3:D:178:LEU:HD23	3:D:178:LEU:HA	1.95	0.41
3:D:207:ALA:O	3:D:208:ASP:C	2.63	0.41
3:C:8:ARG:HA	3:C:120:LEU:CD1	2.46	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:C:242:THR:O	3:C:246:THR:HG23	2.21	0.41
1:M:9:DC:H2"	1:M:10:DT:OP2	2.21	0.41
3:D:74:LEU:O	3:D:78:LEU:HG	2.21	0.41
3:D:190:LYS:HB3	3:D:192:ASP:OD1	2.20	0.41
3:B:236:VAL:O	3:B:240:ILE:HG13	2.21	0.41
3:B:244:TYR:OH	3:B:260:ASP:OD1	2.30	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:NE2	3:D:188:GLN:CA	2.78	0.40
3:C:188:GLN:NE2	3:C:188:GLN:CA	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:LEU:C	3:C:219:LEU:CD2	2.94	0.40
3:B:11:LEU:HD23	3:B:14:LEU:HD12	2.03	0.40
3:B:24:LEU:HD21	3:B:26:ASN:HB2	2.03	0.40
2:P:17:DC:H2"	2:P:18:DT:H6	1.85	0.40
3:D:53:TYR:CE1	3:D:118:LEU:HG	2.57	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:22:LEU:HB2	3:D:81:ARG:HD2	2.04	0.40
3:C:232:LEU:HD12	3:C:278:ASN:HD21	1.85	0.40
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:D:251:LEU:O	3:D:252:ASN:C	2.64	0.40
3:C:17:HIS:C	3:C:19:ASP:N	2.77	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%)	4	9
3	B	284/292 (97%)	239 (84%)	41 (14%)	4 (1%)	9	23
3	C	284/292 (97%)	252 (89%)	27 (10%)	5 (2%)	6	18
3	D	284/292 (97%)	252 (89%)	25 (9%)	7 (2%)	4	11
All	All	1136/1168 (97%)	999 (88%)	113 (10%)	24 (2%)	5	15

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	19	ASP

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	222 (90%)	24 (10%)	7	19
3	B	242/247 (98%)	217 (90%)	25 (10%)	7	18
3	C	246/247 (100%)	221 (90%)	25 (10%)	7	18
3	D	242/247 (98%)	221 (91%)	21 (9%)	9	24
All	All	976/988 (99%)	881 (90%)	95 (10%)	8	20

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	20	GLN
3	A	38	LEU
3	A	43	LYS
3	A	86	GLN
3	A	122	GLU
3	A	132	THR
3	A	139	ILE
3	A	150	GLU
3	A	178	LEU
3	A	188	GLN
3	A	190	LYS
3	A	194	GLN
3	A	202	LEU
3	A	225	VAL
3	A	234	THR
3	A	238	GLU
3	A	243	VAL
3	A	246	THR
3	A	259	GLN
3	A	278	ASN
3	A	280	ARG
3	A	284	LEU
3	A	287	ILE
3	A	291	LEU
3	D	19	ASP
3	D	20	GLN
3	D	43	LYS
3	D	85	GLN
3	D	86	GLN
3	D	122	GLU
3	D	132	THR
3	D	139	ILE
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	284	LEU

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Mol	Chain	Res	Type
3	D	287	ILE
3	D	291	LEU
3	C	20	GLN
3	C	38	LEU
3	C	40	ARG
3	C	43	LYS
3	C	75	ASP
3	C	93	LYS
3	C	122	GLU
3	C	132	THR
3	C	139	ILE
3	C	142	THR
3	C	150	GLU
3	C	178	LEU
3	C	190	LYS
3	C	194	GLN
3	C	202	LEU
3	C	211	VAL
3	C	212	LEU
3	C	219	LEU
3	C	225	VAL
3	C	246	THR
3	C	256	ARG
3	C	259	GLN
3	C	284	LEU
3	C	287	ILE
3	C	291	LEU
3	B	20	GLN
3	B	43	LYS
3	B	85	GLN
3	B	122	GLU
3	B	139	ILE
3	B	142	THR
3	B	150	GLU
3	B	178	LEU
3	B	181	LEU
3	B	190	LYS
3	B	194	GLN
3	B	202	LEU
3	B	204	GLN
3	B	211	VAL
3	B	212	LEU

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Mol	Chain	Res	Type
3	B	225	VAL
3	B	232	LEU
3	B	242	THR
3	B	243	VAL
3	B	246	THR
3	B	256	ARG
3	B	268	GLU
3	B	284	LEU
3	B	287	ILE
3	B	291	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	17	HIS
3	A	20	GLN
3	A	26	ASN
3	A	37	HIS
3	A	79	GLN
3	A	165	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	79	GLN
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	165	HIS
3	C	188	GLN
3	C	204	GLN
3	C	252	ASN
3	C	278	ASN

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Mol	Chain	Res	Type
3	B	17	HIS
3	B	20	GLN
3	B	37	HIS
3	B	98	GLN
3	B	182	ASN
3	B	188	GLN
3	B	278	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.