



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:11 PM UTC

PDB ID : 1LE5 / pdb_00001le5
Title : Crystal structure of a NF-kB heterodimer bound to an IFN γ -kB
Authors : Berkowitz, B.; Huang, D.B.; Chen-Park, F.E.; Sigler, P.B.; Ghosh, G.
Deposited on : 2002-04-09
Resolution : 2.75 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

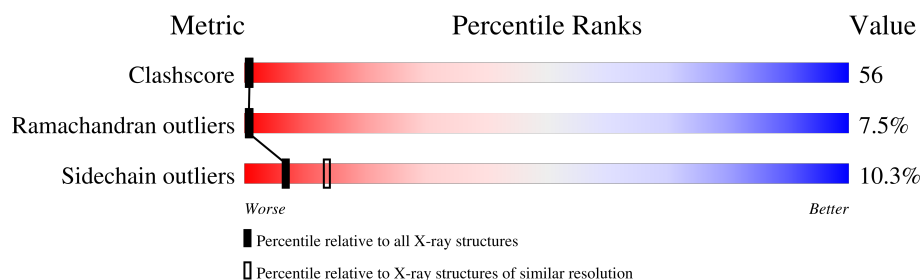
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)

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	C	12	17% 83%
1	G	12	58% 25% 17%
2	D	12	25% 75%
2	H	12	17% 25% 50% 8%
3	A	274	30% 53% 17% .
3	E	274	30% 56% 12% .
4	B	313	26% 64% 10%
4	F	313	31% 52% 15% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10439 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	12	Total	C	N	O	P	0	0	0
			244	118	44	71	11			
1	G	12	Total	C	N	O	P	0	0	0
			244	118	44	71	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			242	117	45	69	11			
2	H	12	Total	C	N	O	P	0	0	0
			242	117	45	69	11			

- Molecule 3 is a protein called Nuclear factor NF-kappa-B p65 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	274	Total	C	N	O	S	0	0	0
			2184	1361	402	409	12			
3	E	274	Total	C	N	O	S	0	0	0
			2184	1361	402	409	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	cloning artifact	UNP Q04207
A	19	ALA	-	cloning artifact	UNP Q04207
E	18	MET	-	cloning artifact	UNP Q04207
E	19	ALA	-	cloning artifact	UNP Q04207

- Molecule 4 is a protein called Nuclear factor NF-kappa-B p50 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	313	Total 2462	C 1559	N 429	O 461	S 13	0	0	0
4	F	313	Total 2462	C 1559	N 429	O 461	S 13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	38	MET	-	initiating methionine	UNP P25799
F	38	MET	-	initiating methionine	UNP P25799

- Molecule 5 is water.

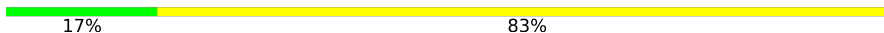
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	4	Total 4	O 4	0	0
5	D	9	Total 9	O 9	0	0
5	G	6	Total 6	O 6	0	0
5	H	8	Total 8	O 8	0	0
5	A	33	Total 33	O 33	0	0
5	B	32	Total 32	O 32	0	0
5	E	32	Total 32	O 32	0	0
5	F	51	Total 51	O 51	0	0

3 Residue-property plots

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.

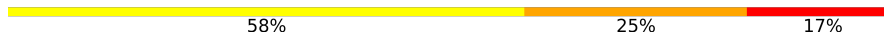
Note EDS was not executed.

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

Chain C: 

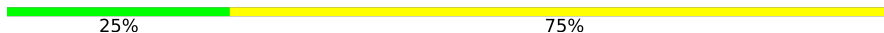


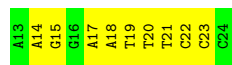
- Molecule 1: 5'-D(*TP*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*T)-3'

Chain G: 



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

Chain D: 

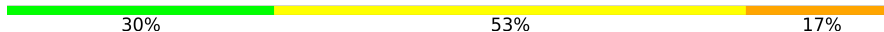


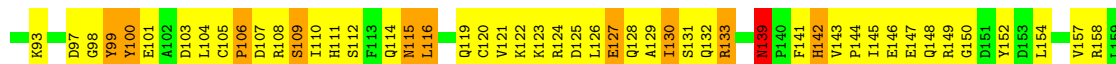
- Molecule 2: 5'-D(*AP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3'

Chain H: 



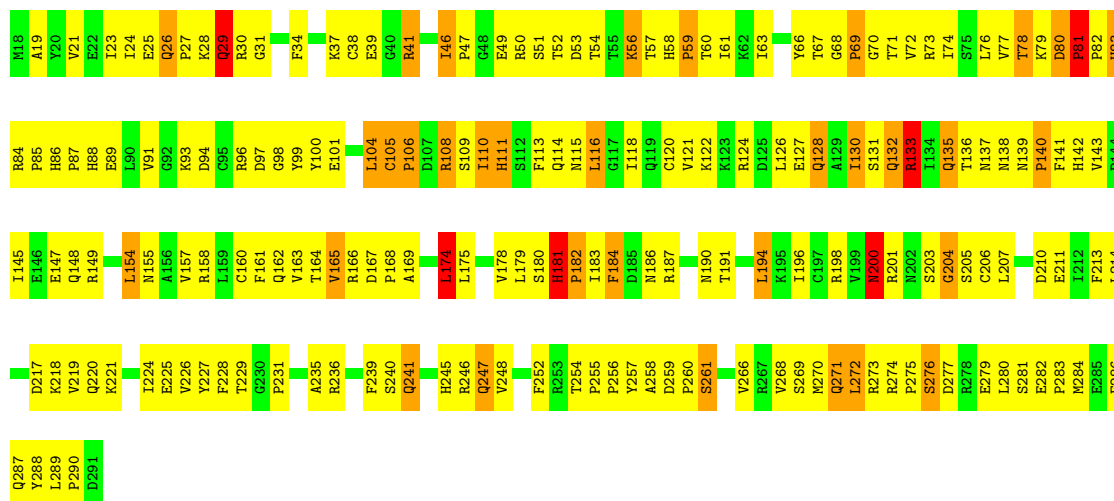
- Molecule 3: Nuclear factor NF-kappa-B p65 subunit

Chain A: 

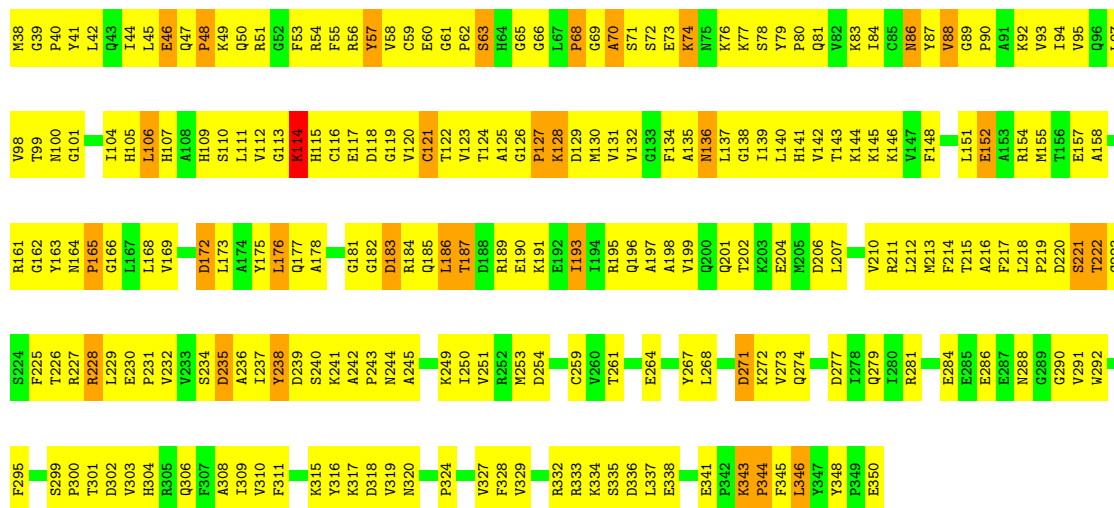




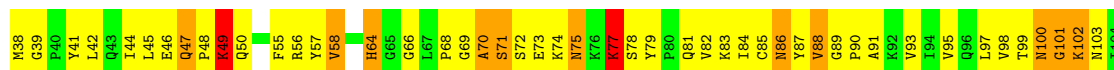
• Molecule 3: Nuclear factor NF-kappa-B p65 subunit



• Molecule 4: Nuclear factor NF-kappa-B p50 subunit



• Molecule 4: Nuclear factor NF-kappa-B p50 subunit



L229	L309	L188	H106
E230	V310	V169	L106
P231	Y316	H170	H107
V232	K317	S171	A108
V233	D318	D172	H109
S234	V319	L173	S110
D235	N320	A174	L111
A236	N320	V175	V112
T237	L322	L176	G113
Y238	K323	Q177	K114
D239	K327	A178	H115
S240	F328	E179	H116
M244	V329	G180	E117
A245	R332	G181	D118
S246	R333	G182	
D247	R334	D183	G121
L248	S335	R184	T122
K249	D336	Q185	V123
L250	L337	L186	T124
		T187	A125
		D188	G126
D254	F338	R189	P127
R255	T339	E190	
	S340	K191	M130
C259	P342	E192	V131
	K343	T193	V132
L266	K344	I194	G133
V267	F345	R195	F134
L268	L346	G196	A135
		A197	N136
D271		A198	L137
K272	P349	V199	G138
V273	E350	Q200	I139
Q274		Q201	L140
K275		T202	H141
		K203	V142
		E204	T143
Q279		M205	K144
L280		D206	K145
R281		L207	K146
F282		S208	V147
Y283		V209	F148
E284		V210	E149
E285			T150
E286		M213	L151
E287		F214	E152
G289		T215	A153
G290		A216	R154
V291		F217	M155
		L218	T156
F298		P219	T157
S299		D220	E157
P300		S221	
		T222	T160
S303		G223	R161
H304		S224	G162
R305		F225	Y163
Q306		T226	N164
F307		R227	P165
L308		P228	G166
			L167

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.53Å 138.01Å 89.32Å 90.00° 97.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75	Depositor
% Data completeness (in resolution range)	88.0 (20.00-2.75)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.260 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10439	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.29	0/273	0.70	0/420
1	G	0.39	0/273	1.16	3/420 (0.7%)
2	D	0.27	0/271	0.70	0/416
2	H	0.44	0/271	1.21	4/416 (1.0%)
3	A	0.48	0/2236	1.04	13/3031 (0.4%)
3	E	0.46	0/2236	1.11	17/3031 (0.6%)
4	B	0.39	0/2514	0.91	10/3394 (0.3%)
4	F	0.48	0/2514	0.99	9/3394 (0.3%)
All	All	0.44	0/10588	1.01	56/14522 (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
1	G	0	5
2	H	0	6
All	All	0	11

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	80	ASP	CA-C-N	9.85	130.53	120.38
3	E	80	ASP	C-N-CA	9.85	130.53	120.38
4	F	191	LYS	N-CA-C	-9.55	101.39	113.23
3	E	81	PRO	CA-C-N	-8.80	108.83	119.84
3	E	81	PRO	C-N-CA	-8.80	108.83	119.84
3	A	80	ASP	CA-C-N	8.68	129.32	120.38
3	A	80	ASP	C-N-CA	8.68	129.32	120.38
3	A	86	HIS	CA-C-N	8.19	130.08	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	86	HIS	C-N-CA	8.19	130.08	119.84
4	F	86	ASN	N-CA-C	-8.04	101.95	112.24
3	A	89	GLU	N-CA-C	7.86	122.11	110.48
4	F	343	LYS	CA-C-N	7.83	129.62	119.84
4	F	343	LYS	C-N-CA	7.83	129.62	119.84
3	E	133	ARG	N-CA-C	-7.60	103.86	113.43
3	E	109	SER	N-CA-C	-7.55	102.38	114.09
3	A	139	ASN	CA-C-N	7.41	127.76	119.32
3	A	139	ASN	C-N-CA	7.41	127.76	119.32
3	E	81	PRO	N-CA-C	7.14	119.42	110.70
3	E	80	ASP	N-CA-C	6.74	120.08	110.24
3	E	287	GLN	N-CA-C	6.37	118.79	108.41
4	B	343	LYS	CA-C-N	6.36	127.79	119.84
4	B	343	LYS	C-N-CA	6.36	127.79	119.84
3	E	182	PRO	N-CA-C	6.30	121.53	111.26
3	E	105	CYS	CA-C-N	6.16	127.54	119.84
3	E	105	CYS	C-N-CA	6.16	127.54	119.84
4	F	271	ASP	N-CA-C	-6.13	102.27	110.55
4	F	64	HIS	N-CA-C	-6.12	105.10	113.30
4	B	348	TYR	CA-C-N	6.08	126.05	119.78
4	B	348	TYR	C-N-CA	6.08	126.05	119.78
1	G	5	DA	N9-C1'-C2'	6.00	122.49	113.50
4	F	167	LEU	N-CA-C	-5.96	106.34	113.97
4	B	172	ASP	N-CA-C	-5.92	105.81	114.39
3	A	187	ARG	N-CA-C	-5.89	105.92	113.23
3	A	123	LYS	N-CA-C	-5.88	104.95	111.36
2	H	15	DG	N9-C1'-C2'	5.86	122.29	113.50
3	A	81	PRO	N-CA-C	5.78	117.75	110.70
4	F	47	GLN	N-CA-C	5.77	113.41	108.22
2	H	19	DT	N1-C1'-C2'	5.72	122.09	113.50
4	B	193	ILE	N-CA-C	-5.51	105.48	110.82
2	H	21	DT	N1-C1'-C2'	5.49	121.73	113.50
1	G	6	DA	N9-C1'-C2'	5.44	121.66	113.50
3	E	240	SER	N-CA-C	5.44	115.42	108.24
4	B	271	ASP	N-CA-C	-5.43	103.21	110.55
2	H	21	DT	C4'-C3'-O3'	-5.36	101.95	110.00
3	E	46	ILE	CA-C-N	5.33	125.09	119.76
3	E	46	ILE	C-N-CA	5.33	125.09	119.76
4	B	86	ASN	N-CA-C	-5.33	104.86	111.90
4	B	61	GLY	CA-C-N	5.31	125.47	119.90
4	B	61	GLY	C-N-CA	5.31	125.47	119.90
3	A	109	SER	N-CA-C	-5.28	105.54	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	287	GLN	N-CA-C	5.23	117.17	108.02
4	F	205	MET	N-CA-C	5.17	116.95	110.24
1	G	5	DA	C4'-C3'-O3'	-5.15	102.27	110.00
3	E	181	HIS	CA-C-N	5.09	125.38	119.93
3	E	181	HIS	C-N-CA	5.09	125.38	119.93
3	A	24	ILE	N-CA-C	5.05	115.72	110.82

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	11	DC	Sidechain
1	G	4	DG	Sidechain
1	G	5	DA	Sidechain
1	G	6	DA	Sidechain
1	G	7	DA	Sidechain
2	H	13	DA	Sidechain
2	H	14	DA	Sidechain
2	H	16	DG	Sidechain
2	H	20	DT	Sidechain
2	H	21	DT	Sidechain
2	H	22	DC	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	C	244	0	138	28	0
1	G	244	0	138	31	0
2	D	242	0	137	23	0
2	H	242	0	137	15	0
3	A	2184	0	2146	251	0
3	E	2184	0	2146	250	0
4	B	2462	0	2458	317	0
4	F	2462	0	2458	269	0
5	A	33	0	0	5	0
5	B	32	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	4	0	0	3	0
5	D	9	0	0	1	0
5	E	32	0	0	7	0
5	F	51	0	0	5	0
5	G	6	0	0	2	0
5	H	8	0	0	1	0
All	All	10439	0	9758	1125	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 56.

All (1125) 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:1:DT:H3'	4:B:65:GLY:HA2	1.30	1.11
4:F:250:ILE:HG23	4:F:268:LEU:HD21	1.29	1.06
4:B:104:ILE:HG22	4:B:211:ARG:HH22	1.23	1.03
3:E:273:ARG:HD2	3:E:280:LEU:HD11	1.41	1.02
4:B:134:PHE:HB3	4:B:137:LEU:HD11	1.42	1.02
3:E:200:ASN:HB2	3:E:213:PHE:H	1.26	0.99
3:A:273:ARG:HE	3:E:81:PRO:HG2	1.26	0.98
3:A:149:ARG:HG2	3:A:150:GLY:H	1.29	0.98
4:F:176:LEU:HD22	4:F:184:ARG:HG3	1.46	0.97
3:E:206:CYS:HA	3:E:288:TYR:HD2	1.28	0.96
3:A:128:GLN:O	3:A:132:GLN:HG3	1.66	0.96
1:G:4:DG:H3'	3:E:246:ARG:NH1	1.80	0.95
3:A:200:ASN:HB2	3:A:213:PHE:H	1.33	0.94
4:F:84:ILE:HB	4:F:130:MET:HB3	1.50	0.93
4:F:332:ARG:HG2	4:F:332:ARG:HH11	1.33	0.93
3:A:165:VAL:HG23	3:A:173:LEU:HB3	1.51	0.92
4:B:195:ARG:HH11	4:B:195:ARG:HA	1.33	0.91
3:E:130:ILE:HD11	3:E:148:GLN:HG2	1.50	0.91
4:B:186:LEU:HD12	4:B:186:LEU:H	1.35	0.91
3:E:74:ILE:HD12	3:E:161:PHE:HD1	1.34	0.90
4:B:84:ILE:HD13	4:B:130:MET:HG2	1.50	0.90
2:D:22:DC:H2''	2:D:23:DC:H5''	1.54	0.90
4:F:88:VAL:HG22	4:F:89:GLY:H	1.34	0.90
3:A:273:ARG:NE	3:E:81:PRO:HG2	1.84	0.90
4:B:111:LEU:HD21	4:B:137:LEU:HB3	1.54	0.89
4:B:244:ASN:HB3	4:B:274:GLN:HE22	1.38	0.89
3:E:174:LEU:H	3:E:174:LEU:HD22	1.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:123:VAL:HG11	4:B:132:VAL:HG11	1.56	0.88
4:F:213:MET:HE3	4:F:233:VAL:HG13	1.56	0.88
3:E:257:TYR:CD2	3:E:258:ALA:N	2.42	0.87
4:F:108:ALA:HB3	4:F:205:MET:HE1	1.53	0.87
3:E:257:TYR:HD2	3:E:258:ALA:N	1.71	0.87
4:F:156:THR:O	4:F:160:ILE:HG23	1.76	0.86
4:B:215:THR:HG23	4:B:228:ARG:HG3	1.57	0.86
3:E:111:HIS:H	3:E:111:HIS:CD2	1.90	0.85
3:A:201:ARG:HG2	3:A:201:ARG:HH21	1.41	0.85
4:F:46:GLU:HG2	4:F:47:GLN:H	1.40	0.85
4:F:108:ALA:CB	4:F:205:MET:HE1	2.06	0.85
3:A:35:ARG:HE	3:A:35:ARG:HA	1.39	0.85
3:A:53:ASP:OD1	3:A:54:THR:HG23	1.75	0.85
1:G:6:DA:H2''	1:G:7:DA:O5'	1.77	0.84
3:A:26:GLN:O	3:A:49:GLU:HB2	1.78	0.83
3:A:63:ILE:HD12	3:A:63:ILE:H	1.43	0.83
4:B:56:ARG:NH1	4:B:56:ARG:HB3	1.94	0.83
4:B:286:GLU:HB2	4:B:290:GLY:HA3	1.57	0.83
4:B:125:ALA:HB3	4:B:132:VAL:HG22	1.60	0.83
4:F:227:ARG:HA	4:F:227:ARG:NE	1.91	0.83
4:B:329:VAL:HG23	4:B:345:PHE:HB2	1.60	0.83
2:D:17:DA:H2'	4:B:306:GLN:HE22	1.43	0.83
4:F:107:HIS:HD2	4:F:109:HIS:H	1.26	0.83
3:A:114:GLN:O	3:A:115:ASN:HB2	1.78	0.82
3:E:81:PRO:HB2	3:E:82:PRO:HD3	1.60	0.82
4:B:116:CYS:HA	4:B:121:CYS:HA	1.62	0.82
3:E:21:VAL:HG13	3:E:63:ILE:HG22	1.60	0.82
3:E:27:PRO:HD2	3:E:180:SER:HB2	1.62	0.82
1:G:8:DT:H72	3:E:187:ARG:HD3	1.60	0.81
4:B:48:PRO:HA	4:B:69:GLY:HA2	1.61	0.81
4:B:45:LEU:HD11	4:B:81:GLN:HB2	1.63	0.81
4:F:123:VAL:HG11	4:F:132:VAL:HG21	1.62	0.81
2:H:21:DT:H2''	2:H:22:DC:O5'	1.79	0.81
3:A:57:THR:HG22	3:A:58:HIS:H	1.45	0.81
3:E:258:ALA:O	3:E:260:PRO:HD3	1.80	0.81
3:A:166:ARG:HG3	3:A:166:ARG:HH11	1.46	0.81
4:B:92:LYS:HB2	4:B:217:PHE:HE1	1.46	0.80
4:F:167:LEU:HD21	4:F:228:ARG:NH2	1.97	0.79
4:F:189:ARG:HD2	4:F:190:GLU:N	1.98	0.79
3:E:76:LEU:HD11	3:E:118:ILE:HD12	1.65	0.79
1:G:4:DG:H3'	3:E:246:ARG:HH12	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:329:VAL:HG23	4:F:345:PHE:HB2	1.64	0.78
4:F:346:LEU:C	4:F:346:LEU:HD23	2.07	0.78
4:B:40:PRO:HB3	4:B:87:TYR:HA	1.64	0.78
3:E:69:PRO:HG2	3:E:166:ARG:NH1	1.98	0.78
3:A:73:ARG:HA	3:A:100:TYR:O	1.84	0.78
2:D:23:DC:H4'	5:D:721:HOH:O	1.84	0.78
3:E:74:ILE:HD12	3:E:161:PHE:CD1	2.18	0.78
4:B:76:LYS:HG3	4:B:77:LYS:H	1.49	0.77
4:B:261:THR:O	4:B:315:LYS:HG2	1.84	0.77
4:F:126:GLY:N	4:F:127:PRO:HD3	2.00	0.77
4:F:88:VAL:HG11	4:F:218:LEU:HD22	1.67	0.77
3:E:79:LYS:HG2	3:E:80:ASP:OD2	1.85	0.77
1:C:9:DT:H2'	3:A:38:CYS:SG	2.24	0.77
3:A:195:LYS:HD2	3:A:217:ASP:OD1	1.84	0.76
4:F:114:LYS:HE2	4:F:134:PHE:HA	1.67	0.76
1:G:5:DA:H2''	1:G:6:DA:O5'	1.86	0.76
4:B:92:LYS:HB2	4:B:217:PHE:CE1	2.20	0.76
3:E:198:ARG:HD2	4:F:310:VAL:HG21	1.67	0.76
1:G:11:DC:O2	2:H:15:DG:N2	2.17	0.76
3:A:262:LEU:HD21	3:A:266:VAL:HG23	1.67	0.76
3:A:169:ALA:HB1	3:A:171:ARG:HH21	1.52	0.75
3:A:79:LYS:HA	3:A:158:ARG:CD	2.17	0.75
3:A:93:LYS:HE2	3:A:115:ASN:HB3	1.66	0.75
3:A:84:ARG:H	3:A:84:ARG:HE	1.34	0.75
4:F:105:HIS:HB3	4:F:201:GLN:NE2	2.02	0.75
3:A:108:ARG:HB3	3:A:111:HIS:CE1	2.22	0.74
4:F:250:ILE:HG23	4:F:268:LEU:CD2	2.12	0.74
3:E:204:GLY:HA2	3:E:210:ASP:OD1	1.86	0.74
4:F:115:HIS:HB3	5:F:800:HOH:O	1.87	0.74
4:B:87:TYR:HD1	4:B:130:MET:HE3	1.53	0.74
4:B:155:MET:HE2	4:B:169:VAL:HG22	1.69	0.74
3:E:111:HIS:H	3:E:111:HIS:HD2	1.33	0.74
4:B:79:TYR:HB3	4:B:80:PRO:HD2	1.69	0.73
4:F:116:CYS:HA	4:F:121:CYS:HA	1.68	0.73
1:G:8:DT:H2''	1:G:9:DT:O5'	1.88	0.73
4:F:84:ILE:HB	4:F:130:MET:CB	2.17	0.73
4:F:97:LEU:HD21	4:F:111:LEU:HD21	1.70	0.73
3:E:58:HIS:HB3	3:E:113:PHE:O	1.87	0.73
3:E:111:HIS:CD2	3:E:111:HIS:N	2.56	0.73
4:B:195:ARG:O	4:B:199:VAL:HG23	1.87	0.73
4:B:173:LEU:HD21	4:B:193:ILE:HG21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:86:HIS:NE2	3:A:154:LEU:HA	2.04	0.72
4:F:184:ARG:H	4:F:184:ARG:HD2	1.54	0.72
4:B:279:GLN:NE2	4:B:332:ARG:HH21	1.88	0.72
1:C:8:DT:H2''	1:C:9:DT:H72	1.72	0.72
4:B:254:ASP:HB2	4:B:267:TYR:HB2	1.72	0.72
4:F:167:LEU:HD12	4:F:167:LEU:N	2.04	0.72
4:B:329:VAL:CG2	4:B:345:PHE:HB2	2.18	0.72
4:B:104:ILE:HG22	4:B:211:ARG:NH2	2.02	0.72
3:E:72:VAL:O	3:E:101:GLU:HA	1.90	0.72
3:E:80:ASP:HB3	3:E:81:PRO:HD2	1.72	0.71
3:A:236:ARG:HE	3:E:82:PRO:HG2	1.54	0.71
3:E:248:VAL:HG11	4:F:305:ARG:HG3	1.71	0.71
3:A:267:ARG:HD2	3:A:285:GLU:HG3	1.71	0.71
3:E:56:LYS:H	3:E:56:LYS:HD3	1.56	0.71
3:E:108:ARG:NH1	3:E:108:ARG:HB2	2.05	0.71
4:F:88:VAL:CG1	4:F:218:LEU:HD22	2.20	0.71
4:F:72:SER:O	4:F:77:LYS:HG3	1.91	0.71
4:F:189:ARG:HD2	4:F:190:GLU:HB2	1.71	0.71
4:B:111:LEU:HD22	4:B:116:CYS:SG	2.31	0.71
4:F:186:LEU:O	4:F:191:LYS:HB2	1.91	0.71
4:B:123:VAL:CG1	4:B:132:VAL:HG11	2.21	0.71
3:A:206:CYS:HA	3:A:288:TYR:HD2	1.56	0.70
4:F:155:MET:HE2	4:F:169:VAL:HG13	1.70	0.70
1:C:3:DG:H1'	1:C:4:DG:C8	2.25	0.70
3:E:241:GLN:HB2	5:E:847:HOH:O	1.90	0.70
4:B:195:ARG:HH11	4:B:195:ARG:CA	2.04	0.70
3:E:271:GLN:NE2	3:E:280:LEU:HD23	2.07	0.69
4:B:39:GLY:CA	4:B:86:ASN:HD22	2.04	0.69
3:A:166:ARG:HG3	3:A:166:ARG:NH1	2.08	0.69
3:E:282:GLU:HG3	3:E:283:PRO:HD2	1.72	0.69
3:A:106:PRO:C	3:A:108:ARG:H	2.00	0.69
4:F:41:TYR:CE2	4:F:85:CYS:HB2	2.26	0.69
3:A:76:LEU:HD11	3:A:88:HIS:O	1.91	0.69
4:B:88:VAL:HG13	4:B:89:GLY:N	2.07	0.69
4:F:42:LEU:HD21	4:F:214:PHE:HB3	1.74	0.69
3:E:49:GLU:HG3	3:E:50:ARG:HG3	1.73	0.69
4:B:155:MET:HE2	4:B:169:VAL:HG13	1.75	0.69
2:H:22:DC:H2'	2:H:23:DC:C6	2.27	0.68
4:B:250:ILE:HG21	4:B:253:MET:HE2	1.75	0.68
4:F:227:ARG:HA	4:F:227:ARG:HE	1.56	0.68
3:A:274:ARG:NH1	3:A:279:GLU:OE1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:69:PRO:HG2	3:E:166:ARG:HH11	1.56	0.68
4:F:332:ARG:HG2	4:F:332:ARG:NH1	2.04	0.68
3:A:129:ALA:HA	3:A:132:GLN:OE1	1.94	0.68
1:C:8:DT:H2"	1:C:9:DT:C7	2.22	0.68
3:A:246:ARG:HD3	5:A:734:HOH:O	1.92	0.68
3:A:88:HIS:HB2	3:A:119:GLN:O	1.93	0.68
3:A:149:ARG:HG2	3:A:150:GLY:N	2.07	0.68
4:B:215:THR:CG2	4:B:228:ARG:HG3	2.23	0.68
5:G:705:HOH:O	3:E:246:ARG:HD3	1.94	0.68
4:B:148:PHE:HE1	4:B:199:VAL:HG22	1.58	0.68
4:B:154:ARG:NE	4:B:154:ARG:HA	2.09	0.68
3:E:73:ARG:HB3	3:E:162:GLN:HB2	1.76	0.68
4:F:250:ILE:CG2	4:F:268:LEU:HD21	2.18	0.67
2:D:22:DC:C2'	2:D:23:DC:H5"	2.23	0.67
3:E:257:TYR:CE1	3:E:266:VAL:HG11	2.30	0.67
4:F:167:LEU:HD21	4:F:228:ARG:HH21	1.57	0.67
3:E:108:ARG:HB2	3:E:108:ARG:HH11	1.59	0.67
3:A:18:MET:HE3	3:A:173:LEU:HG	1.75	0.67
3:E:190:ASN:HB3	3:E:220:GLN:HE22	1.57	0.67
3:E:182:PRO:HB2	3:E:184:PHE:CE1	2.30	0.67
3:A:165:VAL:CG2	3:A:173:LEU:HB3	2.25	0.67
4:B:218:LEU:HG	4:B:229:LEU:HD21	1.74	0.67
4:F:44:ILE:HG22	4:F:46:GLU:O	1.95	0.67
3:A:79:LYS:HA	3:A:158:ARG:NE	2.09	0.67
3:A:88:HIS:CG	3:A:120:CYS:HA	2.30	0.67
3:E:72:VAL:HG13	3:E:100:TYR:HE1	1.59	0.67
4:B:111:LEU:HD23	4:B:112:VAL:H	1.60	0.66
3:A:270:MET:HE2	3:A:286:PHE:HB2	1.75	0.66
4:F:268:LEU:HD12	4:F:280:ILE:HD12	1.78	0.66
4:B:218:LEU:HD21	4:B:229:LEU:HD11	1.78	0.66
3:A:24:ILE:HB	3:A:25:GLU:OE2	1.96	0.66
3:E:122:LYS:NZ	3:E:124:ARG:HH21	1.94	0.66
4:F:88:VAL:HG22	4:F:89:GLY:N	2.08	0.66
4:F:186:LEU:O	4:F:191:LYS:HE3	1.95	0.66
4:B:114:LYS:HD2	4:B:135:ALA:O	1.96	0.66
3:E:70:GLY:HA3	3:E:104:LEU:HD22	1.78	0.66
4:F:162:GLY:C	4:F:163:TYR:HD1	2.04	0.66
4:F:148:PHE:C	4:F:148:PHE:CD2	2.73	0.66
3:A:72:VAL:O	3:A:101:GLU:HA	1.96	0.66
3:A:148:GLN:HG2	3:A:152:TYR:OH	1.95	0.66
4:B:125:ALA:CB	4:B:132:VAL:HG22	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:84:ILE:CB	4:F:130:MET:HB3	2.24	0.65
4:F:107:HIS:NE2	4:F:109:HIS:CD2	2.65	0.65
3:A:262:LEU:HD21	3:A:266:VAL:CG2	2.27	0.65
3:E:84:ARG:HB3	5:E:788:HOH:O	1.96	0.65
3:A:29:GLN:HE22	3:A:181:HIS:HB3	1.61	0.65
4:B:66:GLY:O	4:B:68:PRO:HD3	1.97	0.65
4:F:49:LYS:HE3	4:F:49:LYS:HA	1.77	0.65
4:F:304:HIS:HB3	4:F:308:ALA:HB3	1.79	0.65
4:F:107:HIS:CD2	4:F:109:HIS:H	2.14	0.65
4:B:118:ASP:HB3	4:B:154:ARG:NH2	2.12	0.65
3:E:28:LYS:HG2	3:E:49:GLU:HA	1.79	0.65
4:F:46:GLU:O	4:F:47:GLN:HG2	1.96	0.65
4:B:217:PHE:CD1	4:B:225:PHE:HB3	2.32	0.64
3:E:53:ASP:OD1	3:E:54:THR:HG23	1.97	0.64
3:A:60:THR:HA	3:A:112:SER:HA	1.77	0.64
3:E:31:GLY:CA	3:E:186:ASN:HD22	2.10	0.64
4:F:279:GLN:OE1	4:F:332:ARG:NH1	2.30	0.64
4:B:93:VAL:HG22	4:B:216:ALA:CB	2.27	0.64
4:F:209:VAL:HG22	4:F:238:TYR:HD2	1.62	0.64
3:A:165:VAL:O	3:A:166:ARG:HG3	1.98	0.64
4:B:115:HIS:CE1	4:B:123:VAL:HG23	2.33	0.64
4:B:191:LYS:O	4:B:195:ARG:HG2	1.98	0.64
3:A:88:HIS:ND1	3:A:120:CYS:HA	2.13	0.64
3:E:206:CYS:HA	3:E:288:TYR:CD2	2.21	0.64
3:A:79:LYS:C	3:A:158:ARG:HE	2.06	0.64
4:F:97:LEU:HD21	4:F:111:LEU:CD2	2.28	0.64
4:F:45:LEU:HB3	4:F:81:GLN:O	1.98	0.64
3:A:26:GLN:OE1	3:A:181:HIS:N	2.23	0.63
3:E:58:HIS:CG	3:E:114:GLN:HG2	2.34	0.63
4:B:346:LEU:HD13	4:B:346:LEU:C	2.23	0.63
2:H:14:DA:H2'	2:H:15:DG:C8	2.33	0.63
3:A:208:GLY:HA2	3:A:254:THR:HG22	1.80	0.63
4:B:114:LYS:NZ	4:B:136:ASN:HB3	2.13	0.63
3:A:219:VAL:O	3:A:247:GLN:HG2	1.99	0.63
4:B:92:LYS:HE3	4:B:124:THR:OG1	1.99	0.63
3:E:190:ASN:HB3	3:E:220:GLN:NE2	2.13	0.63
4:F:50:GLN:HG2	4:F:236:ALA:O	1.98	0.63
4:F:123:VAL:CG1	4:F:132:VAL:HG21	2.27	0.63
4:F:192:GLU:O	4:F:196:GLN:HG3	1.98	0.63
4:B:98:VAL:HG11	4:B:213:MET:HE3	1.79	0.63
3:E:246:ARG:O	3:E:248:VAL:HG22	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:56:ARG:HB3	4:B:56:ARG:HH11	1.60	0.63
4:B:73:GLU:O	4:B:74:LYS:HB2	1.99	0.63
4:B:83:LYS:C	4:B:84:ILE:HD12	2.23	0.63
4:F:221:SER:O	4:F:222:THR:HB	1.98	0.63
3:A:88:HIS:HB3	3:A:121:VAL:N	2.14	0.62
3:A:166:ARG:HA	3:A:171:ARG:O	2.00	0.62
4:B:88:VAL:HG22	4:B:89:GLY:H	1.64	0.62
3:E:51:SER:HB2	3:E:57:THR:OG1	1.99	0.62
3:E:79:LYS:HA	3:E:158:ARG:HE	1.64	0.62
3:A:79:LYS:HB3	3:A:79:LYS:NZ	2.14	0.62
4:B:94:ILE:HG12	4:B:215:THR:O	1.99	0.62
4:B:186:LEU:O	4:B:191:LYS:HB3	1.98	0.62
3:E:201:ARG:NH2	4:F:255:ARG:NH2	2.47	0.62
3:E:279:GLU:O	3:E:280:LEU:HD12	1.98	0.62
4:F:163:TYR:O	4:F:164:ASN:C	2.42	0.62
4:B:55:PHE:HB2	4:B:141:HIS:NE2	2.14	0.62
2:D:21:DT:O4	4:B:54:ARG:NH2	2.32	0.62
1:G:10:DC:H2''	1:G:11:DC:C5'	2.30	0.62
4:B:244:ASN:CB	4:B:274:GLN:HE22	2.12	0.62
3:E:201:ARG:NH2	4:F:255:ARG:HH21	1.97	0.62
4:B:45:LEU:HD12	4:B:46:GLU:HB2	1.82	0.62
4:B:114:LYS:HA	4:B:114:LYS:HE3	1.82	0.62
3:E:155:ASN:HB3	3:E:191:THR:HG21	1.81	0.62
4:F:105:HIS:HB3	4:F:201:GLN:HE21	1.63	0.62
3:A:26:GLN:CD	3:A:181:HIS:H	2.06	0.62
3:A:63:ILE:HD12	3:A:63:ILE:N	2.12	0.62
3:A:206:CYS:HA	3:A:288:TYR:CD2	2.33	0.62
3:A:290:PRO:O	3:A:291:ASP:O	2.18	0.62
4:B:98:VAL:HG23	4:B:211:ARG:HB2	1.82	0.62
4:F:237:ILE:N	4:F:237:ILE:HD12	2.14	0.62
4:B:178:ALA:O	4:B:226:THR:HG23	1.99	0.61
4:F:329:VAL:CG2	4:F:345:PHE:HB2	2.30	0.61
4:F:165:PRO:C	4:F:167:LEU:H	2.07	0.61
3:A:24:ILE:HD11	3:A:62:LYS:HB2	1.81	0.61
4:B:244:ASN:HB3	4:B:274:GLN:NE2	2.14	0.61
4:B:279:GLN:HE22	4:B:332:ARG:HH21	1.46	0.61
3:E:131:SER:C	3:E:133:ARG:H	2.09	0.61
4:B:93:VAL:HG22	4:B:216:ALA:HB2	1.83	0.61
4:B:129:ASP:HB3	5:B:827:HOH:O	2.00	0.61
3:E:28:LYS:HG3	3:E:47:PRO:O	2.01	0.61
4:F:42:LEU:HD12	4:F:83:LYS:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:143:VAL:HG13	3:A:147:GLU:OE1	1.99	0.61
4:F:165:PRO:N	4:F:167:LEU:HD13	2.15	0.61
1:G:11:DC:H2'	1:G:12:DT:C6	2.35	0.61
4:F:332:ARG:HD3	4:F:339:THR:HG22	1.83	0.61
4:F:148:PHE:HD2	4:F:148:PHE:O	1.83	0.60
3:A:74:ILE:H	3:A:74:ILE:HD12	1.66	0.60
4:B:143:THR:HG22	4:B:145:LYS:H	1.67	0.60
4:F:254:ASP:HB2	4:F:267:TYR:H	1.65	0.60
4:B:143:THR:HG21	5:B:815:HOH:O	2.01	0.60
3:E:200:ASN:CB	3:E:213:PHE:H	2.08	0.60
3:A:273:ARG:HD2	3:A:280:LEU:HD21	1.82	0.60
4:F:189:ARG:CD	4:F:190:GLU:N	2.64	0.60
1:C:9:DT:OP1	3:A:122:LYS:HD3	2.01	0.60
1:G:6:DA:C2'	1:G:7:DA:O5'	2.50	0.60
3:A:46:ILE:HG13	3:A:116:LEU:O	2.00	0.60
4:B:95:VAL:HG12	4:B:214:PHE:HD1	1.66	0.60
4:B:164:ASN:ND2	4:B:213:MET:SD	2.75	0.60
3:E:77:VAL:HG12	3:E:85:PRO:HA	1.84	0.60
4:F:164:ASN:HA	4:F:167:LEU:HD22	1.84	0.60
3:A:24:ILE:HD11	3:A:62:LYS:CD	2.32	0.60
3:A:201:ARG:HG2	3:A:201:ARG:NH2	2.12	0.60
4:B:57:TYR:N	4:B:57:TYR:CD2	2.68	0.60
4:B:40:PRO:O	4:B:229:LEU:HD22	2.02	0.59
3:A:93:LYS:CE	3:A:115:ASN:HB3	2.32	0.59
4:B:155:MET:SD	4:B:198:ALA:HB2	2.42	0.59
4:B:187:THR:C	4:B:189:ARG:H	2.11	0.59
4:F:99:THR:HG23	4:F:105:HIS:O	2.02	0.59
5:H:760:HOH:O	4:F:145:LYS:HD3	2.00	0.59
3:A:186:ASN:HD21	3:A:193:GLU:HB2	1.67	0.59
4:B:106:LEU:HD22	4:B:168:LEU:CG	2.32	0.59
3:E:46:ILE:HG13	3:E:116:LEU:O	2.01	0.59
1:C:1:DT:H3'	4:B:65:GLY:CA	2.18	0.59
4:B:88:VAL:HG13	4:B:89:GLY:H	1.67	0.59
4:F:240:SER:HA	5:F:859:HOH:O	2.02	0.59
4:B:88:VAL:HG12	4:B:218:LEU:HD22	1.85	0.59
4:B:109:HIS:HE1	4:B:207:LEU:O	1.85	0.59
3:E:70:GLY:HA2	3:E:166:ARG:CZ	2.32	0.59
4:B:158:ALA:HA	4:B:163:TYR:CE1	2.38	0.59
3:E:226:VAL:HG23	3:E:239:PHE:CE1	2.37	0.59
4:F:126:GLY:N	4:F:127:PRO:CD	2.65	0.59
4:F:217:PHE:CE2	4:F:228:ARG:HB3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:DT:H4'	1:G:2:DG:OP1	2.02	0.59
3:E:29:GLN:HA	3:E:29:GLN:HE21	1.68	0.59
4:B:98:VAL:HG22	4:B:211:ARG:O	2.02	0.59
3:E:52:THR:HG22	3:E:53:ASP:N	2.18	0.59
4:F:217:PHE:CD2	4:F:228:ARG:HB3	2.38	0.59
3:A:57:THR:HG22	3:A:58:HIS:N	2.17	0.59
3:A:74:ILE:HD12	3:A:74:ILE:N	2.18	0.59
4:B:240:SER:C	4:B:242:ALA:H	2.10	0.59
3:E:201:ARG:NH1	3:E:210:ASP:HB3	2.18	0.59
4:B:84:ILE:HB	4:B:130:MET:SD	2.43	0.58
3:A:24:ILE:HD11	3:A:62:LYS:CB	2.33	0.58
3:A:124:ARG:HG3	3:A:125:ASP:OD2	2.03	0.58
4:B:114:LYS:HZ3	4:B:136:ASN:HB3	1.68	0.58
2:D:14:DA:H2''	2:D:15:DG:O5'	2.04	0.58
2:D:17:DA:H2''	2:D:18:DA:OP2	2.04	0.58
3:A:108:ARG:HB3	3:A:111:HIS:HE1	1.65	0.58
3:A:163:VAL:O	3:A:174:LEU:HD12	2.03	0.58
3:A:200:ASN:HD21	4:B:254:ASP:CG	2.11	0.58
4:B:76:LYS:CG	4:B:77:LYS:H	2.15	0.58
4:B:165:PRO:HG2	4:B:166:GLY:H	1.68	0.58
1:G:3:DG:H2'	1:G:4:DG:C8	2.38	0.58
3:E:86:HIS:ND1	3:E:87:PRO:HD2	2.18	0.58
4:B:42:LEU:HD23	4:B:84:ILE:HG13	1.84	0.58
3:E:46:ILE:HD12	3:E:116:LEU:HD13	1.84	0.58
3:E:108:ARG:HH11	3:E:108:ARG:CB	2.16	0.58
3:E:198:ARG:NH2	4:F:310:VAL:HG11	2.19	0.58
4:F:66:GLY:O	4:F:68:PRO:HD3	2.04	0.58
1:G:1:DT:H2'	1:G:2:DG:C8	2.39	0.58
3:E:127:GLU:O	3:E:130:ILE:HG22	2.02	0.58
4:F:87:TYR:HD2	4:F:88:VAL:O	1.87	0.58
3:A:40:GLY:O	3:A:41:ARG:C	2.46	0.58
3:A:262:LEU:HD11	3:A:266:VAL:HG21	1.86	0.58
2:D:19:DT:H2''	4:B:57:TYR:OH	2.03	0.58
4:B:76:LYS:HG3	4:B:77:LYS:N	2.18	0.58
4:B:277:ASP:OD2	4:B:334:LYS:HB2	2.04	0.58
3:A:31:GLY:N	3:A:186:ASN:HD22	2.01	0.58
4:B:219:PRO:HG3	4:B:225:PHE:CE1	2.39	0.58
4:F:45:LEU:HD23	4:F:81:GLN:CB	2.33	0.58
3:A:79:LYS:O	3:A:79:LYS:HG2	2.03	0.58
4:B:228:ARG:HG2	4:B:229:LEU:N	2.19	0.58
2:D:21:DT:H2'	4:B:59:CYS:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:333:ARG:HB3	4:B:336:ASP:OD2	2.04	0.57
3:E:273:ARG:CD	3:E:280:LEU:HD11	2.25	0.57
3:A:74:ILE:HD13	3:A:100:TYR:CD1	2.39	0.57
4:F:88:VAL:HG13	4:F:89:GLY:N	2.19	0.57
4:F:254:ASP:HB2	4:F:267:TYR:HB2	1.84	0.57
2:D:21:DT:H3'	4:B:59:CYS:HG	1.69	0.57
4:B:62:PRO:HD2	5:B:843:HOH:O	2.03	0.57
4:B:123:VAL:HG21	4:B:132:VAL:CG1	2.35	0.57
3:E:266:VAL:CG1	3:E:288:TYR:HB2	2.33	0.57
2:H:22:DC:H2'	2:H:23:DC:H6	1.68	0.57
3:A:86:HIS:CE1	3:A:154:LEU:HA	2.39	0.57
2:D:22:DC:OP2	4:B:59:CYS:SG	2.61	0.57
4:F:166:GLY:C	4:F:167:LEU:HD12	2.30	0.57
4:F:343:LYS:HE2	5:F:753:HOH:O	2.04	0.57
3:A:209:GLY:HA2	3:A:253:ARG:CD	2.34	0.57
4:F:101:GLY:O	4:F:102:LYS:C	2.48	0.57
4:F:72:SER:C	4:F:74:LYS:H	2.12	0.57
4:B:38:MET:O	4:B:40:PRO:HD2	2.04	0.57
3:E:122:LYS:HZ2	3:E:124:ARG:HH21	1.52	0.57
4:F:46:GLU:OE1	4:F:78:SER:OG	2.20	0.57
2:H:20:DT:H2''	2:H:21:DT:C5'	2.34	0.57
3:A:79:LYS:CA	3:A:158:ARG:HE	2.18	0.57
3:A:277:ASP:OD1	3:A:279:GLU:HG2	2.05	0.57
4:B:176:LEU:HD21	4:B:184:ARG:HG2	1.87	0.57
3:E:99:TYR:HB3	3:E:138:ASN:HD21	1.70	0.57
1:C:1:DT:H2''	1:C:2:DG:O5'	2.03	0.56
3:A:185:ASP:C	3:A:187:ARG:H	2.13	0.56
3:E:70:GLY:HA2	3:E:166:ARG:NH2	2.19	0.56
3:E:70:GLY:CA	3:E:104:LEU:HD22	2.35	0.56
3:E:70:GLY:O	3:E:104:LEU:HD13	2.04	0.56
3:E:198:ARG:HH21	4:F:310:VAL:HG11	1.70	0.56
3:E:19:ALA:O	3:E:175:LEU:HD22	2.05	0.56
3:E:184:PHE:CD1	3:E:184:PHE:N	2.74	0.56
1:C:5:DA:H3'	3:A:247:GLN:HE22	1.70	0.56
3:A:19:ALA:O	3:A:175:LEU:HD22	2.05	0.56
4:F:175:TYR:CD1	4:F:176:LEU:HG	2.41	0.56
1:G:11:DC:N3	2:H:15:DG:N1	2.40	0.56
4:B:154:ARG:HA	4:B:154:ARG:HE	1.71	0.56
4:B:328:PHE:HE1	4:B:344:PRO:HG3	1.70	0.56
3:E:34:PHE:N	3:E:34:PHE:CD2	2.73	0.56
3:A:86:HIS:CD2	3:A:157:VAL:HG12	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:74:ILE:HG12	3:E:100:TYR:CD1	2.40	0.56
4:F:176:LEU:CD2	4:F:184:ARG:HG3	2.26	0.56
4:F:327:VAL:O	4:F:328:PHE:HD1	1.89	0.56
3:A:71:THR:HG23	3:A:164:THR:HB	1.86	0.56
3:A:229:THR:HG23	3:A:271:GLN:OE1	2.06	0.56
4:F:244:ASN:OD1	4:F:244:ASN:C	2.49	0.56
4:B:40:PRO:CG	4:B:218:LEU:HD11	2.36	0.56
4:B:346:LEU:HD13	4:B:346:LEU:O	2.06	0.56
3:E:56:LYS:H	3:E:56:LYS:CD	2.19	0.56
4:F:187:THR:C	4:F:189:ARG:H	2.14	0.56
2:D:17:DA:C2'	4:B:306:GLN:HE22	2.15	0.56
4:B:39:GLY:HA2	4:B:86:ASN:HD22	1.69	0.56
4:B:143:THR:HB	4:B:146:LYS:HD3	1.88	0.56
3:E:106:PRO:C	3:E:108:ARG:H	2.12	0.56
4:B:58:VAL:HG13	4:B:59:CYS:N	2.20	0.55
3:E:28:LYS:HD3	3:E:47:PRO:CG	2.36	0.55
3:E:81:PRO:O	3:E:83:HIS:N	2.39	0.55
4:F:346:LEU:C	4:F:346:LEU:CD2	2.80	0.55
1:G:2:DG:H2''	1:G:3:DG:C5'	2.36	0.55
3:A:282:GLU:OE1	3:A:283:PRO:HD2	2.06	0.55
1:C:11:DC:H2'	5:C:763:HOH:O	2.04	0.55
3:E:130:ILE:CG2	3:E:131:SER:N	2.69	0.55
3:A:79:LYS:HA	3:A:158:ARG:HE	1.71	0.55
4:B:168:LEU:HD13	4:B:213:MET:HE1	1.88	0.55
4:F:148:PHE:C	4:F:148:PHE:HD2	2.14	0.55
4:F:206:ASP:OD1	4:F:208:SER:OG	2.21	0.55
3:E:24:ILE:HG22	3:E:60:THR:O	2.06	0.55
3:A:79:LYS:HA	3:A:158:ARG:HD2	1.89	0.55
3:E:139:ASN:HD21	3:E:143:VAL:N	2.05	0.55
3:A:60:THR:HG21	3:A:110:ILE:HG22	1.89	0.55
4:F:71:SER:O	4:F:77:LYS:HG2	2.07	0.55
4:F:273:VAL:O	4:F:306:GLN:HB3	2.07	0.55
4:B:187:THR:C	4:B:189:ARG:N	2.64	0.54
4:B:254:ASP:CB	4:B:267:TYR:H	2.21	0.54
3:E:66:TYR:CD1	3:E:67:THR:N	2.75	0.54
4:F:116:CYS:SG	4:F:137:LEU:HD21	2.47	0.54
4:F:254:ASP:CB	4:F:267:TYR:H	2.19	0.54
2:D:19:DT:H4'	2:D:20:DT:OP1	2.06	0.54
4:F:47:GLN:O	4:F:69:GLY:HA2	2.07	0.54
3:E:23:ILE:CD1	3:E:161:PHE:HE2	2.20	0.54
4:F:55:PHE:CE2	4:F:239:ASP:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:167:LEU:N	4:F:167:LEU:CD1	2.69	0.54
3:A:187:ARG:HG2	3:A:187:ARG:HH11	1.71	0.54
4:B:83:LYS:HB2	4:B:131:VAL:HG22	1.89	0.54
3:E:73:ARG:HD2	3:E:99:TYR:CD2	2.42	0.54
1:C:5:DA:H3'	3:A:247:GLN:NE2	2.23	0.54
2:H:15:DG:H2''	2:H:16:DG:O5'	2.08	0.54
3:A:35:ARG:HA	3:A:35:ARG:NE	2.17	0.54
4:B:45:LEU:CD1	4:B:81:GLN:HB2	2.37	0.54
2:H:20:DT:OP2	4:F:57:TYR:OH	2.25	0.54
3:A:93:LYS:HB3	3:A:115:ASN:HB3	1.90	0.54
4:B:161:ARG:HB2	4:B:163:TYR:HE1	1.73	0.54
4:B:308:ALA:C	4:B:309:ILE:HG13	2.33	0.54
3:E:106:PRO:C	3:E:108:ARG:N	2.64	0.54
3:E:272:LEU:H	3:E:281:SER:HB3	1.73	0.54
1:C:5:DA:H61	4:B:54:ARG:HH22	1.54	0.54
4:B:41:TYR:HA	4:B:229:LEU:HB3	1.87	0.54
4:B:111:LEU:HD23	4:B:112:VAL:N	2.22	0.54
4:B:272:LYS:HD2	4:B:306:GLN:OE1	2.08	0.54
3:E:136:THR:HG23	3:E:138:ASN:HB2	1.90	0.54
2:H:21:DT:C2'	2:H:22:DC:O5'	2.53	0.54
4:B:151:LEU:O	4:B:155:MET:HG3	2.08	0.54
4:B:185:GLN:HE21	4:B:185:GLN:HA	1.72	0.54
3:A:61:ILE:HD11	3:A:161:PHE:CE2	2.42	0.54
3:A:61:ILE:HG22	3:A:62:LYS:N	2.23	0.54
4:B:125:ALA:C	4:B:127:PRO:HD2	2.33	0.54
3:A:146:GLU:HA	3:A:149:ARG:NH1	2.23	0.53
3:A:191:THR:HA	3:A:274:ARG:NH1	2.23	0.53
3:E:86:HIS:CD2	3:E:157:VAL:HG12	2.43	0.53
4:F:117:GLU:O	4:F:118:ASP:HB2	2.09	0.53
4:B:172:ASP:C	4:B:173:LEU:HD22	2.34	0.53
3:E:128:GLN:OE1	3:E:128:GLN:O	2.26	0.53
4:F:287:GLU:O	4:F:288:ASN:C	2.51	0.53
4:B:104:ILE:O	4:B:104:ILE:HG13	2.07	0.53
4:F:341:GLU:HA	4:F:341:GLU:OE1	2.08	0.53
3:E:91:VAL:O	3:E:116:LEU:HA	2.08	0.53
4:F:157:GLU:HA	4:F:157:GLU:OE1	2.08	0.53
4:F:160:ILE:HG13	4:F:161:ARG:N	2.22	0.53
3:A:35:ARG:HE	3:A:35:ARG:CA	2.19	0.53
4:B:329:VAL:HG23	4:B:345:PHE:CB	2.37	0.53
3:A:209:GLY:HA2	3:A:253:ARG:NE	2.23	0.53
4:B:84:ILE:HD12	4:B:84:ILE:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:88:HIS:ND1	3:E:120:CYS:HA	2.24	0.53
4:F:45:LEU:HD23	4:F:81:GLN:HB3	1.91	0.53
4:F:219:PRO:HG3	4:F:225:PHE:CE1	2.44	0.53
1:G:10:DC:H2''	1:G:11:DC:H5'	1.91	0.53
3:A:25:GLU:OE2	3:A:60:THR:HB	2.08	0.53
4:F:108:ALA:CB	4:F:142:VAL:HG11	2.38	0.53
4:B:173:LEU:HD22	4:B:173:LEU:N	2.24	0.53
4:F:203:LYS:HD2	4:F:203:LYS:N	2.24	0.53
2:H:16:DG:H2''	2:H:17:DA:C5'	2.39	0.53
3:A:36:TYR:HB2	3:A:39:GLU:HG2	1.91	0.53
3:A:105:CYS:HB3	3:A:108:ARG:CB	2.38	0.53
4:F:300:PRO:O	4:F:303:VAL:HG23	2.09	0.53
3:A:25:GLU:OE2	3:A:25:GLU:N	2.42	0.52
4:B:148:PHE:HZ	4:B:195:ARG:HH22	1.57	0.52
4:B:286:GLU:HB2	4:B:290:GLY:CA	2.33	0.52
3:A:190:ASN:HB3	3:A:220:GLN:OE1	2.09	0.52
3:A:200:ASN:CG	3:A:213:PHE:HB2	2.34	0.52
3:E:27:PRO:HB3	3:E:183:ILE:HD11	1.92	0.52
4:F:209:VAL:HG22	4:F:238:TYR:CD2	2.42	0.52
1:G:3:DG:N7	4:F:56:ARG:NH2	2.53	0.52
3:A:144:PRO:HG2	3:A:147:GLU:HB2	1.89	0.52
4:B:44:ILE:HG22	4:B:46:GLU:O	2.09	0.52
4:B:106:LEU:HD22	4:B:168:LEU:HG	1.90	0.52
3:E:78:THR:HG21	5:E:700:HOH:O	2.08	0.52
3:E:164:THR:HG22	3:E:164:THR:O	2.09	0.52
3:E:210:ASP:O	3:E:254:THR:HG23	2.09	0.52
4:F:165:PRO:HG2	4:F:176:LEU:O	2.09	0.52
3:A:190:ASN:H	3:A:190:ASN:ND2	2.08	0.52
4:F:165:PRO:O	4:F:167:LEU:N	2.41	0.52
1:G:7:DA:H2''	1:G:8:DT:O5'	2.10	0.52
1:G:10:DC:H2''	1:G:11:DC:O5'	2.09	0.52
3:E:96:ARG:O	3:E:98:GLY:N	2.42	0.52
3:E:257:TYR:HB2	3:E:288:TYR:CD2	2.44	0.52
4:F:318:ASP:O	4:F:318:ASP:OD2	2.28	0.52
3:A:255:PRO:HG2	3:A:288:TYR:OH	2.10	0.52
4:B:53:PHE:CD2	4:B:55:PHE:HD1	2.28	0.52
4:F:187:THR:C	4:F:189:ARG:N	2.66	0.52
3:A:232:GLY:O	3:E:141:PHE:HA	2.10	0.52
4:B:107:HIS:ND1	4:B:210:VAL:HG23	2.25	0.52
4:B:143:THR:HB	4:B:146:LYS:H	1.75	0.52
4:B:155:MET:CE	4:B:169:VAL:HG13	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:218:LEU:HD12	4:B:227:ARG:NH2	2.25	0.52
3:A:106:PRO:C	3:A:108:ARG:N	2.68	0.52
3:E:149:ARG:HD2	5:E:741:HOH:O	2.09	0.52
3:E:51:SER:OG	3:E:56:LYS:HA	2.10	0.51
3:A:19:ALA:HB1	3:A:64:ASN:O	2.10	0.51
3:A:79:LYS:HB3	3:A:79:LYS:HZ3	1.75	0.51
4:B:42:LEU:HD13	4:B:214:PHE:HB3	1.92	0.51
4:F:115:HIS:HB3	4:F:122:THR:O	2.09	0.51
3:A:25:GLU:HB2	3:A:59:PRO:HA	1.91	0.51
3:A:187:ARG:HG2	3:A:187:ARG:NH1	2.24	0.51
4:B:47:GLN:NE2	4:B:235:ASP:OD1	2.44	0.51
3:E:19:ALA:HB3	3:E:175:LEU:HD21	1.92	0.51
3:E:130:ILE:O	3:E:133:ARG:HB2	2.11	0.51
3:E:241:GLN:HE21	3:E:241:GLN:HA	1.75	0.51
4:F:175:TYR:HA	4:F:177:GLN:OE1	2.10	0.51
4:F:84:ILE:HG13	4:F:130:MET:O	2.11	0.51
3:A:157:VAL:HG11	5:A:736:HOH:O	2.10	0.51
3:A:190:ASN:N	3:A:190:ASN:HD22	2.08	0.51
4:B:50:GLN:HG3	4:B:236:ALA:O	2.10	0.51
3:E:108:ARG:HH11	3:E:108:ARG:N	2.08	0.51
4:F:179:GLU:HG2	4:F:184:ARG:NH2	2.26	0.51
3:A:24:ILE:HD11	3:A:62:LYS:HD2	1.91	0.51
4:B:56:ARG:HH11	4:B:56:ARG:CB	2.21	0.51
4:B:318:ASP:C	4:B:320:ASN:H	2.19	0.51
3:E:201:ARG:NH1	3:E:211:GLU:O	2.43	0.51
3:E:213:PHE:HB3	4:F:267:TYR:HD2	1.76	0.51
4:F:95:VAL:HA	4:F:213:MET:O	2.10	0.51
4:F:155:MET:SD	4:F:198:ALA:HB2	2.50	0.51
2:D:17:DA:H2'	4:B:306:GLN:NE2	2.21	0.51
3:A:100:TYR:CD1	3:A:100:TYR:C	2.89	0.51
3:A:146:GLU:HA	3:A:149:ARG:NH2	2.26	0.51
3:A:218:LYS:HA	3:A:247:GLN:O	2.11	0.51
4:B:84:ILE:HG22	4:B:87:TYR:HB3	1.92	0.51
4:B:236:ALA:HB3	4:B:238:TYR:CZ	2.46	0.51
3:E:145:ILE:N	3:E:145:ILE:HD12	2.26	0.51
3:A:84:ARG:HB3	3:A:148:GLN:HG3	1.93	0.51
3:A:262:LEU:HD11	3:A:266:VAL:CG2	2.40	0.51
4:B:106:LEU:HD22	4:B:168:LEU:HD23	1.93	0.51
4:F:95:VAL:HG23	4:F:213:MET:O	2.10	0.51
4:F:268:LEU:HD12	4:F:280:ILE:CD1	2.41	0.51
3:A:239:PHE:HB3	3:A:252:PHE:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:84:ILE:CB	4:B:130:MET:SD	2.99	0.51
4:B:126:GLY:N	4:B:127:PRO:CD	2.73	0.51
4:B:291:VAL:HG13	4:B:291:VAL:O	2.11	0.51
3:E:76:LEU:HD22	3:E:157:VAL:HB	1.93	0.51
3:E:257:TYR:OH	3:E:266:VAL:HG21	2.11	0.51
3:E:266:VAL:HG13	3:E:266:VAL:O	2.10	0.51
4:F:97:LEU:HG	4:F:111:LEU:HG	1.93	0.51
4:F:271:ASP:O	4:F:273:VAL:HG13	2.11	0.51
4:B:254:ASP:HB2	4:B:267:TYR:H	1.75	0.51
3:E:67:THR:HG22	3:E:106:PRO:O	2.10	0.51
3:A:36:TYR:O	3:A:37:LYS:C	2.54	0.50
4:B:311:PHE:CD1	4:B:311:PHE:C	2.88	0.50
4:F:172:ASP:C	4:F:174:ALA:H	2.19	0.50
2:D:21:DT:H3'	4:B:59:CYS:SG	2.52	0.50
3:A:77:VAL:HG22	3:A:158:ARG:O	2.11	0.50
3:A:84:ARG:H	3:A:84:ARG:NE	2.05	0.50
3:E:41:ARG:HD3	3:E:41:ARG:N	2.27	0.50
3:E:275:PRO:O	3:E:276:SER:C	2.54	0.50
4:F:93:VAL:HA	4:F:216:ALA:HA	1.93	0.50
4:F:114:LYS:HD2	4:F:135:ALA:O	2.11	0.50
4:F:175:TYR:O	4:F:176:LEU:HB2	2.12	0.50
4:F:272:LYS:HA	4:F:306:GLN:O	2.11	0.50
2:D:21:DT:H73	4:B:60:GLU:HB2	1.93	0.50
3:A:18:MET:HE1	3:A:167:ASP:HB3	1.93	0.50
3:A:46:ILE:HD12	3:A:116:LEU:HD22	1.93	0.50
3:A:145:ILE:HG23	3:A:146:GLU:CD	2.36	0.50
4:B:87:TYR:CD1	4:B:130:MET:HB2	2.46	0.50
3:E:279:GLU:C	3:E:280:LEU:HD12	2.36	0.50
4:F:227:ARG:NE	4:F:227:ARG:CA	2.71	0.50
4:F:286:GLU:HB3	4:F:287:GLU:OE2	2.09	0.50
4:B:87:TYR:HB2	4:B:130:MET:SD	2.51	0.50
4:B:152:GLU:OE2	4:B:195:ARG:NH1	2.45	0.50
4:B:222:THR:HG21	5:B:718:HOH:O	2.12	0.50
4:B:336:ASP:CG	4:B:338:GLU:HB2	2.37	0.50
3:E:31:GLY:HA2	3:E:186:ASN:HD22	1.73	0.50
4:F:73:GLU:O	4:F:75:ASN:N	2.43	0.50
4:F:316:TYR:CG	4:F:317:LYS:N	2.79	0.50
4:B:42:LEU:HD11	4:B:93:VAL:HG13	1.93	0.50
4:B:141:HIS:HE1	4:B:239:ASP:CG	2.20	0.50
4:B:299:SER:OG	4:B:300:PRO:HD2	2.12	0.50
4:F:95:VAL:CG1	4:F:121:CYS:HB2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:81:PRO:C	3:A:83:HIS:H	2.18	0.50
3:A:267:ARG:HD3	5:A:861:HOH:O	2.12	0.50
4:B:53:PHE:C	4:B:240:SER:HB2	2.37	0.50
4:B:117:GLU:HG3	4:B:117:GLU:O	2.11	0.50
4:B:237:ILE:O	4:B:238:TYR:O	2.29	0.50
3:E:27:PRO:O	3:E:181:HIS:NE2	2.44	0.50
3:E:58:HIS:CD2	3:E:114:GLN:HA	2.46	0.50
4:F:189:ARG:HD2	4:F:190:GLU:CB	2.42	0.50
3:A:78:THR:HG22	3:A:79:LYS:N	2.27	0.50
4:B:162:GLY:HA2	4:B:177:GLN:C	2.36	0.50
3:E:27:PRO:CB	3:E:183:ILE:HD11	2.42	0.50
1:G:4:DG:H3'	3:E:246:ARG:HH11	1.73	0.50
4:F:108:ALA:HB2	4:F:205:MET:HE1	1.88	0.50
3:A:127:GLU:OE2	3:A:128:GLN:HG3	2.12	0.50
3:A:203:SER:O	3:A:204:GLY:O	2.30	0.50
4:B:99:THR:HG23	4:B:206:ASP:OD2	2.12	0.50
3:E:130:ILE:HG23	3:E:131:SER:N	2.27	0.50
4:F:49:LYS:O	4:F:49:LYS:HG3	2.12	0.50
4:F:189:ARG:CD	4:F:189:ARG:C	2.85	0.50
1:C:5:DA:H2''	1:C:6:DA:H8	1.77	0.49
3:A:105:CYS:HB3	3:A:108:ARG:HB3	1.92	0.49
3:A:259:ASP:OD2	3:A:262:LEU:HA	2.12	0.49
4:B:157:GLU:HG3	4:B:163:TYR:OH	2.12	0.49
3:E:167:ASP:O	3:E:169:ALA:N	2.44	0.49
4:F:329:VAL:HG23	4:F:345:PHE:CB	2.36	0.49
4:B:88:VAL:CG1	4:B:218:LEU:HD13	2.43	0.49
4:B:118:ASP:HB3	4:B:154:ARG:HH22	1.77	0.49
3:E:200:ASN:HB2	3:E:213:PHE:N	2.10	0.49
3:A:78:THR:O	3:A:158:ARG:HD2	2.12	0.49
3:E:174:LEU:H	3:E:174:LEU:CD2	2.13	0.49
3:E:271:GLN:HG2	3:E:283:PRO:HA	1.94	0.49
1:C:3:DG:H1'	1:C:4:DG:N7	2.27	0.49
3:A:74:ILE:HB	3:A:100:TYR:HB3	1.93	0.49
3:E:53:ASP:CG	3:E:54:THR:N	2.70	0.49
3:E:111:HIS:HD2	3:E:111:HIS:N	2.00	0.49
3:E:255:PRO:HG2	3:E:288:TYR:OH	2.11	0.49
4:F:100:ASN:CG	4:F:101:GLY:H	2.21	0.49
4:F:284:GLU:OE1	4:F:316:TYR:OH	2.30	0.49
1:G:1:DT:H2''	1:G:2:DG:O5'	2.11	0.49
4:B:53:PHE:CE2	4:B:55:PHE:HA	2.47	0.49
4:B:112:VAL:HG12	4:B:113:GLY:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:176:LEU:CD2	4:B:184:ARG:HG2	2.42	0.49
4:B:236:ALA:HB3	4:B:238:TYR:CE1	2.47	0.49
1:G:2:DG:C2'	1:G:3:DG:O5'	2.61	0.49
2:H:20:DT:H2''	2:H:21:DT:H5'	1.93	0.49
3:A:89:GLU:HB3	3:A:98:GLY:HA2	1.95	0.49
3:E:178:VAL:HG22	3:E:179:LEU:N	2.28	0.49
3:E:228:PHE:CD2	3:E:255:PRO:HG3	2.48	0.49
4:F:100:ASN:OD1	4:F:101:GLY:N	2.45	0.49
4:F:237:ILE:N	4:F:237:ILE:CD1	2.75	0.49
1:C:8:DT:C2'	1:C:9:DT:H72	2.39	0.49
3:E:84:ARG:HG2	3:E:143:VAL:HG11	1.95	0.49
4:F:103:ASN:HB3	4:F:105:HIS:CE1	2.48	0.49
3:A:26:GLN:OE1	3:A:27:PRO:HD2	2.13	0.49
3:A:60:THR:CG2	3:A:110:ILE:HG22	2.43	0.49
4:F:282:PHE:CD2	4:F:329:VAL:HG22	2.48	0.49
3:A:74:ILE:HG13	3:A:161:PHE:CE1	2.48	0.49
4:B:83:LYS:HB3	4:B:131:VAL:HG13	1.95	0.49
4:B:115:HIS:HB3	4:B:122:THR:O	2.13	0.49
4:B:215:THR:HG23	4:B:228:ARG:CG	2.38	0.49
4:F:108:ALA:HB3	4:F:142:VAL:HG11	1.94	0.49
4:B:88:VAL:HG22	4:B:89:GLY:N	2.27	0.48
3:E:26:GLN:O	3:E:49:GLU:HB3	2.13	0.48
4:F:286:GLU:OE1	4:F:317:LYS:HE2	2.13	0.48
3:A:205:SER:C	3:A:207:LEU:H	2.21	0.48
4:B:143:THR:CB	4:B:146:LYS:HD3	2.43	0.48
4:B:228:ARG:HD2	4:B:231:PRO:CG	2.43	0.48
4:B:284:GLU:O	4:B:291:VAL:HA	2.13	0.48
4:B:333:ARG:HG2	4:B:335:SER:OG	2.13	0.48
1:C:1:DT:H2'	1:C:2:DG:C8	2.49	0.48
1:G:1:DT:H3'	4:F:64:HIS:C	2.38	0.48
3:A:28:LYS:HD2	3:A:49:GLU:OE2	2.13	0.48
4:B:115:HIS:N	4:B:115:HIS:CD2	2.80	0.48
4:B:195:ARG:CA	4:B:195:ARG:NH1	2.74	0.48
3:E:201:ARG:HH21	4:F:255:ARG:HH21	1.60	0.48
4:F:187:THR:OG1	4:F:189:ARG:HG3	2.13	0.48
4:F:318:ASP:C	4:F:320:ASN:H	2.21	0.48
4:B:148:PHE:CE1	4:B:199:VAL:HG22	2.45	0.48
3:E:136:THR:O	3:E:137:ASN:C	2.56	0.48
3:A:74:ILE:H	3:A:74:ILE:CD1	2.27	0.48
3:A:216:CYS:O	4:B:304:HIS:HE1	1.96	0.48
4:B:42:LEU:HD12	4:B:214:PHE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:186:LEU:H	4:B:186:LEU:CD1	2.12	0.48
3:E:66:TYR:CE1	3:E:68:GLY:N	2.81	0.48
3:E:282:GLU:CG	3:E:283:PRO:HD2	2.42	0.48
4:F:321:ILE:HG13	4:F:323:LYS:H	1.79	0.48
3:A:62:LYS:HG2	3:A:64:ASN:HD21	1.78	0.48
3:A:80:ASP:O	3:A:84:ARG:NH2	2.46	0.48
4:B:186:LEU:HD12	4:B:186:LEU:N	2.16	0.48
3:E:37:LYS:O	3:E:39:GLU:N	2.47	0.48
3:E:132:GLN:O	3:E:136:THR:HG22	2.14	0.48
3:E:181:HIS:HB2	3:E:182:PRO:HD2	1.95	0.48
4:F:197:ALA:C	4:F:199:VAL:H	2.22	0.48
1:G:2:DG:H2''	1:G:3:DG:H5'	1.94	0.48
3:A:185:ASP:C	3:A:187:ARG:N	2.70	0.48
4:B:57:TYR:CD1	4:B:141:HIS:HB2	2.48	0.48
4:B:110:SER:HB3	4:B:119:GLY:CA	2.44	0.48
3:E:71:THR:HG22	3:E:72:VAL:N	2.29	0.48
3:E:274:ARG:NE	3:E:277:ASP:OD1	2.45	0.48
4:F:90:PRO:HA	4:F:126:GLY:O	2.14	0.48
4:F:259:CYS:SG	4:F:350:GLU:HG2	2.54	0.48
3:E:196:ILE:HG23	3:E:214:LEU:HD21	1.94	0.48
2:D:22:DC:H2''	2:D:23:DC:C5'	2.36	0.48
3:A:62:LYS:HG2	3:A:64:ASN:ND2	2.28	0.48
3:A:127:GLU:O	3:A:130:ILE:HG22	2.14	0.48
4:F:170:HIS:O	4:F:172:ASP:N	2.47	0.48
4:B:53:PHE:O	4:B:240:SER:HB2	2.14	0.47
3:E:248:VAL:CG1	4:F:305:ARG:HG3	2.43	0.47
4:F:170:HIS:O	4:F:171:SER:C	2.56	0.47
4:B:109:HIS:CD2	4:B:142:VAL:HG12	2.49	0.47
4:B:114:LYS:HE3	4:B:114:LYS:CA	2.43	0.47
4:B:218:LEU:CG	4:B:229:LEU:HD21	2.43	0.47
3:E:63:ILE:O	3:E:63:ILE:HG13	2.13	0.47
3:E:218:LYS:HA	3:E:247:GLN:O	2.14	0.47
1:C:6:DA:H5'	5:C:806:HOH:O	2.13	0.47
3:E:59:PRO:O	3:E:113:PHE:HD1	1.97	0.47
3:E:205:SER:C	3:E:207:LEU:H	2.22	0.47
4:B:111:LEU:HD23	4:B:138:GLY:O	2.15	0.47
4:F:84:ILE:CG1	4:F:130:MET:HB3	2.44	0.47
4:F:125:ALA:C	4:F:127:PRO:HD3	2.39	0.47
3:A:146:GLU:HA	3:A:149:ARG:CZ	2.44	0.47
3:A:173:LEU:HD13	3:A:173:LEU:C	2.39	0.47
3:E:41:ARG:HD3	3:E:41:ARG:H	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:333:ARG:HD2	4:F:336:ASP:OD1	2.14	0.47
4:B:219:PRO:HG3	4:B:225:PHE:HE1	1.78	0.47
4:F:154:ARG:C	4:F:156:THR:H	2.23	0.47
4:F:321:ILE:O	4:F:349:PRO:HB3	2.15	0.47
1:C:9:DT:H2''	1:C:10:DC:OP2	2.15	0.47
1:G:6:DA:H2'	1:G:7:DA:C8	2.50	0.47
3:A:75:SER:OG	3:A:162:GLN:NE2	2.48	0.47
3:A:233:TRP:HA	3:E:141:PHE:O	2.15	0.47
3:A:240:SER:OG	3:A:243:ASP:OD2	2.31	0.47
3:A:273:ARG:NH1	3:E:81:PRO:HD2	2.30	0.47
4:B:41:TYR:O	4:B:84:ILE:HG23	2.15	0.47
4:B:93:VAL:HA	4:B:216:ALA:HA	1.97	0.47
4:B:97:LEU:HD12	4:B:109:HIS:C	2.40	0.47
4:B:117:GLU:O	4:B:118:ASP:HB2	2.14	0.47
3:E:116:LEU:O	3:E:116:LEU:HD12	2.15	0.47
3:E:194:LEU:HB3	3:E:281:SER:HB2	1.97	0.47
4:F:50:GLN:NE2	4:F:235:ASP:HB3	2.29	0.47
4:F:70:ALA:O	4:F:71:SER:HB2	2.15	0.47
4:F:183:ASP:OD1	4:F:183:ASP:O	2.32	0.47
3:A:84:ARG:HG2	3:A:148:GLN:HA	1.97	0.47
3:A:275:PRO:O	3:A:276:SER:C	2.58	0.47
4:B:57:TYR:N	4:B:57:TYR:HD2	2.12	0.47
4:B:216:ALA:O	4:B:229:LEU:HG	2.15	0.47
3:E:23:ILE:HB	3:E:26:GLN:HG3	1.97	0.47
3:E:227:TYR:CE2	3:E:229:THR:HG22	2.49	0.47
4:F:57:TYR:O	4:F:58:VAL:C	2.57	0.47
2:D:19:DT:H2''	2:D:20:DT:H71	1.96	0.47
3:A:190:ASN:ND2	3:A:190:ASN:N	2.62	0.47
4:F:116:CYS:SG	4:F:137:LEU:CD2	3.03	0.47
3:A:46:ILE:CG1	3:A:116:LEU:HD13	2.45	0.46
3:A:60:THR:OG1	3:A:112:SER:HB2	2.15	0.46
3:A:63:ILE:H	3:A:63:ILE:CD1	2.20	0.46
3:A:261:SER:HA	3:A:291:ASP:OD2	2.15	0.46
4:B:69:GLY:O	4:B:71:SER:N	2.48	0.46
4:B:79:TYR:O	4:B:81:GLN:HG2	2.15	0.46
4:B:95:VAL:HA	4:B:213:MET:O	2.15	0.46
4:B:316:TYR:CG	4:B:317:LYS:N	2.83	0.46
3:A:200:ASN:OD1	4:B:254:ASP:OD1	2.33	0.46
3:A:245:HIS:CE1	4:B:251:VAL:HG21	2.50	0.46
3:E:140:PRO:HB3	3:E:160:CYS:SG	2.54	0.46
4:F:55:PHE:CD2	4:F:239:ASP:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:121:CYS:SG	4:F:137:LEU:HD21	2.55	0.46
1:C:9:DT:OP2	3:A:36:TYR:HB3	2.14	0.46
3:A:139:ASN:OD1	3:A:142:HIS:HA	2.14	0.46
3:A:41:ARG:HD3	3:A:41:ARG:N	2.29	0.46
3:A:191:THR:O	3:A:191:THR:HG23	2.15	0.46
4:F:173:LEU:HB3	4:F:176:LEU:HD12	1.96	0.46
3:E:160:CYS:HA	3:E:178:VAL:O	2.16	0.46
4:F:247:ASN:HD22	4:F:247:ASN:HA	1.57	0.46
3:A:236:ARG:NE	3:E:82:PRO:HG2	2.26	0.46
4:B:125:ALA:HB3	4:B:132:VAL:CG2	2.40	0.46
3:E:135:GLN:HA	3:E:135:GLN:OE1	2.15	0.46
4:B:93:VAL:HG13	4:B:216:ALA:HB2	1.96	0.46
4:F:77:LYS:HG2	5:F:755:HOH:O	2.15	0.46
4:F:146:LYS:O	4:F:150:THR:HB	2.14	0.46
3:A:46:ILE:HB	3:A:116:LEU:HD13	1.98	0.46
4:B:62:PRO:O	4:B:63:SER:C	2.57	0.46
3:E:78:THR:O	3:E:83:HIS:HD2	1.99	0.46
3:E:81:PRO:HB2	3:E:82:PRO:CD	2.39	0.46
3:E:196:ILE:HG12	3:E:272:LEU:HD22	1.97	0.46
3:E:227:TYR:CD2	3:E:280:LEU:HD21	2.50	0.46
4:F:175:TYR:HA	4:F:177:GLN:CD	2.41	0.46
3:A:160:CYS:SG	3:A:177:PRO:HB2	2.55	0.46
3:E:141:PHE:CZ	3:E:179:LEU:HD11	2.51	0.46
3:E:148:GLN:C	3:E:149:ARG:HG3	2.41	0.46
3:E:214:LEU:C	3:E:214:LEU:HD23	2.41	0.46
4:F:287:GLU:O	4:F:289:GLY:N	2.48	0.46
3:A:71:THR:HA	3:A:103:ASP:HA	1.97	0.46
3:A:236:ARG:HG2	3:E:147:GLU:OE2	2.16	0.46
4:B:42:LEU:HD12	4:B:214:PHE:C	2.41	0.46
4:B:69:GLY:N	4:B:78:SER:O	2.49	0.46
4:B:195:ARG:HA	4:B:195:ARG:NH1	2.16	0.46
3:E:105:CYS:HB2	3:E:108:ARG:HB2	1.97	0.46
3:E:155:ASN:CB	3:E:191:THR:HG21	2.46	0.46
3:E:203:SER:O	3:E:204:GLY:O	2.34	0.46
3:E:245:HIS:O	3:E:246:ARG:C	2.59	0.46
4:F:160:ILE:HD12	4:F:160:ILE:C	2.41	0.46
4:F:161:ARG:HG2	4:F:163:TYR:CE1	2.50	0.46
4:F:248:LEU:HB2	4:F:340:SER:HB3	1.98	0.46
4:B:93:VAL:HG22	4:B:216:ALA:HB1	1.98	0.45
3:E:86:HIS:CG	3:E:157:VAL:HG12	2.51	0.45
3:E:217:ASP:O	3:E:218:LYS:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:42:LEU:CD2	4:F:214:PHE:HB3	2.46	0.45
4:F:97:LEU:HD12	4:F:109:HIS:C	2.42	0.45
4:F:177:GLN:O	4:F:184:ARG:NH2	2.49	0.45
4:B:143:THR:C	4:B:145:LYS:H	2.23	0.45
3:E:139:ASN:ND2	3:E:142:HIS:HA	2.31	0.45
4:F:179:GLU:HG2	4:F:184:ARG:HH21	1.81	0.45
4:F:222:THR:HG22	4:F:223:GLY:N	2.30	0.45
4:F:267:TYR:CE1	4:F:310:VAL:HG22	2.51	0.45
3:A:26:GLN:HG3	3:A:181:HIS:CD2	2.52	0.45
3:A:33:ARG:HB2	3:A:187:ARG:HD3	1.99	0.45
3:A:165:VAL:O	3:A:172:PRO:HA	2.16	0.45
3:A:200:ASN:HD22	3:A:200:ASN:HA	1.54	0.45
3:A:214:LEU:C	3:A:214:LEU:HD23	2.40	0.45
4:B:176:LEU:HD11	4:B:184:ARG:HB2	1.98	0.45
4:F:87:TYR:CD2	4:F:88:VAL:O	2.69	0.45
4:B:185:GLN:HA	4:B:185:GLN:NE2	2.31	0.45
4:B:249:LYS:HG2	4:B:250:ILE:N	2.32	0.45
4:B:292:TRP:HZ2	4:B:315:LYS:O	2.00	0.45
4:B:299:SER:O	4:B:302:ASP:HB2	2.16	0.45
3:E:72:VAL:HB	3:E:104:LEU:HD11	1.97	0.45
3:E:200:ASN:HD21	4:F:254:ASP:CG	2.24	0.45
4:F:107:HIS:CE1	4:F:210:VAL:HG12	2.51	0.45
1:C:8:DT:H2'	3:A:36:TYR:CZ	2.52	0.45
3:A:61:ILE:CG2	3:A:62:LYS:N	2.80	0.45
3:A:81:PRO:O	3:A:83:HIS:N	2.44	0.45
3:E:93:LYS:HG2	3:E:94:ASP:OD2	2.17	0.45
4:F:112:VAL:HG22	4:F:138:GLY:C	2.41	0.45
4:F:229:LEU:O	4:F:230:GLU:C	2.59	0.45
4:F:346:LEU:HD23	4:F:346:LEU:O	2.16	0.45
3:A:28:LYS:O	3:A:29:GLN:C	2.60	0.45
3:A:185:ASP:O	3:A:187:ARG:N	2.50	0.45
3:E:72:VAL:CG1	3:E:100:TYR:HE1	2.28	0.45
4:F:107:HIS:HD2	4:F:109:HIS:N	2.04	0.45
4:F:286:GLU:HB3	4:F:287:GLU:H	1.61	0.45
3:A:194:LEU:HD12	3:A:280:LEU:C	2.42	0.45
4:B:56:ARG:HB3	4:B:56:ARG:CZ	2.46	0.45
4:F:113:GLY:O	4:F:114:LYS:C	2.59	0.45
4:F:236:ALA:C	4:F:237:ILE:HD12	2.41	0.45
1:G:11:DC:H2'	1:G:12:DT:H6	1.82	0.45
3:A:58:HIS:CD2	3:A:114:GLN:NE2	2.85	0.45
3:A:214:LEU:HD21	3:A:216:CYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:288:ASN:C	4:B:288:ASN:HD22	2.25	0.45
3:E:257:TYR:HD2	3:E:259:ASP:H	1.64	0.45
3:A:129:ALA:HA	3:A:132:GLN:CD	2.41	0.45
4:B:42:LEU:HD13	4:B:214:PHE:CB	2.46	0.45
4:B:73:GLU:O	4:B:74:LYS:CB	2.65	0.45
4:B:88:VAL:CG1	4:B:218:LEU:HD22	2.45	0.45
4:B:143:THR:C	4:B:145:LYS:N	2.75	0.45
3:A:77:VAL:HA	3:A:86:HIS:H	1.82	0.44
3:E:53:ASP:CG	3:E:54:THR:H	2.25	0.44
4:F:237:ILE:O	4:F:237:ILE:HG22	2.16	0.44
4:B:173:LEU:C	4:B:175:TYR:H	2.25	0.44
4:B:288:ASN:C	4:B:288:ASN:ND2	2.74	0.44
3:E:77:VAL:HA	3:E:86:HIS:H	1.81	0.44
4:F:69:GLY:O	4:F:71:SER:N	2.50	0.44
4:F:71:SER:HB3	4:F:78:SER:OG	2.17	0.44
4:F:181:GLY:O	4:F:182:GLY:C	2.60	0.44
4:F:327:VAL:C	4:F:328:PHE:HD1	2.24	0.44
3:A:52:THR:HG22	3:A:53:ASP:N	2.32	0.44
3:A:121:VAL:O	3:A:121:VAL:HG13	2.17	0.44
4:B:55:PHE:CB	4:B:141:HIS:NE2	2.81	0.44
4:F:126:GLY:HA2	4:F:130:MET:HE2	2.00	0.44
4:F:155:MET:O	4:F:194:ILE:HD13	2.18	0.44
3:A:60:THR:HG23	3:A:111:HIS:C	2.42	0.44
3:A:72:VAL:HG12	3:A:163:VAL:HG12	2.00	0.44
4:B:189:ARG:O	4:B:189:ARG:NH1	2.51	0.44
3:E:255:PRO:HA	5:E:732:HOH:O	2.17	0.44
3:E:259:ASP:C	3:E:261:SER:H	2.26	0.44
4:F:193:ILE:HD13	4:F:193:ILE:HA	1.86	0.44
4:F:343:LYS:HA	4:F:344:PRO:HD3	1.71	0.44
1:C:1:DT:H2'	1:C:2:DG:H8	1.81	0.44
3:A:81:PRO:C	3:A:83:HIS:N	2.76	0.44
3:A:99:TYR:CD2	3:A:100:TYR:N	2.86	0.44
3:A:183:ILE:O	3:A:183:ILE:HG22	2.18	0.44
3:E:30:ARG:HG3	3:E:30:ARG:HH11	1.83	0.44
3:E:266:VAL:HG13	3:E:288:TYR:HB2	1.99	0.44
4:F:56:ARG:O	4:F:140:LEU:HA	2.17	0.44
1:G:2:DG:H2''	1:G:3:DG:O5'	2.18	0.44
3:A:217:ASP:O	3:A:218:LYS:C	2.60	0.44
4:B:40:PRO:HG3	4:B:218:LEU:HD11	1.98	0.44
4:B:210:VAL:HG22	4:B:211:ARG:N	2.31	0.44
4:B:237:ILE:O	4:B:237:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:193:ILE:HD13	4:F:196:GLN:NE2	2.33	0.44
4:F:275:LYS:HG2	4:F:303:VAL:HB	1.99	0.44
2:H:20:DT:H2''	2:H:21:DT:O5'	2.18	0.44
3:A:273:ARG:CZ	3:E:81:PRO:HG2	2.47	0.44
4:B:58:VAL:HG13	4:B:59:CYS:H	1.83	0.44
3:E:141:PHE:CD1	3:E:141:PHE:N	2.86	0.44
1:C:10:DC:P	4:B:144:LYS:HD3	2.58	0.44
1:G:2:DG:O6	4:F:64:HIS:CE1	2.71	0.44
3:A:139:ASN:HD22	3:A:139:ASN:HA	1.64	0.44
4:B:109:HIS:CD2	4:B:142:VAL:H	2.36	0.44
4:B:120:VAL:O	4:B:120:VAL:HG13	2.18	0.44
4:B:271:ASP:O	4:B:273:VAL:HG13	2.18	0.44
4:F:151:LEU:C	4:F:151:LEU:HD12	2.42	0.44
4:F:152:GLU:HG3	4:F:198:ALA:HB3	1.99	0.44
2:D:17:DA:C2	2:D:18:DA:C4	3.06	0.44
3:A:77:VAL:O	3:A:86:HIS:HB2	2.18	0.44
3:A:282:GLU:HB2	5:A:873:HOH:O	2.18	0.44
3:E:86:HIS:CE1	3:E:87:PRO:HD2	2.53	0.44
4:F:45:LEU:HD23	4:F:81:GLN:HB2	1.99	0.44
4:F:78:SER:C	4:F:79:TYR:CD1	2.96	0.44
4:F:153:ALA:O	4:F:156:THR:HB	2.18	0.44
5:G:731:HOH:O	3:E:221:LYS:HG2	2.18	0.43
4:B:98:VAL:HG11	4:B:213:MET:CE	2.47	0.43
3:E:25:GLU:HG3	3:E:25:GLU:O	2.18	0.43
3:E:29:GLN:NE2	3:E:182:PRO:O	2.51	0.43
3:E:88:HIS:ND1	3:E:121:VAL:HG22	2.33	0.43
4:B:56:ARG:O	4:B:140:LEU:HA	2.17	0.43
4:B:106:LEU:HD22	4:B:168:LEU:CD2	2.47	0.43
4:B:250:ILE:HD13	4:B:268:LEU:HD11	1.99	0.43
4:B:328:PHE:CE1	4:B:344:PRO:HG3	2.52	0.43
4:F:46:GLU:HG2	4:F:47:GLN:N	2.21	0.43
3:A:259:ASP:C	3:A:261:SER:H	2.25	0.43
3:E:164:THR:HG23	3:E:174:LEU:HD13	2.00	0.43
3:E:180:SER:O	3:E:181:HIS:C	2.62	0.43
3:E:200:ASN:CG	3:E:213:PHE:HB2	2.43	0.43
4:B:217:PHE:CD1	4:B:225:PHE:CB	3.01	0.43
4:F:280:ILE:HG12	4:F:298:PHE:CE1	2.54	0.43
2:D:20:DT:O2	2:D:21:DT:O4'	2.36	0.43
3:A:198:ARG:HD3	4:B:310:VAL:HG21	2.00	0.43
4:F:48:PRO:C	4:F:50:GLN:H	2.26	0.43
4:F:88:VAL:HG12	4:F:218:LEU:HD22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:184:PHE:HB3	3:A:191:THR:HG21	2.00	0.43
4:B:143:THR:HB	4:B:146:LYS:HB2	2.00	0.43
4:B:189:ARG:HB3	4:B:189:ARG:CZ	2.49	0.43
3:E:61:ILE:O	3:E:110:ILE:HA	2.18	0.43
1:C:3:DG:C2	1:C:4:DG:C6	3.07	0.43
3:A:104:LEU:HD22	3:A:111:HIS:CD2	2.54	0.43
3:A:255:PRO:HG2	3:A:288:TYR:HH	1.84	0.43
4:B:40:PRO:C	4:B:229:LEU:HD13	2.43	0.43
4:B:49:LYS:C	4:B:51:ARG:H	2.27	0.43
4:B:106:LEU:N	4:B:168:LEU:HG	2.34	0.43
4:B:113:GLY:O	4:B:114:LYS:C	2.60	0.43
4:B:182:GLY:O	4:B:183:ASP:HB2	2.19	0.43
4:B:303:VAL:HG22	4:B:309:ILE:HG12	2.01	0.43
4:F:333:ARG:O	4:F:337:LEU:HA	2.18	0.43
1:C:4:DG:H2''	1:C:5:DA:C8	2.53	0.43
1:C:11:DC:H6	5:C:763:HOH:O	2.02	0.43
2:D:22:DC:H41	4:B:60:GLU:HG3	1.82	0.43
3:A:34:PHE:CE1	3:A:185:ASP:HB2	2.54	0.43
4:B:228:ARG:HD2	4:B:231:PRO:HG3	2.01	0.43
3:E:104:LEU:N	3:E:104:LEU:CD1	2.81	0.43
3:E:224:ILE:HG13	3:E:225:GLU:N	2.34	0.43
3:E:257:TYR:CE1	3:E:266:VAL:HG21	2.54	0.43
4:F:109:HIS:CE1	4:F:142:VAL:H	2.37	0.43
4:F:271:ASP:O	4:F:272:LYS:C	2.61	0.43
3:A:87:PRO:O	3:A:129:ALA:HB1	2.18	0.43
4:B:110:SER:HB3	4:B:119:GLY:HA2	2.01	0.43
4:B:240:SER:C	4:B:242:ALA:N	2.76	0.43
3:E:228:PHE:CE1	3:E:270:MET:HB2	2.54	0.43
4:F:164:ASN:C	4:F:167:LEU:HD13	2.44	0.43
3:E:31:GLY:HA2	3:E:186:ASN:ND2	2.33	0.42
3:E:89:GLU:HG3	3:E:133:ARG:HH12	1.84	0.42
3:E:205:SER:C	3:E:207:LEU:N	2.77	0.42
3:E:226:VAL:HG21	3:E:252:PHE:CD2	2.54	0.42
4:F:46:GLU:CG	4:F:47:GLN:H	2.19	0.42
4:F:47:GLN:OE1	4:F:234:SER:HB2	2.19	0.42
4:F:88:VAL:CG2	4:F:89:GLY:H	2.11	0.42
4:F:148:PHE:HB2	4:F:202:THR:HG21	2.01	0.42
2:D:18:DA:P	4:B:243:PRO:HG2	2.59	0.42
1:G:9:DT:H2''	1:G:10:DC:O4'	2.20	0.42
2:H:22:DC:H2'	2:H:23:DC:O4'	2.19	0.42
4:B:116:CYS:N	4:B:121:CYS:SG	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:259:CYS:SG	4:B:350:GLU:HG2	2.60	0.42
4:B:271:ASP:O	4:B:272:LYS:C	2.62	0.42
3:E:52:THR:HG22	3:E:53:ASP:H	1.84	0.42
3:E:52:THR:CG2	3:E:53:ASP:N	2.81	0.42
3:E:73:ARG:HD2	3:E:99:TYR:HD2	1.81	0.42
4:B:221:SER:O	4:B:222:THR:HB	2.19	0.42
4:F:163:TYR:O	4:F:165:PRO:N	2.52	0.42
3:A:167:ASP:HB2	3:A:168:PRO:CD	2.48	0.42
4:B:84:ILE:HG21	4:B:130:MET:SD	2.59	0.42
4:B:123:VAL:HG21	4:B:132:VAL:HG11	2.01	0.42
4:B:259:CYS:H	4:B:264:GLU:CD	2.27	0.42
4:B:281:ARG:HG3	4:B:295:PHE:CE2	2.54	0.42
3:E:219:VAL:O	3:E:247:GLN:HG2	2.19	0.42
4:F:173:LEU:HD21	4:F:190:GLU:HG3	2.01	0.42
4:B:90:PRO:HA	4:B:126:GLY:O	2.20	0.42
4:B:92:LYS:HG2	4:B:124:THR:HA	2.01	0.42
4:B:105:HIS:CB	4:B:201:GLN:HE22	2.32	0.42
3:E:28:LYS:HB3	3:E:28:LYS:HE2	1.79	0.42
3:E:41:ARG:N	3:E:41:ARG:CD	2.82	0.42
4:F:85:CYS:C	4:F:87:TYR:N	2.72	0.42
4:F:91:ALA:O	4:F:124:THR:O	2.38	0.42
4:F:175:TYR:CE1	4:F:176:LEU:HG	2.54	0.42
4:F:202:THR:O	4:F:202:THR:HG22	2.19	0.42
4:F:318:ASP:O	4:F:318:ASP:CG	2.63	0.42
3:A:106:PRO:O	3:A:108:ARG:N	2.52	0.42
3:A:146:GLU:HA	3:A:149:ARG:HH12	1.84	0.42
3:E:23:ILE:HA	3:E:61:ILE:HA	2.01	0.42
3:E:30:ARG:NH2	3:E:277:ASP:OD2	2.53	0.42
4:F:206:ASP:OD1	4:F:206:ASP:C	2.63	0.42
4:F:215:THR:OG1	4:F:231:PRO:HB3	2.19	0.42
4:B:181:GLY:HA3	4:B:184:ARG:NE	2.34	0.42
3:E:34:PHE:HA	5:E:719:HOH:O	2.18	0.42
4:F:136:ASN:HD22	4:F:136:ASN:HA	1.70	0.42
2:H:13:DA:H2'	2:H:14:DA:C8	2.55	0.42
3:A:50:ARG:HE	3:A:50:ARG:HB3	1.49	0.42
3:A:86:HIS:HA	3:A:87:PRO:HD2	1.72	0.42
3:E:131:SER:C	3:E:133:ARG:N	2.71	0.42
3:E:154:LEU:H	3:E:154:LEU:HD22	1.85	0.42
1:G:7:DA:H2''	1:G:8:DT:C5'	2.50	0.42
3:A:28:LYS:HD2	3:A:28:LYS:HA	1.92	0.42
3:A:168:PRO:HB3	5:A:726:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:55:PHE:HB2	4:B:141:HIS:CE1	2.54	0.42
4:B:88:VAL:HG12	4:B:130:MET:HE1	2.02	0.42
4:B:97:LEU:HB3	4:B:210:VAL:HG21	2.02	0.42
3:E:130:ILE:O	3:E:133:ARG:N	2.46	0.42
3:E:145:ILE:N	3:E:145:ILE:CD1	2.83	0.42
3:E:163:VAL:HG12	3:E:164:THR:N	2.34	0.42
4:F:144:LYS:HD2	4:F:144:LYS:HA	1.78	0.42
4:F:284:GLU:O	4:F:291:VAL:HG13	2.20	0.42
4:B:97:LEU:HD12	4:B:109:HIS:O	2.20	0.42
4:B:187:THR:HG22	4:B:189:ARG:H	1.85	0.42
4:F:113:GLY:O	4:F:116:CYS:HB2	2.20	0.42
4:F:165:PRO:HB2	4:F:166:GLY:H	1.70	0.42
4:F:254:ASP:O	4:F:255:ARG:NH1	2.50	0.42
3:A:34:PHE:CD1	3:A:185:ASP:HB2	2.55	0.41
3:A:39:GLU:O	3:A:40:GLY:C	2.62	0.41
3:A:93:LYS:HE2	3:A:93:LYS:HB3	1.81	0.41
3:A:116:LEU:N	3:A:116:LEU:HD12	2.35	0.41
3:A:144:PRO:HG2	3:A:147:GLU:CB	2.50	0.41
4:B:232:VAL:O	4:B:232:VAL:HG23	2.20	0.41
3:E:113:PHE:CD1	3:E:113:PHE:N	2.87	0.41
4:F:77:LYS:HB3	4:F:78:SER:H	1.71	0.41
1:G:10:DC:C2'	1:G:11:DC:O5'	2.68	0.41
3:A:186:ASN:HA	3:A:192:ALA:HA	2.01	0.41
4:B:105:HIS:HA	4:B:168:LEU:HD12	2.02	0.41
4:F:184:ARG:HD2	4:F:184:ARG:N	2.29	0.41
4:B:41:TYR:HD2	4:B:229:LEU:HB3	1.86	0.41
4:B:73:GLU:HB2	4:B:76:LYS:O	2.21	0.41
4:B:173:LEU:C	4:B:175:TYR:N	2.77	0.41
4:B:187:THR:HB	4:B:190:GLU:HG2	2.02	0.41
4:B:333:ARG:O	4:B:337:LEU:HA	2.20	0.41
3:E:29:GLN:HB3	5:E:727:HOH:O	2.19	0.41
4:F:39:GLY:C	4:F:86:ASN:HD22	2.26	0.41
4:F:232:VAL:HA	5:F:803:HOH:O	2.18	0.41
1:C:5:DA:O5'	3:A:247:GLN:NE2	2.53	0.41
1:C:8:DT:H2''	1:C:9:DT:H73	2.01	0.41
3:A:245:HIS:O	3:A:246:ARG:C	2.63	0.41
4:B:49:LYS:HG2	4:B:70:ALA:HA	2.01	0.41
4:B:181:GLY:HA3	4:B:184:ARG:CD	2.50	0.41
4:F:163:TYR:C	4:F:165:PRO:HD3	2.46	0.41
4:F:333:ARG:HG2	4:F:335:SER:OG	2.21	0.41
3:A:105:CYS:HA	3:A:106:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:130:ILE:HG22	3:A:131:SER:N	2.35	0.41
3:A:165:VAL:HG22	3:A:173:LEU:O	2.20	0.41
3:A:239:PHE:HB3	3:A:252:PHE:HB3	2.01	0.41
3:A:272:LEU:HB2	3:A:281:SER:HB3	2.01	0.41
3:E:28:LYS:HG2	3:E:49:GLU:CA	2.49	0.41
3:E:70:GLY:N	3:E:166:ARG:NH1	2.68	0.41
3:E:130:ILE:O	3:E:130:ILE:HD13	2.21	0.41
3:E:255:PRO:HA	3:E:256:PRO:HD3	1.96	0.41
4:F:72:SER:C	4:F:74:LYS:N	2.76	0.41
4:F:183:ASP:O	4:F:185:GLN:N	2.54	0.41
3:A:258:ALA:O	3:A:260:PRO:HD3	2.20	0.41
4:B:324:PRO:HB3	4:B:346:LEU:HD21	2.02	0.41
4:B:343:LYS:HA	4:B:344:PRO:HD3	1.82	0.41
4:F:50:GLN:HE21	4:F:236:ALA:H	1.69	0.41
3:A:85:PRO:HB2	3:A:133:ARG:HG3	2.02	0.41
4:B:46:GLU:C	4:B:47:GLN:HG3	2.44	0.41
4:B:128:LYS:HE3	4:B:128:LYS:HB2	1.92	0.41
4:B:175:TYR:O	4:B:176:LEU:CB	2.68	0.41
3:E:257:TYR:CD2	3:E:257:TYR:C	2.95	0.41
3:A:36:TYR:H	3:A:39:GLU:HG3	1.84	0.41
3:A:46:ILE:HB	3:A:116:LEU:CD1	2.51	0.41
3:A:60:THR:HG23	3:A:112:SER:HB2	2.02	0.41
3:A:188:ALA:HA	3:A:189:PRO:HD3	1.94	0.41
4:B:42:LEU:HD21	4:B:216:ALA:HB2	2.02	0.41
4:B:229:LEU:O	4:B:230:GLU:C	2.64	0.41
3:E:165:VAL:O	3:E:166:ARG:HG3	2.20	0.41
4:F:184:ARG:O	4:F:184:ARG:HG2	2.20	0.41
2:D:19:DT:O3'	4:B:57:TYR:HE1	2.03	0.41
3:A:78:THR:HG22	3:A:79:LYS:H	1.85	0.41
3:A:86:HIS:CD2	3:A:157:VAL:CG1	3.04	0.41
4:B:142:VAL:HG22	4:B:143:THR:N	2.36	0.41
4:B:177:GLN:HG2	4:B:178:ALA:H	1.86	0.41
4:B:189:ARG:NH1	4:B:189:ARG:HB3	2.36	0.41
3:E:100:TYR:CD1	3:E:101:GLU:N	2.89	0.41
3:E:235:ALA:C	3:E:236:ARG:HD3	2.46	0.41
3:A:198:ARG:CZ	4:B:310:VAL:HG11	2.51	0.41
3:A:205:SER:C	3:A:207:LEU:N	2.78	0.41
4:B:84:ILE:HB	4:B:130:MET:CG	2.50	0.41
4:B:141:HIS:CE1	4:B:239:ASP:CG	2.98	0.41
4:B:218:LEU:HD12	4:B:227:ARG:CZ	2.51	0.41
3:E:217:ASP:O	3:E:219:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:DG:H2"	1:C:5:DA:H8	1.85	0.40
3:E:127:GLU:HG3	3:E:128:GLN:N	2.35	0.40
4:F:114:LYS:HE2	4:F:134:PHE:CA	2.45	0.40
3:A:229:THR:CG2	3:A:271:GLN:OE1	2.69	0.40
3:E:19:ALA:HB3	3:E:175:LEU:CD2	2.52	0.40
3:E:79:LYS:HA	3:E:158:ARG:NE	2.33	0.40
4:F:72:SER:O	4:F:77:LYS:NZ	2.49	0.40
4:F:95:VAL:O	4:F:95:VAL:HG13	2.21	0.40
4:F:332:ARG:NH1	4:F:332:ARG:CG	2.77	0.40
3:A:29:GLN:NE2	3:A:181:HIS:HB3	2.33	0.40
3:A:141:PHE:HE1	3:A:179:LEU:HD21	1.86	0.40
4:B:72:SER:C	4:B:74:LYS:H	2.29	0.40
4:B:212:LEU:HD23	4:B:212:LEU:HA	1.97	0.40
4:F:49:LYS:HE3	4:F:49:LYS:CA	2.48	0.40
4:F:162:GLY:O	4:F:163:TYR:HD1	2.04	0.40
3:A:109:SER:C	3:A:110:ILE:HG13	2.46	0.40
4:B:54:ARG:HA	4:B:240:SER:CB	2.52	0.40
4:B:56:ARG:O	4:B:139:ILE:O	2.38	0.40
4:B:155:MET:HE2	4:B:169:VAL:CG2	2.46	0.40
4:B:304:HIS:HB3	4:B:308:ALA:HB3	2.04	0.40
3:E:72:VAL:HB	3:E:104:LEU:CD1	2.51	0.40
3:E:178:VAL:CG2	3:E:179:LEU:N	2.85	0.40
3:E:289:LEU:HB3	3:E:290:PRO:HD2	2.03	0.40
4:F:44:ILE:HA	4:F:82:VAL:HG23	2.02	0.40
3:A:81:PRO:HB2	3:A:82:PRO:CD	2.51	0.40
3:A:225:GLU:HG3	3:A:273:ARG:HB3	2.03	0.40
4:B:148:PHE:HB2	4:B:202:THR:HG21	2.03	0.40
4:B:165:PRO:HG2	4:B:166:GLY:N	2.34	0.40
4:B:197:ALA:C	4:B:199:VAL:H	2.30	0.40
3:E:167:ASP:C	3:E:169:ALA:N	2.80	0.40
3:E:184:PHE:N	3:E:184:PHE:HD1	2.19	0.40
3:E:268:VAL:HG22	3:E:286:PHE:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	272/274 (99%)	204 (75%)	49 (18%)	19 (7%)	1	1
3	E	272/274 (99%)	201 (74%)	50 (18%)	21 (8%)	1	1
4	B	311/313 (99%)	236 (76%)	54 (17%)	21 (7%)	1	1
4	F	311/313 (99%)	240 (77%)	44 (14%)	27 (9%)	0	0
All	All	1166/1174 (99%)	881 (76%)	197 (17%)	88 (8%)	1	1

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	81	PRO
3	A	83	HIS
3	A	115	ASN
3	A	204	GLY
4	B	101	GLY
4	B	127	PRO
4	B	165	PRO
4	B	183	ASP
4	B	187	THR
4	B	238	TYR
3	E	81	PRO
3	E	97	ASP
4	F	70	ALA
4	F	102	LYS
4	F	127	PRO
4	F	238	TYR
4	F	288	ASN
4	B	63	SER
4	B	68	PRO
4	B	100	ASN
4	B	114	LYS
4	B	245	ALA
3	E	38	CYS
3	E	83	HIS
3	E	165	VAL
3	E	204	GLY
3	E	247	GLN
4	F	49	LYS

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Mol	Chain	Res	Type
4	F	71	SER
4	F	77	LYS
4	F	101	GLY
4	F	114	LYS
4	F	165	PRO
4	F	171	SER
4	F	183	ASP
4	F	184	ARG
4	F	187	THR
4	F	221	SER
3	A	41	ARG
3	A	97	ASP
3	A	99	TYR
3	A	126	LEU
3	A	142	HIS
3	A	186	ASN
3	A	191	THR
3	A	261	SER
4	B	70	ALA
4	B	221	SER
4	B	223	GLY
3	E	106	PRO
3	E	174	LEU
3	E	261	SER
4	F	100	ASN
4	F	175	TYR
4	F	222	THR
4	F	223	GLY
3	A	106	PRO
3	A	107	ASP
3	A	185	ASP
4	B	241	LYS
3	E	168	PRO
4	F	173	LEU
4	B	74	LYS
4	B	88	VAL
4	B	222	THR
3	E	59	PRO
3	E	115	ASN
3	E	132	GLN
3	E	200	ASN
3	E	276	SER

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Mol	Chain	Res	Type
4	F	88	VAL
4	F	164	ASN
4	F	182	GLY
3	A	31	GLY
4	B	48	PRO
3	E	29	GLN
3	E	41	ARG
3	E	69	PRO
3	A	165	VAL
4	B	319	VAL
3	E	110	ILE
4	F	319	VAL
3	A	231	PRO
4	B	344	PRO
3	E	231	PRO
3	A	77	VAL
4	F	344	PRO
4	F	166	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	243/243 (100%)	212 (87%)	31 (13%)	4	7
3	E	243/243 (100%)	217 (89%)	26 (11%)	6	12
4	B	269/269 (100%)	249 (93%)	20 (7%)	13	24
4	F	269/269 (100%)	241 (90%)	28 (10%)	7	13
All	All	1024/1024 (100%)	919 (90%)	105 (10%)	7	13

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	20	TYR
3	A	37	LYS
3	A	50	ARG

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Mol	Chain	Res	Type
3	A	58	HIS
3	A	63	ILE
3	A	71	THR
3	A	74	ILE
3	A	76	LEU
3	A	79	LYS
3	A	81	PRO
3	A	84	ARG
3	A	100	TYR
3	A	116	LEU
3	A	127	GLU
3	A	130	ILE
3	A	133	ARG
3	A	139	ASN
3	A	181	HIS
3	A	183	ILE
3	A	190	ASN
3	A	199	VAL
3	A	200	ASN
3	A	201	ARG
3	A	207	LEU
3	A	231	PRO
3	A	254	THR
3	A	263	GLN
3	A	270	MET
3	A	272	LEU
3	A	277	ASP
3	A	290	PRO
4	B	46	GLU
4	B	57	TYR
4	B	106	LEU
4	B	114	LYS
4	B	121	CYS
4	B	128	LYS
4	B	136	ASN
4	B	152	GLU
4	B	176	LEU
4	B	186	LEU
4	B	196	GLN
4	B	204	GLU
4	B	220	ASP
4	B	228	ARG

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Mol	Chain	Res	Type
4	B	234	SER
4	B	235	ASP
4	B	301	THR
4	B	327	VAL
4	B	341	GLU
4	B	346	LEU
3	E	26	GLN
3	E	29	GLN
3	E	56	LYS
3	E	78	THR
3	E	81	PRO
3	E	104	LEU
3	E	108	ARG
3	E	111	HIS
3	E	116	LEU
3	E	126	LEU
3	E	128	GLN
3	E	130	ILE
3	E	133	ARG
3	E	135	GLN
3	E	140	PRO
3	E	154	LEU
3	E	174	LEU
3	E	181	HIS
3	E	184	PHE
3	E	194	LEU
3	E	200	ASN
3	E	241	GLN
3	E	269	SER
3	E	271	GLN
3	E	272	LEU
3	E	284	MET
4	F	38	MET
4	F	49	LYS
4	F	58	VAL
4	F	75	ASN
4	F	77	LYS
4	F	98	VAL
4	F	121	CYS
4	F	148	PHE
4	F	150	THR
4	F	152	GLU

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Mol	Chain	Res	Type
4	F	160	ILE
4	F	167	LEU
4	F	184	ARG
4	F	188	ASP
4	F	189	ARG
4	F	190	GLU
4	F	220	ASP
4	F	227	ARG
4	F	246	SER
4	F	247	ASN
4	F	266	ILE
4	F	268	LEU
4	F	279	GLN
4	F	280	ILE
4	F	285	GLU
4	F	287	GLU
4	F	303	VAL
4	F	332	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	29	GLN
3	A	58	HIS
3	A	83	HIS
3	A	111	HIS
3	A	114	GLN
3	A	138	ASN
3	A	162	GLN
3	A	181	HIS
3	A	186	ASN
3	A	190	ASN
3	A	200	ASN
3	A	247	GLN
3	A	287	GLN
4	B	43	GLN
4	B	47	GLN
4	B	81	GLN
4	B	86	ASN
4	B	109	HIS
4	B	185	GLN
4	B	196	GLN

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Mol	Chain	Res	Type
4	B	200	GLN
4	B	201	GLN
4	B	247	ASN
4	B	274	GLN
4	B	288	ASN
4	B	306	GLN
4	B	330	GLN
3	E	26	GLN
3	E	29	GLN
3	E	111	HIS
3	E	119	GLN
3	E	128	GLN
3	E	139	ASN
3	E	186	ASN
3	E	200	ASN
3	E	241	GLN
3	E	247	GLN
3	E	263	GLN
3	E	271	GLN
3	E	287	GLN
4	F	50	GLN
4	F	103	ASN
4	F	105	HIS
4	F	115	HIS
4	F	136	ASN
4	F	141	HIS
4	F	164	ASN
4	F	170	HIS
4	F	196	GLN
4	F	201	GLN
4	F	247	ASN
4	F	306	GLN
4	F	320	ASN
4	F	330	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 [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.