



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:59 PM BST

PDB ID : 6N62
Title : Escherichia coli RNA polymerase sigma70-holoenzyme bound to upstream fork promoter DNA
Authors : Braffman, N.; Hauver, J.; Campbell, E.A.; Darst, S.A.
Deposited on : 2018-11-24
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

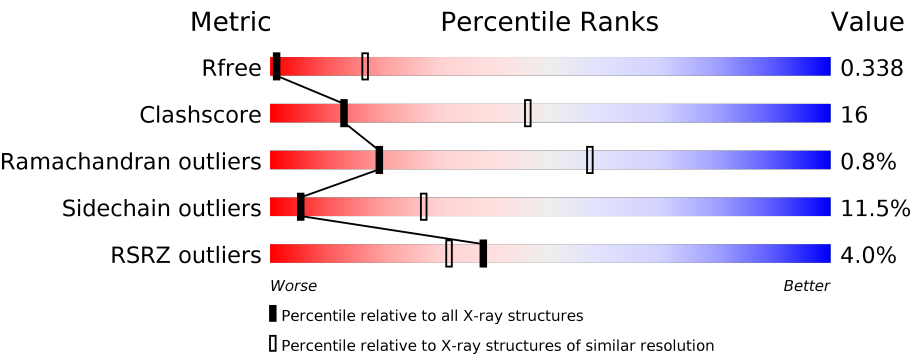
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




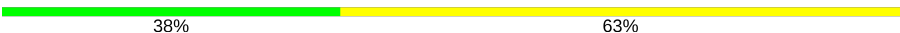
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	239	<div><div>10%</div><div><div></div><div>58%</div><div>34%</div><div>• 5%</div></div></div>
1	B	239	<div><div>3%</div><div><div></div><div>56%</div><div>30%</div><div>• 9%</div></div></div>
2	C	1342	<div><div>%</div><div><div></div><div>60%</div><div>34%</div><div>5%</div></div></div>
3	D	1409	<div><div>4%</div><div><div></div><div>51%</div><div>31%</div><div>5%</div><div>13%</div></div></div>
4	E	91	<div><div>2%</div><div><div></div><div>51%</div><div>25%</div><div>11%</div><div>13%</div></div></div>
5	F	613	<div><div>7%</div><div><div></div><div>50%</div><div>24%</div><div>•</div><div>23%</div></div></div>

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Mol	Chain	Length	Quality of chain
6	N	29	 28% 69% .
7	T	24	 38% 63%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 29075 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1750	1088	312	344	6			
1	B	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP P0A7Z6
A	236	VAL	-	expression tag	UNP P0A7Z6
A	237	LEU	-	expression tag	UNP P0A7Z6
A	238	PHE	-	expression tag	UNP P0A7Z6
A	239	GLN	-	expression tag	UNP P0A7Z6
B	235	GLU	-	expression tag	UNP P0A7Z6
B	236	VAL	-	expression tag	UNP P0A7Z6
B	237	LEU	-	expression tag	UNP P0A7Z6
B	238	PHE	-	expression tag	UNP P0A7Z6
B	239	GLN	-	expression tag	UNP P0A7Z6

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1337	Total	C	N	O	S	0	0	0
			10545	6616	1838	2048	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1226	Total	C	N	O	S	0	0	0
			9557	6006	1714	1791	46			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	expression tag	UNP P0A8T8
D	1408	LEU	-	expression tag	UNP P0A8T8
D	1409	GLU	-	expression tag	UNP P0A8T8

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	471	Total	C	N	O	S	0	0	0
			3839	2405	684	727	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	149	ASN	ASP	conflict	UNP Q0P6L9

- Molecule 6 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	29	Total	C	N	O	P	0	0	0
			595	284	106	176	29			

- Molecule 7 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	T	24	Total	C	N	O	P	0	0	0
			492	233	94	141	24			

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Mg	0	0
			1	1		

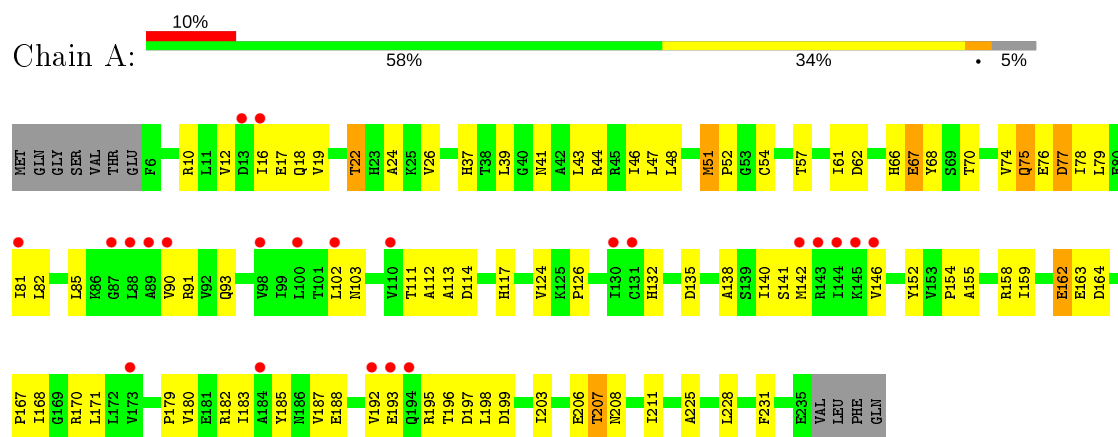
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total 2	Zn 2	0	0

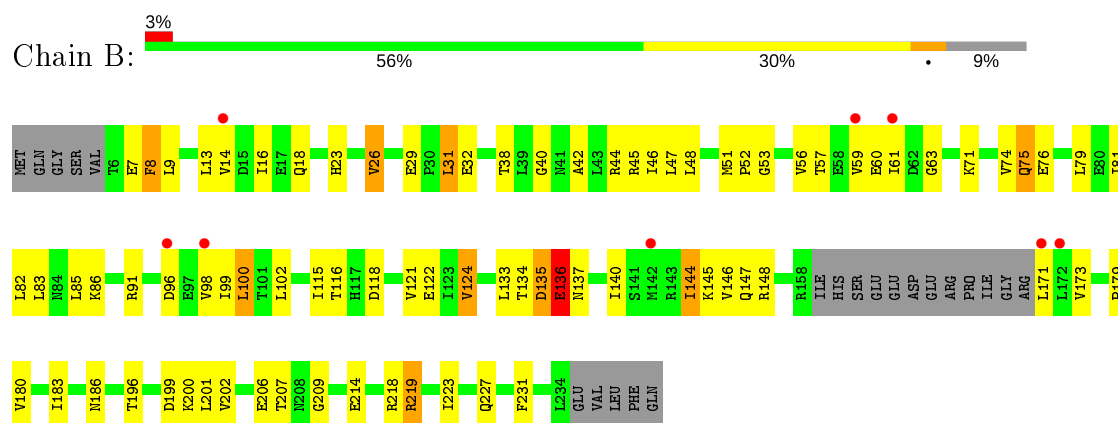
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

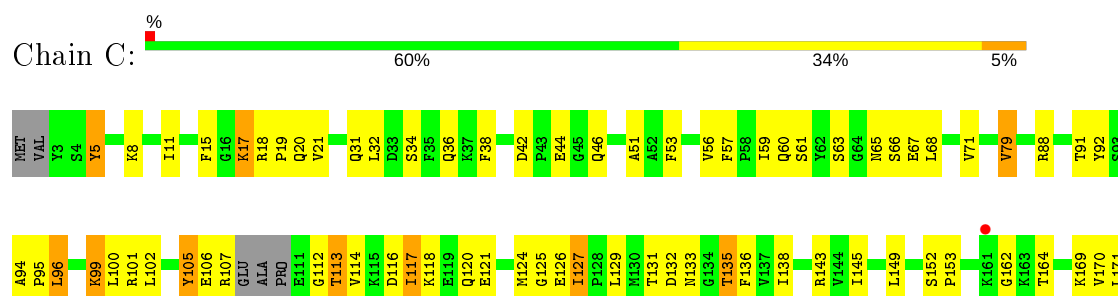
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

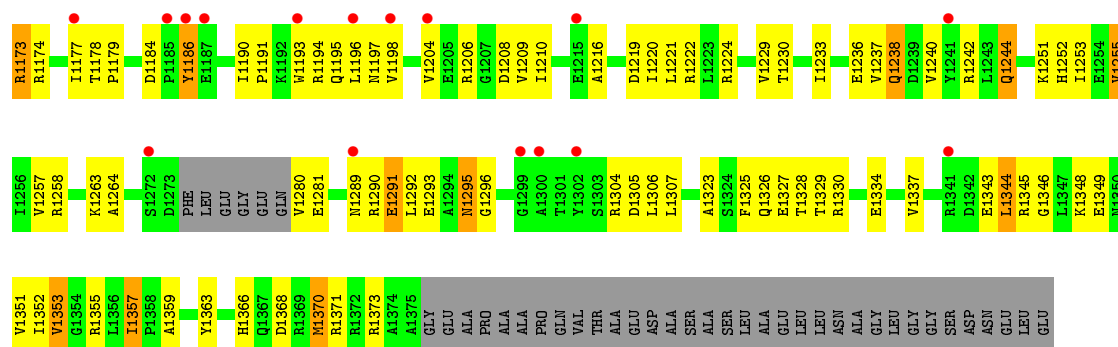


• Molecule 2: DNA-directed RNA polymerase subunit beta

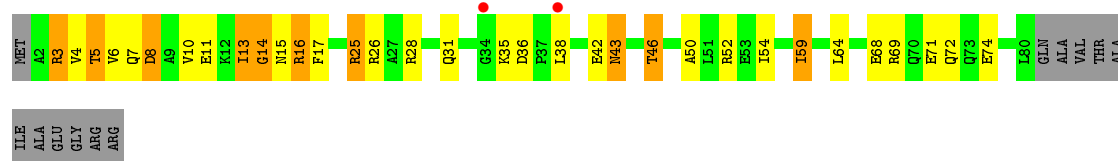




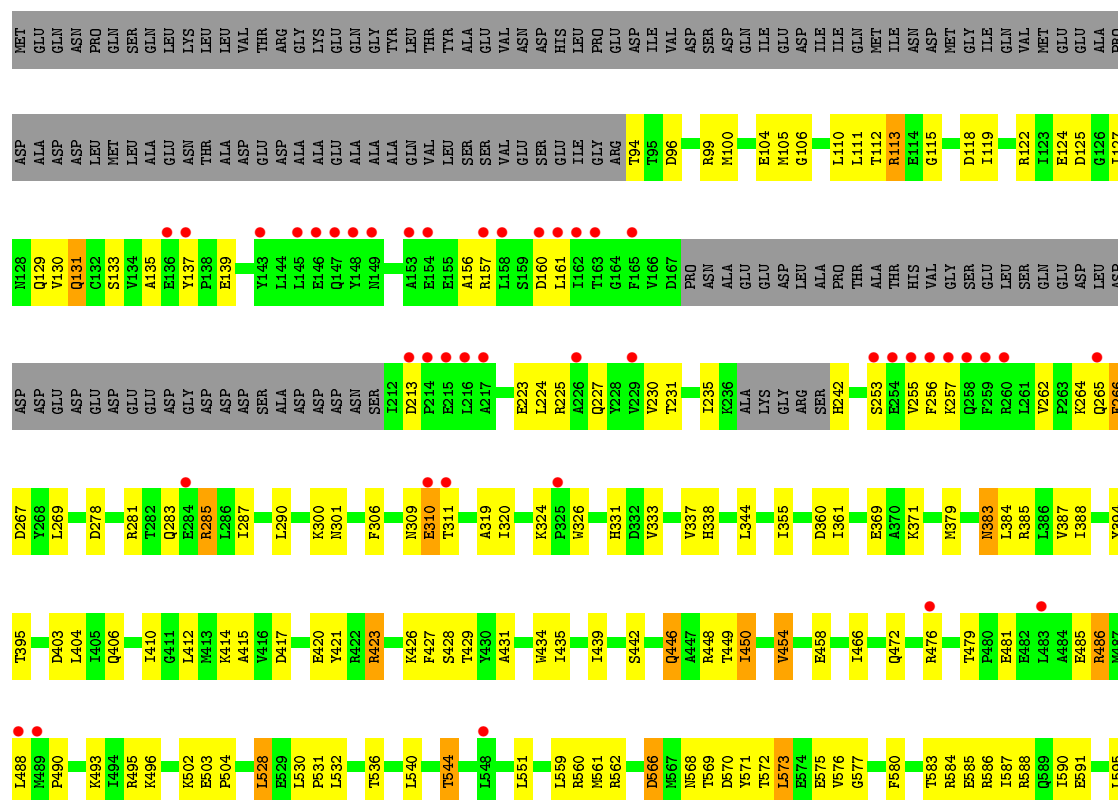




• Molecule 4: DNA-directed RNA polymerase subunit omega

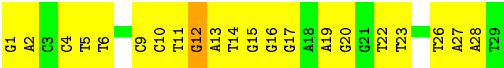


• Molecule 5: RNA polymerase sigma factor RpoD

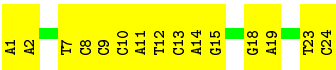




● Molecule 6: non-template strand DNA



● Molecule 7: template strand DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.77Å 173.77Å 388.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.88 – 3.80 49.77 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.88-3.80) 99.7 (49.77-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.286 , 0.334 0.297 , 0.338	Depositor DCC
R_{free} test set	1999 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å ²)	171.7	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 101.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29075	wwPDB-VP
Average B, all atoms (Å ²)	164.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/1771	0.51	0/2401
1	B	0.30	0/1686	0.53	0/2285
2	C	0.28	0/10712	0.50	3/14450 (0.0%)
3	D	0.27	0/9702	0.48	1/13092 (0.0%)
4	E	0.26	0/629	0.48	0/847
5	F	0.27	0/3891	0.44	0/5231
6	N	0.58	1/666 (0.2%)	0.91	0/1026
7	T	0.56	0/552	0.83	0/849
All	All	0.29	1/29609 (0.0%)	0.51	4/40181 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	7
3	D	0	2
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	12	DG	C1'-N9	-7.88	1.36	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1161	LEU	CA-CB-CG	6.94	131.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1151	LEU	CA-CB-CG	6.74	130.80	115.30
2	C	1151	LEU	CB-CG-CD2	6.11	121.39	111.00
3	D	1343	GLU	C-N-CA	5.53	135.52	121.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	135	ASP	Peptide
2	C	1150	ASP	Peptide
2	C	1164	PHE	Peptide
2	C	1340	GLU	Peptide
2	C	169	LYS	Peptide
2	C	572	ILE	Peptide
2	C	811	ASN	Peptide
2	C	985	GLU	Peptide
3	D	416	ILE	Peptide
3	D	45	ASN	Peptide

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	A	1750	0	1764	47	0
1	B	1667	0	1689	45	0
2	C	10545	0	10559	371	0
3	D	9557	0	9764	356	0
4	E	627	0	634	28	0
5	F	3839	0	3904	97	0
6	N	595	0	329	51	0
7	T	492	0	269	32	0
8	D	1	0	0	0	0
9	D	2	0	0	0	0
All	All	29075	0	28912	946	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 16.

All (946) 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)
2:C:116:ASP:O	2:C:117:ILE:HG23	1.37	1.20
2:C:116:ASP:O	2:C:117:ILE:CG2	1.94	1.14
6:N:13:DA:H1'	6:N:14:DT:H5'	1.27	1.07
2:C:106:GLU:O	2:C:114:VAL:HG22	1.55	1.06
6:N:12:DG:H4'	6:N:13:DA:OP1	1.52	1.05
6:N:10:DC:H2''	6:N:11:DT:H5'	1.38	1.04
6:N:15:DG:H2''	6:N:16:DG:H5'	1.40	1.02
6:N:10:DC:H2''	6:N:11:DT:C5'	1.90	1.02
2:C:1242:LYS:O	2:C:1244:HIS:HD2	1.43	1.00
6:N:13:DA:C1'	6:N:14:DT:H5'	1.94	0.96
1:A:162:GLU:O	1:A:164:ASP:N	2.01	0.93
7:T:10:DC:C6	7:T:10:DC:H5'	2.06	0.91
2:C:107:ARG:C	2:C:112:GLY:HA2	1.89	0.91
2:C:106:GLU:O	2:C:114:VAL:CG2	2.19	0.90
3:D:1263:LYS:NZ	3:D:1281:GLU:OE2	2.05	0.89
7:T:9:DC:H1'	7:T:10:DC:H5'	1.54	0.89
2:C:118:LYS:NZ	2:C:485:ASP:O	2.07	0.88
2:C:116:ASP:OD1	2:C:117:ILE:N	2.08	0.87
6:N:11:DT:H1'	6:N:12:DG:H5'	1.56	0.86
2:C:1242:LYS:O	2:C:1244:HIS:CD2	2.28	0.86
7:T:10:DC:H5'	7:T:10:DC:H6	1.37	0.85
2:C:1080:ASN:HD21	2:C:1084:ASP:HB2	1.42	0.83
6:N:13:DA:H1'	6:N:14:DT:C5'	2.08	0.83
2:C:398:SER:O	2:C:401:GLY:N	2.10	0.83
3:D:358:GLY:H	3:D:359:PRO:HD3	1.44	0.83
7:T:10:DC:H2'	7:T:11:DA:C8	2.14	0.83
2:C:1212:LEU:HB2	2:C:1225:VAL:HG11	1.61	0.82
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.61	0.82
7:T:11:DA:H2''	7:T:12:DT:OP2	1.80	0.82
2:C:1142:ARG:HD3	2:C:1161:LEU:HB2	1.60	0.82
3:D:746:LEU:HG	3:D:758:PRO:HB3	1.63	0.81
2:C:985:GLU:HB3	2:C:989:LEU:HB2	1.63	0.80
3:D:282:LEU:HD21	5:F:410:ILE:HD12	1.61	0.80
6:N:15:DG:H2''	6:N:16:DG:C5'	2.12	0.80
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.64	0.80
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.63	0.80
7:T:13:DC:OP2	7:T:13:DC:H6	1.63	0.79
2:C:1244:HIS:CE1	3:D:352:ARG:NE	2.50	0.79
2:C:1341:ASP:N	2:C:1341:ASP:OD1	2.14	0.79
2:C:1070:HIS:HB3	2:C:1108:ASN:HD21	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:745:GLU:HG3	2:C:1021:LEU:HD11	1.63	0.78
2:C:741:MET:SD	2:C:974:ARG:NH1	2.57	0.78
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.67	0.77
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.49	0.77
2:C:557:ARG:HG2	2:C:587:LEU:HB3	1.65	0.77
1:A:90:VAL:HG11	1:A:146:VAL:HG11	1.67	0.77
2:C:229:ILE:HB	2:C:240:GLU:HB2	1.66	0.77
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.66	0.76
2:C:106:GLU:HB3	2:C:114:VAL:HG21	1.68	0.76
1:A:51:MET:HB3	1:A:179:PRO:HD2	1.69	0.75
2:C:339:ASN:HB3	2:C:343:HIS:H	1.49	0.75
2:C:400:VAL:HG12	2:C:584:TYR:HB3	1.68	0.75
3:D:1263:LYS:HB2	3:D:1307:LEU:HD11	1.69	0.75
2:C:1032:LYS:HA	2:C:1035:LYS:HE3	1.68	0.74
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.68	0.74
5:F:106:GLY:HA2	5:F:385:ARG:HH22	1.51	0.74
2:C:1341:ASP:O	3:D:17:PHE:HA	1.87	0.74
2:C:116:ASP:C	2:C:117:ILE:HG23	2.08	0.74
6:N:13:DA:H61	7:T:12:DT:H3	1.34	0.74
2:C:765:ILE:HG13	2:C:787:PRO:HG3	1.69	0.74
6:N:14:DT:H2"	6:N:15:DG:N7	2.03	0.74
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.70	0.74
3:D:961:SER:HB2	3:D:981:GLU:HB3	1.69	0.73
2:C:888:THR:HG23	2:C:914:LYS:HB3	1.69	0.73
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.69	0.73
6:N:12:DG:C4'	6:N:13:DA:OP1	2.35	0.73
6:N:13:DA:C2'	6:N:14:DT:H5'	2.18	0.73
2:C:189:ASP:HB3	2:C:193:ASN:HB2	1.71	0.73
5:F:572:THR:HG22	5:F:575:GLU:HB2	1.71	0.73
2:C:670:PHE:HB3	2:C:673:HIS:HD2	1.53	0.72
3:D:1344:LEU:O	3:D:1346:GLY:N	2.22	0.72
3:D:515:ARG:HB3	3:D:545:HIS:HD2	1.53	0.72
7:T:10:DC:H2"	7:T:11:DA:O4'	1.89	0.72
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.71	0.72
3:D:747:MET:HB2	3:D:774:ILE:HG22	1.72	0.72
3:D:483:LEU:HD21	4:E:17:PHE:HE1	1.54	0.71
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.71	0.71
3:D:679:TYR:OH	3:D:754:ILE:O	2.08	0.71
3:D:667:GLN:HE21	3:D:672:LEU:HD22	1.53	0.70
6:N:12:DG:H1'	6:N:13:DA:H5"	1.73	0.70
2:C:1290:MET:HG3	3:D:347:VAL:HG11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:415:ALA:HB2	5:F:434:TRP:HB2	1.74	0.70
6:N:14:DT:H1'	6:N:15:DG:C8	2.27	0.70
7:T:12:DT:H2''	7:T:13:DC:C6	2.27	0.70
3:D:1159:ILE:HG21	3:D:1179:PRO:HG3	1.74	0.69
5:F:135:ALA:HB1	5:F:253:SER:HB3	1.73	0.69
6:N:10:DC:H2'	6:N:11:DT:H71	1.72	0.69
3:D:1173:ARG:HB3	3:D:1190:ILE:O	1.93	0.69
3:D:860:ARG:HD2	3:D:861:ASN:HD22	1.55	0.69
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.75	0.69
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.75	0.68
2:C:1221:PHE:HD1	3:D:634:ARG:HA	1.57	0.68
7:T:9:DC:C4	7:T:10:DC:N4	2.61	0.68
2:C:200:ARG:HE	2:C:200:ARG:HA	1.59	0.68
2:C:131:THR:HG22	2:C:135:THR:H	1.58	0.68
2:C:116:ASP:O	2:C:117:ILE:HG22	1.91	0.68
2:C:131:THR:HG23	2:C:133:ASN:H	1.59	0.68
3:D:342:LEU:HD13	3:D:1352:ILE:HG23	1.74	0.67
1:B:99:ILE:HB	1:B:145:LYS:HG2	1.75	0.67
3:D:559:ALA:O	3:D:560:ASN:ND2	2.28	0.67
3:D:362:ARG:H	3:D:365:GLN:HE21	1.41	0.67
6:N:14:DT:H2''	6:N:15:DG:C8	2.30	0.67
5:F:224:LEU:HD21	5:F:225:ARG:HH11	1.59	0.67
2:C:1244:HIS:HB3	2:C:1264:GLN:HB3	1.77	0.67
3:D:819:GLY:HA2	3:D:883:ARG:HA	1.77	0.67
6:N:14:DT:H1'	6:N:15:DG:N7	2.10	0.67
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.76	0.67
2:C:107:ARG:C	2:C:112:GLY:CA	2.63	0.66
6:N:11:DT:H2''	6:N:12:DG:O5'	1.94	0.66
7:T:9:DC:H1'	7:T:10:DC:C5'	2.23	0.66
3:D:1237:VAL:HG11	3:D:1253:ILE:HG21	1.77	0.66
2:C:1191:LYS:HD2	2:C:1192:GLU:H	1.60	0.66
1:A:16:ILE:HG22	1:A:26:VAL:HG12	1.78	0.66
5:F:530:LEU:HD12	5:F:532:LEU:HD13	1.77	0.66
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.78	0.66
7:T:18:DG:H2''	7:T:19:DA:H5''	1.77	0.66
3:D:20:ILE:HD13	3:D:1344:LEU:HD21	1.78	0.65
1:A:74:VAL:HG22	1:A:76:GLU:H	1.60	0.65
3:D:161:THR:HG22	3:D:164:GLN:HG3	1.78	0.65
2:C:71:VAL:HB	2:C:99:LYS:HB3	1.77	0.65
2:C:521:LEU:HB2	2:C:794:LEU:HD21	1.78	0.65
1:B:81:ILE:O	1:B:85:LEU:HG	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:ARG:HA	2:C:200:ARG:NE	2.12	0.65
2:C:247:ARG:HE	2:C:274:ILE:HD13	1.62	0.65
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	1.79	0.65
3:D:194:LEU:H	3:D:194:LEU:HD23	1.60	0.65
2:C:530:ILE:HD11	2:C:575:LEU:HD12	1.78	0.65
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.79	0.65
2:C:99:LYS:HA	2:C:121:GLU:HA	1.79	0.64
3:D:417:ARG:HH21	4:E:43:ASN:HB3	1.63	0.64
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.79	0.64
2:C:112:GLY:O	2:C:113:THR:HG22	1.97	0.64
2:C:560:PRO:HB2	3:D:776:THR:HG21	1.80	0.64
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.29	0.64
2:C:118:LYS:NZ	2:C:487:LEU:O	2.31	0.64
4:E:3:ARG:NH1	4:E:5:THR:O	2.30	0.64
2:C:1255:THR:HG21	3:D:341:ASN:HD21	1.61	0.63
2:C:528:ARG:NH2	2:C:576:SER:O	2.31	0.63
2:C:883:LEU:HD13	2:C:1052:VAL:HG11	1.79	0.63
3:D:490:ILE:HG13	3:D:491:LEU:HD23	1.79	0.63
3:D:1221:LEU:HD11	3:D:1304:ARG:HB2	1.79	0.62
2:C:1005:GLU:HG2	2:C:1007:LYS:H	1.64	0.62
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.82	0.62
2:C:935:THR:HG23	2:C:1048:LYS:HG2	1.82	0.62
2:C:65:ASN:HB3	2:C:105:TYR:CD2	2.34	0.62
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.81	0.62
3:D:1326:GLN:HG2	3:D:1327:GLU:H	1.63	0.62
3:D:516:ASP:HA	3:D:545:HIS:HB3	1.82	0.62
3:D:614:LEU:HD23	4:E:7:GLN:HB2	1.81	0.62
6:N:13:DA:H2''	6:N:14:DT:C6	2.34	0.62
7:T:14:DA:H1'	7:T:15:DG:H5'	1.81	0.62
2:C:1073:LYS:HG3	3:D:462:ASP:HB2	1.82	0.62
5:F:156:ALA:HB1	5:F:161:LEU:HD11	1.82	0.62
6:N:10:DC:C2'	6:N:11:DT:H5'	2.23	0.61
3:D:1229:VAL:O	3:D:1233:ILE:HG13	2.00	0.61
5:F:442:SER:O	5:F:446:GLN:HG2	2.01	0.61
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.82	0.61
2:C:606:LEU:HD23	2:C:611:GLU:HA	1.82	0.61
2:C:1269:ARG:HH22	3:D:340:GLN:HA	1.65	0.61
2:C:407:ARG:HH21	2:C:414:ILE:HG21	1.65	0.61
3:D:557:LYS:HA	3:D:563:LEU:HA	1.83	0.61
3:D:1170:LYS:H	3:D:1170:LYS:HD3	1.65	0.61
2:C:448:LEU:HB2	2:C:553:THR:HB	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.83	0.60
3:D:844:THR:HG23	3:D:864:LEU:HD11	1.81	0.60
5:F:283:GLN:HG3	5:F:344:LEU:HB2	1.82	0.60
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.83	0.60
5:F:571:TYR:HB3	5:F:575:GLU:HB3	1.83	0.60
6:N:10:DC:C2	6:N:11:DT:C7	2.84	0.60
1:B:74:VAL:HG12	1:B:76:GLU:H	1.63	0.60
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.83	0.60
2:C:551:HIS:H	2:C:554:HIS:CD2	2.19	0.60
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.83	0.60
2:C:1062:PRO:HG3	2:C:1078:LYS:HA	1.84	0.60
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.83	0.60
3:D:1005:LYS:HD2	3:D:1009:GLU:HB3	1.83	0.60
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.82	0.60
3:D:667:GLN:HA	3:D:672:LEU:HD13	1.83	0.60
3:D:697:MET:O	3:D:701:LEU:HB2	2.00	0.60
2:C:444:ASP:HB3	2:C:447:HIS:HB2	1.83	0.60
2:C:701:GLY:HA2	2:C:1069:ARG:HH22	1.66	0.60
1:A:152:TYR:HB2	2:C:824:GLN:HE21	1.66	0.60
1:B:82:LEU:HA	1:B:85:LEU:HD12	1.84	0.60
3:D:762:ASN:HD21	3:D:764:ARG:HB2	1.67	0.60
3:D:264:ASP:HB3	3:D:324:LEU:HB2	1.84	0.60
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.83	0.60
1:B:71:LYS:HE3	1:B:140:ILE:HD13	1.84	0.60
2:C:960:LEU:HB3	2:C:1025:PHE:HE1	1.67	0.60
6:N:13:DA:C2'	6:N:14:DT:C6	2.85	0.60
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.82	0.59
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.84	0.59
2:C:102:LEU:HB3	2:C:489:PRO:HG3	1.84	0.59
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.85	0.59
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.84	0.59
2:C:19:PRO:HA	2:C:1156:ARG:HH11	1.68	0.59
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.84	0.59
3:D:401:VAL:HG12	3:D:408:VAL:HG21	1.83	0.59
6:N:13:DA:H2''	6:N:14:DT:OP2	2.02	0.59
2:C:678:ARG:HD2	2:C:1071:GLY:O	2.03	0.59
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.85	0.59
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.84	0.59
3:D:481:ARG:HD3	4:E:3:ARG:HG2	1.84	0.59
3:D:1170:LYS:HE2	3:D:1174:ARG:HG3	1.84	0.58
2:C:922:ASN:HD22	2:C:923:GLY:N	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:10:DC:H6	7:T:10:DC:C5'	2.11	0.58
2:C:1077:SER:HB2	3:D:357:VAL:HG22	1.84	0.58
2:C:1125:GLY:HA2	2:C:1128:ILE:HD12	1.85	0.58
2:C:114:VAL:O	2:C:114:VAL:HG23	2.03	0.58
3:D:587:LEU:HD21	3:D:608:CYS:HB2	1.85	0.58
2:C:106:GLU:C	2:C:114:VAL:CG2	2.71	0.58
1:A:78:ILE:HD13	1:A:81:ILE:HD12	1.86	0.58
5:F:466:ILE:HG12	5:F:486:ARG:HG2	1.85	0.58
6:N:14:DT:C2'	6:N:15:DG:C8	2.87	0.58
2:C:107:ARG:O	2:C:112:GLY:HA2	2.03	0.58
2:C:1234:LYS:HE2	2:C:1238:LEU:HD11	1.86	0.58
2:C:230:PHE:HD2	2:C:335:THR:HG21	1.67	0.58
2:C:543:ALA:HB1	2:C:547:VAL:HG21	1.85	0.58
3:D:520:ALA:HB1	3:D:543:SER:OG	2.04	0.58
3:D:1370:MET:HA	3:D:1373:ARG:HB3	1.86	0.57
2:C:582:ASN:HD21	2:C:586:PHE:H	1.51	0.57
2:C:1107:MET:N	2:C:1107:MET:SD	2.77	0.57
3:D:950:ILE:HB	3:D:1018:ALA:HB3	1.85	0.57
7:T:12:DT:H2"	7:T:13:DC:C5	2.39	0.57
5:F:490:PRO:HD2	5:F:493:LYS:HD2	1.86	0.57
5:F:540:LEU:O	5:F:544:THR:OG1	2.20	0.57
1:A:188:GLU:O	1:A:199:ASP:HA	2.04	0.57
2:C:400:VAL:HG11	2:C:452:ARG:NH1	2.20	0.57
3:D:1220:ILE:HG23	3:D:1224:ARG:HD2	1.85	0.57
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.86	0.57
2:C:1254:VAL:HG22	2:C:1255:THR:HG23	1.87	0.57
3:D:518:VAL:HA	3:D:547:ARG:HD2	1.86	0.57
2:C:243:PRO:HB3	2:C:277:LEU:HB2	1.87	0.56
3:D:664:ILE:HG23	3:D:681:LYS:HD3	1.86	0.56
4:E:31:GLN:HB2	4:E:46:THR:HG21	1.86	0.56
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.86	0.56
2:C:237:LEU:HD22	2:C:292:ILE:HD12	1.86	0.56
3:D:1173:ARG:HG2	3:D:1174:ARG:H	1.70	0.56
5:F:420:GLU:H	5:F:423:ARG:HH22	1.51	0.56
3:D:1323:ALA:HB1	3:D:1328:THR:HG23	1.87	0.56
3:D:704:GLU:H	3:D:718:SER:HB2	1.70	0.56
3:D:875:ASN:HB2	3:D:877:VAL:HG12	1.88	0.56
2:C:545:PHE:HA	2:C:548:ARG:HD2	1.87	0.56
2:C:865:LEU:HB3	2:C:869:GLY:HA2	1.88	0.56
2:C:1258:PRO:HG2	3:D:346:ARG:HB2	1.86	0.56
3:D:644:MET:O	3:D:764:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:613:GLY:O	3:D:617:THR:OG1	2.22	0.56
3:D:789:LYS:HA	3:D:792:ASN:HD22	1.71	0.56
5:F:426:LYS:HD3	6:N:27:DA:H3'	1.87	0.56
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.88	0.56
2:C:271:ALA:HA	2:C:274:ILE:HD12	1.87	0.56
2:C:976:ARG:HH12	2:C:990:ASP:HB3	1.70	0.56
5:F:278:ASP:OD1	5:F:281:ARG:NH2	2.39	0.56
5:F:105:MET:HE2	5:F:384:LEU:HB3	1.88	0.56
1:B:180:VAL:HA	1:B:207:THR:HA	1.88	0.55
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.89	0.55
2:C:812:PHE:CE1	3:D:503:SER:HB2	2.40	0.55
3:D:1349:GLU:CD	3:D:1349:GLU:H	2.10	0.55
3:D:27:PRO:HB3	3:D:240:THR:HB	1.87	0.55
5:F:306:PHE:CZ	5:F:310:GLU:HG3	2.42	0.55
2:C:1070:HIS:CB	2:C:1108:ASN:HD21	2.18	0.55
2:C:257:ALA:HB2	2:C:285:ILE:HG22	1.88	0.55
3:D:491:LEU:HA	3:D:498:PRO:HA	1.89	0.55
2:C:1295:SER:HB2	3:D:346:ARG:O	2.06	0.55
2:C:262:TYR:HD2	2:C:276:GLN:HE21	1.55	0.55
2:C:705:GLU:HB3	2:C:794:LEU:H	1.71	0.55
3:D:93:THR:HG22	3:D:94:GLN:H	1.72	0.55
6:N:5:DT:H1'	6:N:6:DT:H5'	1.88	0.55
2:C:1313:HIS:H	4:E:31:GLN:NE2	2.04	0.55
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.88	0.55
3:D:417:ARG:HG3	3:D:418:GLU:HG2	1.88	0.55
5:F:488:LEU:H	5:F:488:LEU:HD12	1.72	0.55
2:C:1244:HIS:CE1	3:D:352:ARG:CZ	2.90	0.55
2:C:125:GLY:HA3	2:C:499:SER:HB2	1.89	0.55
3:D:186:GLN:O	3:D:190:LYS:HG3	2.07	0.55
5:F:410:ILE:HG22	5:F:414:LYS:HE3	1.87	0.55
2:C:1069:ARG:HD3	2:C:1231:TYR:HB3	1.89	0.54
3:D:1344:LEU:O	3:D:1349:GLU:HG3	2.07	0.54
3:D:194:LEU:HD12	3:D:228:VAL:HG22	1.89	0.54
2:C:1282:GLY:H	3:D:483:LEU:HD22	1.72	0.54
2:C:1221:PHE:CD1	3:D:634:ARG:HA	2.40	0.54
7:T:9:DC:C1'	7:T:10:DC:H5'	2.33	0.54
2:C:164:THR:HG21	2:C:171:LEU:HD12	1.88	0.54
2:C:948:ILE:O	2:C:951:MET:HG3	2.07	0.54
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.90	0.54
3:D:797:THR:O	3:D:801:VAL:HG13	2.07	0.54
3:D:760:THR:H	3:D:771:GLN:NE2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1167:LYS:HB3	3:D:1174:ARG:HD2	1.89	0.54
3:D:557:LYS:HB3	3:D:563:LEU:HG	1.89	0.54
2:C:1103:VAL:HG21	2:C:1112:ILE:HD11	1.90	0.54
2:C:831:ILE:HG12	2:C:1057:LYS:HG3	1.90	0.54
3:D:483:LEU:HD21	4:E:17:PHE:CE1	2.41	0.54
3:D:793:SER:O	3:D:797:THR:HG22	2.08	0.54
1:B:79:LEU:HA	1:B:82:LEU:HD12	1.90	0.54
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.42	0.54
3:D:1177:ILE:HG22	3:D:1179:PRO:HD3	1.89	0.54
5:F:324:LYS:HD2	5:F:326:TRP:HE1	1.72	0.54
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.90	0.54
5:F:571:TYR:HD1	5:F:575:GLU:HG2	1.73	0.54
7:T:23:DT:H2"	7:T:24:DC:H5"	1.90	0.54
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.88	0.53
2:C:452:ARG:HH21	2:C:454:ARG:HG2	1.73	0.53
2:C:60:GLN:HA	2:C:67:GLU:HA	1.88	0.53
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.54	0.53
1:B:214:GLU:O	1:B:218:ARG:HG3	2.08	0.53
2:C:65:ASN:HB3	2:C:105:TYR:HD2	1.72	0.53
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.90	0.53
3:D:289:ASP:HA	3:D:292:VAL:HG22	1.90	0.53
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.91	0.53
3:D:551:ARG:HA	3:D:569:LEU:HA	1.91	0.53
5:F:112:THR:HG22	5:F:113:ARG:HD2	1.91	0.53
2:C:1297:ASP:O	2:C:1300:GLY:N	2.41	0.53
3:D:515:ARG:NH2	3:D:718:SER:O	2.37	0.53
2:C:674:ASP:N	2:C:674:ASP:OD1	2.41	0.53
3:D:56:LEU:HD21	3:D:273:ILE:HD12	1.90	0.53
1:B:7:GLU:HG2	1:B:8:PHE:H	1.74	0.53
2:C:1120:ALA:O	2:C:1124:ILE:HG12	2.08	0.53
2:C:582:ASN:HD21	2:C:586:PHE:N	2.07	0.53
3:D:650:LYS:HZ1	3:D:762:ASN:HB3	1.74	0.53
3:D:835:LEU:HD21	3:D:880:VAL:HG23	1.89	0.53
4:E:10:VAL:HG12	4:E:14:GLY:HA2	1.91	0.53
1:A:61:ILE:HG22	1:A:62:ASP:H	1.73	0.53
2:C:1109:ILE:HD12	3:D:763:PHE:HB3	1.91	0.53
1:B:83:LEU:HA	1:B:86:LYS:HG3	1.91	0.52
2:C:275:ARG:HB2	2:C:275:ARG:HH11	1.74	0.52
5:F:115:GLY:O	5:F:119:ILE:HG12	2.09	0.52
6:N:10:DC:H2"	6:N:11:DT:H5"	1.88	0.52
2:C:68:LEU:HD21	2:C:100:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:332:LYS:HB3	3:D:1328:THR:HB	1.90	0.52
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.91	0.52
3:D:701:LEU:HD22	3:D:723:TYR:HB2	1.90	0.52
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.90	0.52
2:C:669:PRO:HD3	2:C:1069:ARG:HH21	1.73	0.52
7:T:9:DC:C2	7:T:10:DC:C4	2.97	0.52
3:D:201:LEU:HD22	3:D:217:LEU:HD21	1.91	0.52
6:N:13:DA:H2''	6:N:14:DT:H5'	1.90	0.52
2:C:101:ARG:HA	2:C:118:LYS:O	2.09	0.52
2:C:618:GLN:HG3	2:C:620:ASN:H	1.74	0.52
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.45	0.52
2:C:745:GLU:HB2	2:C:1017:GLN:HB3	1.90	0.52
3:D:1238:GLN:HB3	3:D:1242:ARG:HH21	1.74	0.52
3:D:349:TYR:HD2	3:D:472:LEU:HD21	1.74	0.52
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.92	0.52
3:D:667:GLN:HG3	3:D:672:LEU:HB2	1.91	0.52
2:C:1101:LEU:O	3:D:731:ARG:HG2	2.10	0.52
5:F:100:MET:O	5:F:104:GLU:HB2	2.09	0.52
2:C:710:VAL:HA	2:C:715:THR:HG21	1.90	0.52
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.44	0.52
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.92	0.52
2:C:38:PHE:HE2	2:C:127:ILE:HD13	1.74	0.52
2:C:877:VAL:HG21	2:C:883:LEU:HD21	1.90	0.52
2:C:987:GLU:O	2:C:991:LYS:HG2	2.09	0.52
3:D:278:ARG:HH12	5:F:403:ASP:HA	1.75	0.52
6:N:14:DT:C1'	6:N:15:DG:N7	2.73	0.52
3:D:1138:LEU:HG	3:D:1139:PRO:HD3	1.92	0.52
3:D:514:THR:HG21	3:D:596:LEU:HG	1.92	0.52
3:D:638:SER:O	3:D:721:SER:HB3	2.10	0.52
2:C:1115:THR:HA	2:C:1229:TYR:O	2.09	0.52
2:C:686:GLN:HE21	2:C:796:LEU:HD22	1.75	0.52
2:C:812:PHE:HE1	3:D:503:SER:HB2	1.74	0.52
3:D:358:GLY:H	3:D:359:PRO:CD	2.20	0.52
3:D:963:VAL:HG23	3:D:975:ILE:HG23	1.92	0.52
6:N:1:DG:H2''	6:N:2:DA:C8	2.44	0.52
2:C:31:GLN:HG3	2:C:527:LYS:HB3	1.92	0.51
7:T:9:DC:C2	7:T:10:DC:C5	2.98	0.51
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.92	0.51
2:C:1280:ALA:HB1	3:D:431:ARG:HD2	1.93	0.51
2:C:836:LEU:HD13	2:C:921:PRO:HD3	1.91	0.51
2:C:976:ARG:HB2	2:C:997:TRP:CZ3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:134:ASP:O	3:D:138:VAL:HG23	2.10	0.51
6:N:26:DT:H2"	6:N:27:DA:H8	1.74	0.51
6:N:10:DC:C2	6:N:11:DT:H71	2.46	0.51
2:C:1247:SER:O	3:D:348:ASP:HB3	2.10	0.51
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.91	0.51
3:D:978:ARG:NE	3:D:1197:ASN:HD21	2.09	0.51
5:F:309:ASN:O	5:F:311:THR:HG23	2.10	0.51
6:N:14:DT:C2'	6:N:15:DG:N7	2.71	0.51
2:C:745:GLU:HA	2:C:971:LEU:HD13	1.92	0.51
2:C:197:ARG:NH1	2:C:201:ARG:O	2.43	0.51
2:C:702:THR:HA	2:C:1184:THR:H	1.74	0.51
2:C:657:THR:HB	2:C:1187:PHE:HB2	1.93	0.51
5:F:224:LEU:HB2	5:F:255:VAL:HB	1.93	0.51
1:B:82:LEU:HD11	1:B:171:LEU:HD13	1.93	0.51
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.76	0.51
5:F:110:LEU:HD12	5:F:110:LEU:H	1.75	0.51
5:F:122:ARG:HG3	5:F:371:LYS:HE3	1.91	0.51
5:F:562:ARG:HH21	5:F:573:LEU:HA	1.76	0.51
1:B:86:LYS:HG2	1:B:173:VAL:HG13	1.92	0.51
2:C:1270:PHE:CZ	2:C:1274:GLU:HB3	2.45	0.51
2:C:182:SER:HB3	2:C:199:ASP:OD2	2.11	0.51
2:C:834:GLN:HE22	2:C:924:VAL:HG21	1.76	0.51
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.93	0.51
3:D:51:PRO:HG2	3:D:71:LEU:HD11	1.92	0.51
2:C:786:GLY:N	2:C:789:THR:OG1	2.44	0.51
3:D:1149:ARG:HH21	3:D:1153:PRO:HG2	1.76	0.51
3:D:549:LYS:HG2	3:D:571:ASP:HA	1.93	0.51
3:D:964:LYS:HE3	3:D:976:THR:HB	1.92	0.51
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.93	0.51
2:C:1258:PRO:HD3	2:C:1295:SER:HA	1.93	0.50
2:C:5:TYR:CE2	2:C:776:PRO:HB2	2.46	0.50
2:C:1340:GLU:HB2	3:D:19:ALA:HB3	1.94	0.50
7:T:7:DT:H1'	7:T:8:DC:H5'	1.92	0.50
2:C:576:SER:HB2	2:C:579:ALA:HB2	1.93	0.50
5:F:454:VAL:O	5:F:458:GLU:HG2	2.10	0.50
2:C:672:GLU:HB3	3:D:767:LEU:O	2.11	0.50
2:C:1105:SER:HB3	3:D:731:ARG:HG3	1.92	0.50
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.93	0.50
2:C:1315:MET:HG3	2:C:1317:PRO:HD3	1.92	0.50
4:E:8:ASP:HA	4:E:11:GLU:HG2	1.93	0.50
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:849:LEU:HB3	3:D:855:ASP:O	2.12	0.50
3:D:960:LEU:HD13	3:D:963:VAL:HG11	1.94	0.50
7:T:10:DC:H2"	7:T:11:DA:H5'	1.93	0.50
2:C:106:GLU:CB	2:C:114:VAL:HG21	2.39	0.50
2:C:635:THR:HG23	2:C:644:LEU:HD22	1.93	0.50
2:C:975:ILE:HG12	2:C:1014:LEU:HD23	1.93	0.50
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.93	0.50
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	1.94	0.50
2:C:808:ASN:H	3:D:633:ALA:HB2	1.77	0.49
2:C:976:ARG:HH22	2:C:990:ASP:HB3	1.76	0.49
3:D:1179:PRO:HG2	3:D:1184:ASP:HA	1.94	0.49
3:D:843:VAL:HG13	3:D:883:ARG:HB2	1.94	0.49
3:D:259:ARG:HG3	5:F:502:LYS:HD2	1.94	0.49
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.94	0.49
3:D:1012:ALA:HB3	3:D:1015:GLU:HG3	1.93	0.49
2:C:1289:GLU:OE2	3:D:473:THR:HG23	2.12	0.49
3:D:506:VAL:HG11	3:D:625:MET:HA	1.94	0.49
3:D:650:LYS:NZ	3:D:762:ASN:HB3	2.26	0.49
3:D:309:ASN:HB2	3:D:326:SER:HB3	1.94	0.49
2:C:1211:ARG:HD3	2:C:1220:GLN:HE22	1.77	0.49
3:D:904:ALA:HB3	4:E:16:ARG:HH22	1.78	0.49
2:C:690:VAL:HG13	2:C:830:THR:HG21	1.94	0.49
2:C:960:LEU:HB3	2:C:1025:PHE:CE1	2.47	0.49
2:C:1101:LEU:HD13	3:D:504:GLN:HB3	1.94	0.49
2:C:548:ARG:HE	2:C:569:ILE:HD12	1.78	0.49
2:C:540:ARG:HD2	2:C:540:ARG:H	1.76	0.49
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.95	0.49
3:D:1295:ASN:HD22	3:D:1296:GLY:N	2.11	0.49
3:D:361:LEU:HD13	3:D:366:CYS:HA	1.94	0.49
1:A:57:THR:HB	1:A:158:ARG:HH21	1.78	0.49
2:C:213:LEU:HD13	2:C:422:LYS:HG2	1.94	0.49
6:N:14:DT:H1'	6:N:15:DG:C5	2.48	0.49
3:D:385:LEU:HD21	3:D:411:ILE:HG13	1.94	0.49
3:D:349:TYR:CD2	3:D:472:LEU:HD21	2.48	0.49
3:D:973:LEU:HB3	3:D:1003:LEU:HB2	1.94	0.49
6:N:9:DC:H2"	6:N:10:DC:C5	2.48	0.49
7:T:9:DC:N1	7:T:10:DC:C5	2.81	0.49
2:C:822:VAL:HG13	2:C:827:ARG:HD3	1.95	0.49
3:D:84:ILE:HG23	3:D:91:GLU:HB3	1.94	0.49
1:B:14:VAL:HG11	1:B:29:GLU:HG2	1.95	0.48
2:C:1142:ARG:HH11	2:C:1161:LEU:HA	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:518:ASN:O	2:C:691:PRO:HD3	2.13	0.48
3:D:1002:VAL:HB	3:D:1019:ASN:HB3	1.95	0.48
2:C:96:LEU:HD23	2:C:124:MET:HG3	1.94	0.48
2:C:539:THR:HB	2:C:542:ARG:HB2	1.94	0.48
1:B:61:ILE:HG22	1:B:63:GLY:H	1.78	0.48
4:E:6:VAL:O	4:E:10:VAL:HG23	2.12	0.48
7:T:10:DC:C6	7:T:10:DC:C5'	2.88	0.48
7:T:11:DA:H8	7:T:11:DA:OP2	1.96	0.48
2:C:106:GLU:HB3	2:C:114:VAL:CG2	2.41	0.48
2:C:980:VAL:HG13	2:C:984:VAL:HG23	1.95	0.48
3:D:450:HIS:HB3	3:D:453:VAL:HG23	1.95	0.48
1:B:48:LEU:HD22	3:D:539:SER:HB3	1.96	0.48
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.95	0.48
1:A:195:ARG:HG2	1:A:198:LEU:CG	2.39	0.48
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.94	0.48
2:C:767:GLN:HA	2:C:786:GLY:HA2	1.95	0.48
3:D:1280:VAL:HG22	3:D:1281:GLU:H	1.77	0.48
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.95	0.48
3:D:650:LYS:O	3:D:654:ILE:HG13	2.14	0.48
2:C:234:ASP:O	2:C:235:ASN:HB2	2.13	0.48
1:B:136:GLU:CD	1:B:137:ASN:H	2.15	0.48
2:C:383:SER:O	2:C:387:ASN:HB2	2.13	0.48
2:C:899:GLU:O	2:C:903:ARG:HG2	2.13	0.48
3:D:797:THR:HA	3:D:800:LEU:HD12	1.95	0.48
3:D:113:HIS:CD2	3:D:239:LEU:HD11	2.48	0.48
1:A:44:ARG:HA	1:A:47:LEU:HD12	1.94	0.47
2:C:120:GLN:OE1	2:C:488:MET:HB3	2.15	0.47
3:D:1170:LYS:N	3:D:1170:LYS:HD3	2.29	0.47
3:D:1252:HIS:O	3:D:1255:VAL:HG12	2.13	0.47
3:D:269:TYR:O	3:D:273:ILE:HG13	2.14	0.47
3:D:609:TYR:HA	3:D:617:THR:OG1	2.14	0.47
5:F:131:GLN:HG3	5:F:266:PHE:HZ	1.79	0.47
1:B:57:THR:OG1	1:B:147:GLN:HB2	2.14	0.47
2:C:1070:HIS:HB3	2:C:1108:ASN:ND2	2.24	0.47
2:C:1244:HIS:HB3	2:C:1264:GLN:CB	2.42	0.47
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.96	0.47
3:D:210:SER:O	3:D:212:THR:N	2.48	0.47
2:C:1304:MET:O	2:C:1308:ILE:HG12	2.13	0.47
2:C:206:ALA:O	2:C:209:ILE:HG22	2.15	0.47
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.78	0.47
3:D:1290:ARG:HA	3:D:1293:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:919:ALA:O	3:D:923:ILE:HG13	2.14	0.47
4:E:13:ILE:O	4:E:15:ASN:N	2.47	0.47
2:C:176:ILE:HB	2:C:184:LEU:HB3	1.95	0.47
2:C:1281:TYR:HD2	3:D:484:MET:HG2	1.79	0.47
2:C:842:ASP:HA	2:C:847:PRO:HA	1.96	0.47
2:C:1191:LYS:O	2:C:1195:ILE:HG12	2.15	0.47
1:A:26:VAL:HG23	1:A:203:ILE:HB	1.97	0.47
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.96	0.47
3:D:481:ARG:NH1	4:E:3:ARG:O	2.48	0.47
3:D:772:TYR:O	3:D:776:THR:OG1	2.30	0.47
1:B:44:ARG:HG2	1:B:183:ILE:HD13	1.97	0.47
2:C:1314:GLN:HG3	4:E:28:ARG:HH21	1.79	0.47
2:C:592:ARG:HH22	2:C:623:LEU:HD12	1.80	0.47
2:C:744:GLY:C	2:C:746:ALA:H	2.19	0.47
2:C:1244:HIS:NE2	3:D:352:ARG:CD	2.78	0.47
5:F:137:TYR:CE2	5:F:139:GLU:HB2	2.50	0.47
5:F:591:GLU:O	5:F:595:LEU:HG	2.14	0.47
6:N:22:DT:H1'	6:N:23:DT:H5''	1.96	0.47
7:T:14:DA:H2''	7:T:15:DG:OP2	2.15	0.47
1:A:102:LEU:HB3	1:A:142:MET:CG	2.45	0.47
2:C:670:PHE:HB3	2:C:673:HIS:CD2	2.41	0.47
3:D:1005:LYS:HD3	3:D:1005:LYS:HA	1.67	0.47
3:D:118:LYS:HD3	3:D:312:ARG:NH1	2.30	0.47
3:D:1191:PRO:HB2	3:D:1194:ARG:HG2	1.97	0.47
3:D:886:VAL:HG11	3:D:1230:THR:HG21	1.97	0.47
3:D:503:SER:O	3:D:506:VAL:HG23	2.15	0.47
5:F:406:GLN:O	5:F:410:ILE:HG12	2.14	0.47
1:A:77:ASP:O	1:A:81:ILE:HG13	2.15	0.47
2:C:696:ASP:OD2	2:C:1178:LYS:HE2	2.14	0.47
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.96	0.47
3:D:1005:LYS:O	3:D:1009:GLU:HG3	2.15	0.47
3:D:1253:ILE:H	3:D:1253:ILE:HD12	1.80	0.47
3:D:1264:ALA:O	3:D:1280:VAL:N	2.48	0.47
3:D:1348:LYS:O	3:D:1351:VAL:HG22	2.15	0.47
3:D:857:LEU:HD13	3:D:872:LEU:HD23	1.97	0.47
3:D:47:ARG:HH12	5:F:496:LYS:HE3	1.80	0.47
2:C:268:ARG:HH22	2:C:270:THR:HA	1.79	0.46
2:C:591:TYR:CE1	2:C:616:ILE:HG21	2.49	0.46
3:D:325:LYS:HE3	3:D:330:MET:HG2	1.95	0.46
3:D:358:GLY:N	3:D:359:PRO:HD3	2.23	0.46
3:D:405:GLU:O	3:D:408:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HD23	1:A:85:LEU:HD12	1.98	0.46
1:B:44:ARG:NH2	1:B:45:ARG:HG2	2.30	0.46
2:C:225:PHE:CZ	2:C:347:ILE:HB	2.50	0.46
2:C:273:HIS:HD2	2:C:276:GLN:NE2	2.13	0.46
3:D:805:GLN:OE1	3:D:1348:LYS:HB2	2.15	0.46
2:C:92:TYR:CE2	2:C:129:LEU:HB2	2.49	0.46
3:D:597:GLY:O	3:D:601:ILE:HG13	2.16	0.46
5:F:111:LEU:HB3	5:F:115:GLY:HA3	1.97	0.46
5:F:532:LEU:H	5:F:532:LEU:HD12	1.81	0.46
6:N:13:DA:N6	7:T:12:DT:H3	2.09	0.46
2:C:32:LEU:O	2:C:36:GLN:HB2	2.15	0.46
3:D:335:GLN:HE21	3:D:335:GLN:HB2	1.51	0.46
5:F:310:GLU:HG2	5:F:355:ILE:HG21	1.97	0.46
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.97	0.46
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.98	0.46
2:C:1030:GLU:HG2	2:C:1033:ARG:HH12	1.80	0.46
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.48	0.46
2:C:646:SER:HB2	2:C:649:GLN:HG3	1.98	0.46
3:D:44:ILE:O	5:F:450:ILE:HG22	2.15	0.46
3:D:507:VAL:HG12	3:D:601:ILE:HD12	1.97	0.46
5:F:105:MET:HE1	5:F:388:ILE:HD13	1.97	0.46
2:C:1120:ALA:HB1	2:C:1198:LEU:HD12	1.96	0.46
2:C:42:ASP:OD2	2:C:46:GLN:HB3	2.16	0.46
3:D:536:LEU:HB3	3:D:542:ALA:HB3	1.97	0.46
3:D:701:LEU:HD11	3:D:722:ILE:HD11	1.98	0.46
2:C:199:ASP:O	2:C:200:ARG:HG2	2.15	0.46
6:N:14:DT:O3'	6:N:15:DG:H8	1.99	0.46
1:A:192:VAL:HG22	1:A:193:GLU:H	1.80	0.46
2:C:1244:HIS:NE2	3:D:352:ARG:NE	2.63	0.46
3:D:201:LEU:O	3:D:217:LEU:HD11	2.16	0.46
6:N:14:DT:C1'	6:N:15:DG:C8	2.98	0.46
2:C:598:VAL:HG22	2:C:628:HIS:CD2	2.51	0.46
3:D:1357:ILE:H	3:D:1357:ILE:HG13	1.42	0.46
3:D:334:LYS:HA	3:D:339:ARG:HD2	1.98	0.46
3:D:411:ILE:O	3:D:415:VAL:HG13	2.15	0.46
4:E:50:ALA:O	4:E:54:ILE:HG12	2.15	0.46
5:F:429:THR:HA	6:N:28:DA:N7	2.31	0.46
2:C:1261:GLY:C	2:C:1263:ALA:H	2.18	0.46
2:C:1313:HIS:CD2	3:D:477:GLN:HE22	2.34	0.46
2:C:379:GLU:CD	2:C:379:GLU:H	2.19	0.46
2:C:414:ILE:HG13	2:C:414:ILE:H	1.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:617:ALA:HA	2:C:636:CYS:SG	2.56	0.46
3:D:952:VAL:HG13	3:D:1014:GLY:HA2	1.98	0.46
3:D:212:THR:HA	3:D:215:LYS:HE2	1.97	0.46
2:C:59:ILE:HG21	2:C:475:VAL:HB	1.97	0.45
3:D:114:ILE:HG13	3:D:118:LYS:HG3	1.98	0.45
3:D:121:PRO:HB2	3:D:123:ARG:HH21	1.82	0.45
6:N:27:DA:H2''	6:N:28:DA:H5'	1.98	0.45
2:C:1223:ARG:HE	2:C:1223:ARG:HB3	1.64	0.45
2:C:1244:HIS:HE1	3:D:352:ARG:CZ	2.29	0.45
3:D:475:GLU:N	3:D:475:GLU:OE1	2.45	0.45
1:A:102:LEU:HB3	1:A:142:MET:HG3	1.97	0.45
1:B:8:PHE:HE1	1:B:32:GLU:HG3	1.80	0.45
2:C:1243:MET:O	2:C:1243:MET:HE2	2.16	0.45
2:C:465:ARG:O	2:C:469:VAL:HG23	2.16	0.45
2:C:562:GLU:HG2	2:C:574:SER:CB	2.43	0.45
2:C:734:ILE:HD12	2:C:777:VAL:HG11	1.99	0.45
3:D:268:LEU:CB	3:D:306:LEU:HD23	2.46	0.45
3:D:596:LEU:HD11	3:D:604:MET:HE1	1.98	0.45
3:D:750:PRO:HG3	3:D:777:HIS:CE1	2.52	0.45
2:C:802:VAL:HG23	2:C:1098:LEU:HD13	1.99	0.45
2:C:138:ILE:HG12	2:C:506:PHE:O	2.17	0.45
3:D:1216:ALA:O	3:D:1220:ILE:HG13	2.17	0.45
3:D:144:TYR:CD1	3:D:180:MET:HB2	2.51	0.45
2:C:1244:HIS:HE1	3:D:352:ARG:NE	2.06	0.45
1:B:13:LEU:HD11	1:B:26:VAL:HG12	1.97	0.45
2:C:1100:PRO:HG2	3:D:637:ALA:O	2.16	0.45
3:D:963:VAL:HB	3:D:980:THR:HG23	1.99	0.45
4:E:26:ARG:NH2	4:E:38:LEU:HD13	2.31	0.45
5:F:486:ARG:HB2	5:F:486:ARG:HH11	1.80	0.45
2:C:1176:LEU:HD23	2:C:1176:LEU:HA	1.72	0.45
3:D:1230:THR:HB	3:D:1257:VAL:HG11	1.98	0.45
3:D:148:GLU:H	3:D:156:ARG:HG3	1.81	0.45
3:D:532:GLU:O	3:D:536:LEU:HD23	2.16	0.45
3:D:797:THR:HB	3:D:924:GLY:HA3	1.98	0.45
5:F:423:ARG:HB2	5:F:423:ARG:HH11	1.81	0.45
5:F:584:ARG:NH1	5:F:584:ARG:O	2.49	0.45
2:C:145:ILE:HB	2:C:456:VAL:HB	1.97	0.45
2:C:56:VAL:HG11	2:C:468:LEU:HD13	1.99	0.45
2:C:611:GLU:HG3	2:C:616:ILE:HD13	1.98	0.45
2:C:563:THR:O	2:C:680:LEU:HD11	2.17	0.45
7:T:1:DA:H2''	7:T:2:DA:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASN:O	1:A:44:ARG:HG2	2.16	0.45
1:A:91:ARG:NH2	1:A:211:ILE:HA	2.32	0.45
3:D:362:ARG:H	3:D:365:GLN:NE2	2.13	0.45
4:E:54:ILE:HD13	4:E:59:ILE:HG22	1.98	0.45
5:F:572:THR:O	5:F:576:VAL:HG23	2.17	0.45
2:C:11:ILE:HB	2:C:1149:TYR:OH	2.17	0.45
2:C:273:HIS:O	2:C:277:LEU:HG	2.17	0.45
2:C:364:VAL:HG13	2:C:376:PRO:HG3	1.98	0.45
3:D:83:VAL:O	3:D:91:GLU:HA	2.17	0.45
6:N:14:DT:O3'	6:N:15:DG:C8	2.70	0.45
2:C:1120:ALA:HB2	2:C:1199:LEU:HD23	1.99	0.45
2:C:205:PRO:HG2	2:C:354:ASP:HA	1.98	0.45
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.32	0.45
2:C:564:PRO:HD2	2:C:572:ILE:HB	1.99	0.45
3:D:674:THR:HG23	3:D:677:GLU:HB2	1.98	0.45
7:T:18:DG:H2'	7:T:18:DG:OP2	2.17	0.45
1:A:154:PRO:HB2	2:C:1059:ARG:HH22	1.82	0.44
1:A:182:ARG:O	1:A:183:ILE:HG13	2.16	0.44
2:C:1281:TYR:CD2	3:D:484:MET:HG2	2.51	0.44
2:C:131:THR:HG23	2:C:133:ASN:N	2.28	0.44
3:D:1156:LEU:HD23	3:D:1219:ASP:HB3	1.98	0.44
3:D:154:LEU:HD12	3:D:176:PHE:HE1	1.82	0.44
5:F:394:TYR:HB2	5:F:404:LEU:HD13	1.97	0.44
2:C:171:LEU:HD21	2:C:190:PRO:HA	1.99	0.44
2:C:246:LEU:HD12	2:C:246:LEU:H	1.82	0.44
3:D:950:ILE:HD13	3:D:995:TYR:HB3	1.98	0.44
5:F:281:ARG:HD2	5:F:285:ARG:CZ	2.48	0.44
6:N:9:DC:H2''	6:N:10:DC:C6	2.52	0.44
1:A:62:ASP:OD1	1:A:141:SER:HB2	2.17	0.44
2:C:1143:GLU:HG2	2:C:1147:ARG:NH1	2.32	0.44
2:C:1244:HIS:CE1	3:D:352:ARG:HE	2.34	0.44
2:C:136:PHE:CE1	2:C:456:VAL:HG21	2.52	0.44
2:C:238:GLN:HA	2:C:286:GLU:HA	1.98	0.44
2:C:705:GLU:CB	2:C:794:LEU:H	2.30	0.44
3:D:850:LYS:HZ3	3:D:857:LEU:HD21	1.82	0.44
2:C:964:LEU:HD13	2:C:1025:PHE:HB2	1.99	0.44
2:C:1059:ARG:HG2	2:C:1060:ILE:H	1.83	0.44
2:C:171:LEU:HD13	2:C:188:PHE:O	2.18	0.44
3:D:205:LEU:HD22	3:D:214:ARG:HG2	1.99	0.44
3:D:325:LYS:HG3	3:D:329:ASP:HB3	2.00	0.44
3:D:337:ARG:HA	3:D:341:ASN:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:515:ARG:HG3	3:D:516:ASP:H	1.82	0.44
3:D:811:GLU:O	3:D:895:CYS:HA	2.17	0.44
5:F:127:ILE:HA	5:F:130:VAL:HG22	2.00	0.44
5:F:503:GLU:OE1	5:F:504:PRO:HD2	2.18	0.44
1:A:207:THR:HG22	1:A:208:ASN:H	1.83	0.44
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.87	0.44
2:C:841:ARG:HB2	2:C:1045:GLY:O	2.18	0.44
3:D:1021:ASP:HB3	3:D:1023:HIS:HD2	1.82	0.44
3:D:430:HIS:CE1	3:D:432:LEU:HB2	2.53	0.44
3:D:664:ILE:HD12	3:D:681:LYS:HD3	1.99	0.44
3:D:689:ALA:HA	3:D:692:ARG:HD3	1.99	0.44
3:D:913:GLU:HG3	4:E:17:PHE:HZ	1.82	0.44
1:A:155:ALA:HA	1:A:158:ARG:HB2	2.00	0.44
1:B:115:ILE:HG22	1:B:116:THR:H	1.83	0.44
2:C:210:LEU:HD21	2:C:429:MET:HE1	2.00	0.44
2:C:732:ILE:HG13	2:C:753:LEU:HD11	2.00	0.44
3:D:1138:LEU:HD23	3:D:1138:LEU:H	1.83	0.44
3:D:1158:GLU:O	3:D:1206:ARG:NH1	2.51	0.44
3:D:127:LEU:HD21	3:D:234:PRO:HB3	2.00	0.44
3:D:506:VAL:CG1	3:D:625:MET:HA	2.47	0.44
3:D:733:SER:O	3:D:737:ILE:HG12	2.17	0.44
3:D:991:THR:O	3:D:992:LYS:HD2	2.18	0.44
5:F:528:LEU:HG	5:F:528:LEU:H	1.54	0.44
1:A:22:THR:OG1	1:A:206:GLU:HG3	2.18	0.44
1:B:23:HIS:HB2	1:B:206:GLU:HG2	1.99	0.44
2:C:810:TYR:HE2	2:C:1078:LYS:HE3	1.81	0.44
3:D:1263:LYS:HB2	3:D:1307:LEU:CD1	2.42	0.44
3:D:537:TYR:CD1	3:D:544:LEU:HD23	2.52	0.44
2:C:1077:SER:HB2	3:D:357:VAL:CG2	2.48	0.44
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.53	0.44
2:C:658:GLN:HE21	2:C:658:GLN:HB2	1.61	0.44
2:C:903:ARG:HD2	2:C:908:GLU:O	2.18	0.44
3:D:670:SER:HB2	3:D:672:LEU:HD12	2.00	0.44
2:C:1276:TRP:HH2	3:D:798:ARG:HG3	1.83	0.44
5:F:426:LYS:H	6:N:27:DA:P	2.41	0.44
1:A:168:ILE:H	1:A:168:ILE:HD12	1.83	0.44
3:D:1136:GLY:HA2	3:D:1140:ARG:HB2	2.00	0.44
3:D:1291:GLU:HG3	3:D:1292:LEU:N	2.33	0.44
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.00	0.44
4:E:26:ARG:NH1	4:E:35:LYS:HD3	2.33	0.44
2:C:1296:ASP:HB3	2:C:1320:PRO:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:238:GLN:HB3	2:C:284:LEU:HD11	2.00	0.43
2:C:367:TYR:HD2	2:C:381:ALA:HA	1.83	0.43
2:C:582:ASN:N	2:C:582:ASN:HD22	2.15	0.43
3:D:258:GLY:C	5:F:502:LYS:HE3	2.38	0.43
2:C:1085:MET:HA	2:C:1085:MET:HE2	1.99	0.43
2:C:20:GLN:HG2	2:C:20:GLN:H	1.64	0.43
3:D:118:LYS:HE2	3:D:311:ARG:HB3	2.00	0.43
3:D:525:MET:O	3:D:548:VAL:HG13	2.19	0.43
5:F:449:THR:OG1	5:F:504:PRO:HG3	2.18	0.43
7:T:11:DA:C8	7:T:12:DT:C7	3.01	0.43
2:C:445:ILE:H	2:C:445:ILE:HG13	1.51	0.43
3:D:950:ILE:HG13	3:D:1020:TRP:CZ3	2.53	0.43
4:E:69:ARG:HE	4:E:69:ARG:HB2	1.65	0.43
6:N:4:DC:H2'	6:N:5:DT:H71	1.99	0.43
2:C:205:PRO:O	2:C:208:ILE:HG22	2.18	0.43
2:C:262:TYR:HD2	2:C:276:GLN:NE2	2.15	0.43
3:D:1155:ILE:HB	3:D:1210:ILE:HB	1.99	0.43
3:D:1230:THR:CB	3:D:1257:VAL:HG11	2.48	0.43
3:D:850:LYS:HB3	3:D:851:PRO:HD2	2.00	0.43
2:C:823:VAL:HG23	2:C:1060:ILE:HG23	2.00	0.43
2:C:1340:GLU:O	2:C:1341:ASP:O	2.36	0.43
2:C:273:HIS:HA	2:C:276:GLN:HB3	2.00	0.43
3:D:1330:ARG:O	3:D:1334:GLU:HG3	2.18	0.43
3:D:902:ASP:H	3:D:1251:LYS:NZ	2.16	0.43
2:C:1070:HIS:NE2	2:C:1114:GLU:OE2	2.51	0.43
2:C:398:SER:O	2:C:400:VAL:N	2.51	0.43
2:C:678:ARG:HD3	2:C:678:ARG:HA	1.78	0.43
3:D:646:ILE:HG13	3:D:764:ARG:HH21	1.84	0.43
3:D:990:ARG:HD2	3:D:992:LYS:HD3	2.01	0.43
5:F:96:ASP:OD1	5:F:96:ASP:N	2.52	0.43
2:C:189:ASP:O	2:C:192:ASP:N	2.52	0.43
2:C:494:ASN:O	2:C:498:ILE:HD13	2.19	0.43
3:D:397:ALA:O	3:D:401:VAL:HG13	2.19	0.43
3:D:661:VAL:HG12	3:D:685:ILE:HD11	2.00	0.43
1:A:37:HIS:CE1	1:A:187:VAL:HG21	2.53	0.43
2:C:34:SER:O	2:C:457:GLY:HA3	2.18	0.43
2:C:609:ILE:H	2:C:609:ILE:HD13	1.84	0.43
3:D:421:VAL:O	3:D:436:ALA:HA	2.19	0.43
3:D:504:GLN:CD	3:D:731:ARG:HH21	2.22	0.43
5:F:379:MET:O	5:F:383:ASN:ND2	2.52	0.43
2:C:138:ILE:HG21	2:C:507:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:242:VAL:HG12	2:C:244:GLU:H	1.83	0.43
2:C:633:LEU:HB3	2:C:644:LEU:HD12	2.00	0.43
3:D:1238:GLN:O	3:D:1242:ARG:HB2	2.19	0.43
5:F:287:ILE:HG23	5:F:337:VAL:HG13	2.01	0.43
5:F:573:LEU:H	5:F:573:LEU:HD23	1.84	0.43
2:C:1313:HIS:HD2	3:D:477:GLN:HE22	1.67	0.43
3:D:255:LEU:HA	3:D:255:LEU:HD12	1.88	0.43
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.54	0.43
5:F:125:ASP:O	5:F:129:GLN:HG3	2.19	0.43
1:B:219:ARG:O	1:B:223:ILE:HG13	2.18	0.42
2:C:494:ASN:HD22	2:C:495:ALA:H	1.66	0.42
2:C:639:LYS:C	2:C:641:GLU:H	2.23	0.42
3:D:122:SER:O	3:D:126:LEU:HD23	2.19	0.42
3:D:159:ILE:HG12	3:D:160:LEU:N	2.34	0.42
3:D:593:ASN:O	3:D:594:GLN:NE2	2.52	0.42
3:D:615:LYS:HG3	3:D:615:LYS:H	1.62	0.42
5:F:281:ARG:HD2	5:F:285:ARG:NE	2.34	0.42
6:N:12:DG:H1'	6:N:13:DA:C5'	2.46	0.42
2:C:996:ARG:O	2:C:1000:LEU:HG	2.19	0.42
2:C:1211:ARG:HD3	2:C:1220:GLN:NE2	2.34	0.42
2:C:1305:TYR:CD2	5:F:531:PRO:HB2	2.54	0.42
3:D:755:ILE:HG13	3:D:757:THR:H	1.84	0.42
5:F:124:GLU:O	5:F:127:ILE:HG13	2.19	0.42
7:T:12:DT:C2'	7:T:13:DC:C5	3.02	0.42
2:C:1073:LYS:HG2	2:C:1073:LYS:H	1.71	0.42
2:C:1268:GLN:HE22	3:D:352:ARG:NE	2.16	0.42
3:D:1368:ASP:HA	3:D:1371:ARG:HH11	1.84	0.42
3:D:744:ARG:HD2	3:D:763:PHE:CE2	2.54	0.42
7:T:9:DC:H1'	7:T:10:DC:C6	2.54	0.42
2:C:1119:MET:HE1	2:C:1208:GLY:O	2.19	0.42
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.84	0.42
2:C:149:LEU:HD12	2:C:452:ARG:O	2.20	0.42
2:C:467:GLY:HA2	2:C:470:ARG:HG2	2.02	0.42
2:C:403:MET:HG3	2:C:584:TYR:CE2	2.55	0.42
2:C:582:ASN:ND2	2:C:586:PHE:H	2.15	0.42
2:C:724:VAL:HG11	2:C:727:VAL:HG22	2.01	0.42
3:D:223:LEU:O	3:D:227:PHE:HB2	2.19	0.42
3:D:306:LEU:HD13	3:D:307:LEU:HD23	2.01	0.42
3:D:430:HIS:NE2	3:D:432:LEU:HB2	2.34	0.42
3:D:361:LEU:HD11	3:D:448:GLN:HB3	2.00	0.42
3:D:901:ARG:HD2	3:D:906:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:O	1:A:43:LEU:HB2	2.19	0.42
2:C:1089:GLU:H	2:C:1089:GLU:HG3	1.47	0.42
2:C:949:GLU:O	2:C:953:LEU:HG	2.18	0.42
2:C:974:ARG:O	2:C:978:VAL:HG22	2.19	0.42
3:D:495:ASN:HD22	3:D:497:GLU:HB2	1.84	0.42
4:E:7:GLN:O	4:E:11:GLU:HG2	2.19	0.42
1:B:51:MET:HB3	1:B:179:PRO:HD2	2.01	0.42
2:C:804:PHE:HE2	2:C:1112:ILE:HD13	1.84	0.42
2:C:1191:LYS:HE3	2:C:1191:LYS:HB3	1.74	0.42
2:C:1230:MET:HE3	2:C:1230:MET:HB2	1.87	0.42
2:C:538:LEU:HB3	2:C:542:ARG:CZ	2.49	0.42
3:D:1162:ILE:O	3:D:1178:THR:HB	2.19	0.42
3:D:900:GLY:O	3:D:909:ILE:HG22	2.20	0.42
5:F:562:ARG:NH1	5:F:591:GLU:OE2	2.53	0.42
1:B:40:GLY:O	1:B:44:ARG:HB2	2.19	0.42
2:C:1308:ILE:HD12	3:D:380:PHE:CE1	2.54	0.42
2:C:669:PRO:HD3	2:C:1069:ARG:HE	1.85	0.42
3:D:1195:GLN:HG2	3:D:1196:LEU:N	2.35	0.42
3:D:553:THR:OG1	3:D:567:THR:HB	2.20	0.42
3:D:674:THR:OG1	3:D:675:ALA:N	2.52	0.42
3:D:767:LEU:HA	3:D:767:LEU:HD13	1.93	0.42
3:D:814:CYS:SG	3:D:816:THR:HG22	2.60	0.42
5:F:585:GLU:OE2	5:F:588:ARG:HD3	2.20	0.42
1:A:103:ASN:ND2	1:A:141:SER:HA	2.35	0.42
1:B:124:VAL:HG11	1:B:209:GLY:HA3	2.02	0.42
2:C:153:PRO:HD3	2:C:452:ARG:HD3	2.02	0.42
2:C:857:VAL:HG21	2:C:862:LEU:HD21	2.01	0.42
2:C:5:TYR:CZ	2:C:8:LYS:HE3	2.54	0.42
3:D:118:LYS:HD3	3:D:312:ARG:HH11	1.84	0.42
3:D:582:ILE:HG12	3:D:627:THR:HG21	2.01	0.42
3:D:980:THR:O	3:D:996:LYS:HD3	2.20	0.42
6:N:4:DC:C2'	6:N:5:DT:H71	2.49	0.42
1:A:75:GLN:HG2	1:A:132:HIS:HB2	2.02	0.42
3:D:1144:LEU:HD11	3:D:1236:GLU:HG2	2.02	0.42
3:D:123:ARG:HD2	3:D:1337:VAL:HG11	2.00	0.42
3:D:190:LYS:HG2	3:D:235:GLU:HG2	2.02	0.42
5:F:157:ARG:HB2	5:F:160:ASP:HB2	2.02	0.42
5:F:265:GLN:O	5:F:269:LEU:HG	2.19	0.42
5:F:404:LEU:HD22	5:F:439:ILE:HG23	2.01	0.42
7:T:9:DC:H6	7:T:9:DC:H2'	1.75	0.42
1:B:8:PHE:HD1	1:B:9:LEU:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:THR:HG21	2:C:755:LYS:HE2	2.01	0.42
3:D:1159:ILE:HG23	3:D:1160:SER:O	2.20	0.42
3:D:394:ILE:HG23	5:F:536:THR:HG22	2.01	0.42
3:D:744:ARG:HB2	3:D:744:ARG:HE	1.72	0.42
3:D:789:LYS:HA	3:D:792:ASN:ND2	2.35	0.42
3:D:973:LEU:HB3	3:D:1003:LEU:HD12	2.02	0.42
4:E:68:GLU:O	4:E:72:GLN:HG3	2.20	0.42
2:C:79:VAL:HG21	5:F:476:ARG:HH11	1.85	0.42
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.88	0.41
1:B:31:LEU:HB3	1:B:199:ASP:HB2	2.02	0.41
2:C:17:LYS:N	2:C:1188:ASP:OD2	2.51	0.41
2:C:127:ILE:O	2:C:127:ILE:HG13	2.18	0.41
2:C:871:VAL:HG11	2:C:883:LEU:HD22	2.02	0.41
3:D:1138:LEU:HA	3:D:1141:VAL:HG22	2.02	0.41
3:D:1172:LYS:HA	3:D:1193:TRP:HZ3	1.85	0.41
3:D:317:THR:HG22	3:D:322:ARG:O	2.20	0.41
3:D:586:GLY:HA3	3:D:612:LEU:HD21	2.02	0.41
3:D:810:THR:O	3:D:911:LYS:HG3	2.20	0.41
5:F:320:ILE:HD13	5:F:331:HIS:CE1	2.55	0.41
2:C:1034:ARG:O	2:C:1038:GLN:HB2	2.20	0.41
2:C:1138:VAL:HG21	2:C:1166:ASP:OD2	2.20	0.41
2:C:138:ILE:HD13	2:C:143:ARG:HD3	2.02	0.41
2:C:496:LYS:HB3	2:C:497:PRO:HD3	2.03	0.41
2:C:727:VAL:H	2:C:773:LEU:HD23	1.84	0.41
3:D:21:LYS:HE3	3:D:23:ALA:HB2	2.03	0.41
3:D:502:PRO:HG2	3:D:601:ILE:HG21	2.01	0.41
5:F:601:PRO:C	5:F:603:ARG:H	2.24	0.41
1:A:46:ILE:HD11	1:B:38:THR:HG21	2.01	0.41
2:C:453:ILE:HD13	2:C:530:ILE:HD13	2.03	0.41
2:C:662:SER:O	2:C:666:SER:HB3	2.20	0.41
2:C:99:LYS:HG3	2:C:121:GLU:HB3	2.02	0.41
3:D:1244:GLN:HE21	3:D:1244:GLN:HB2	1.58	0.41
3:D:382:TYR:HB3	3:D:394:ILE:HD12	2.02	0.41
3:D:798:ARG:O	3:D:801:VAL:HG22	2.20	0.41
5:F:227:GLN:CD	5:F:230:VAL:HG11	2.40	0.41
1:A:18:GLN:HG3	1:A:24:ALA:HB2	2.02	0.41
1:B:100:LEU:CD2	1:B:121:VAL:HG11	2.50	0.41
1:B:79:LEU:HA	1:B:82:LEU:HB2	2.01	0.41
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.21	0.41
2:C:909:LYS:HE3	2:C:909:LYS:HB2	1.83	0.41
3:D:160:LEU:HD12	3:D:165:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:870:ASP:O	3:D:874:GLU:HG2	2.21	0.41
4:E:25:ARG:HD2	4:E:64:LEU:HD13	2.01	0.41
5:F:133:SER:HB3	5:F:361:ILE:HG23	2.01	0.41
5:F:105:MET:CE	5:F:384:LEU:HB3	2.49	0.41
2:C:378:ARG:O	2:C:382:GLU:HB2	2.20	0.41
2:C:582:ASN:HD21	2:C:585:GLY:N	2.18	0.41
2:C:61:SER:HB3	2:C:479:LEU:HB3	2.01	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.85	0.41
3:D:528:THR:O	3:D:551:ARG:HB3	2.20	0.41
5:F:262:VAL:HG12	5:F:264:LYS:H	1.85	0.41
1:A:67:GLU:H	1:A:67:GLU:HG3	1.52	0.41
1:A:78:ILE:HA	1:A:81:ILE:HD12	2.03	0.41
2:C:820:GLU:N	2:C:1080:ASN:O	2.54	0.41
2:C:475:VAL:HG12	2:C:479:LEU:HD12	2.01	0.41
2:C:754:THR:O	2:C:755:LYS:HD2	2.20	0.41
3:D:362:ARG:HB2	3:D:365:GLN:HG2	2.02	0.41
3:D:362:ARG:N	3:D:365:GLN:HE21	2.14	0.41
2:C:563:THR:HG21	3:D:780:ARG:NH1	2.35	0.41
3:D:800:LEU:O	3:D:803:VAL:HG12	2.20	0.41
2:C:1334:GLY:H	3:D:113:HIS:HE2	1.69	0.41
3:D:1177:ILE:HD12	3:D:1186:TYR:HB3	2.02	0.41
3:D:154:LEU:HD12	3:D:176:PHE:CE1	2.56	0.41
3:D:664:ILE:HG21	3:D:681:LYS:HB3	2.01	0.41
5:F:560:ARG:HD3	5:F:566:ASP:OD1	2.20	0.41
6:N:16:DG:H1'	6:N:17:DG:H5'	2.01	0.41
1:A:195:ARG:HG3	1:A:196:THR:N	2.35	0.41
1:B:102:LEU:HD23	1:B:115:ILE:HG23	2.02	0.41
2:C:806:PRO:HD3	2:C:1100:PRO:HG2	2.03	0.41
2:C:46:GLN:O	2:C:51:ALA:HB2	2.21	0.41
3:D:198:CYS:O	3:D:202:ARG:HG3	2.20	0.41
3:D:904:ALA:HB3	4:E:16:ARG:NH2	2.35	0.41
4:E:4:VAL:HG13	4:E:5:THR:HG22	2.02	0.41
6:N:19:DA:H1'	6:N:20:DG:H5''	2.03	0.41
1:B:227:GLN:HA	1:B:227:GLN:HE21	1.84	0.41
2:C:548:ARG:HB3	2:C:569:ILE:O	2.21	0.41
3:D:105:ILE:HD13	3:D:273:ILE:HG12	2.03	0.41
3:D:1359:ALA:HA	3:D:1363:TYR:HB2	2.02	0.41
5:F:235:ILE:HD12	5:F:242:HIS:ND1	2.36	0.41
5:F:598:LEU:O	5:F:604:SER:HB3	2.21	0.41
5:F:600:HIS:ND1	5:F:601:PRO:HD2	2.36	0.41
1:A:90:VAL:HG22	1:A:91:ARG:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:HD12	1:B:202:VAL:H	1.86	0.41
2:C:189:ASP:HA	2:C:190:PRO:HD3	1.93	0.41
2:C:395:TYR:HE2	2:C:420:LEU:HG	1.85	0.41
2:C:524:ILE:HD13	2:C:712:SER:HB3	2.02	0.41
3:D:1233:ILE:HG13	3:D:1233:ILE:H	1.76	0.41
3:D:216:LYS:HE3	3:D:216:LYS:HB2	1.90	0.41
3:D:442:ILE:HG21	3:D:448:GLN:OE1	2.21	0.41
4:E:71:GLU:HA	4:E:74:GLU:HG3	2.03	0.41
5:F:106:GLY:HA2	5:F:385:ARG:NH2	2.27	0.41
5:F:427:PHE:CZ	5:F:431:ALA:HB2	2.56	0.41
2:C:1296:ASP:HB3	2:C:1321:GLU:H	1.85	0.40
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.52	0.40
2:C:409:LEU:HD22	2:C:427:ASP:HB3	2.03	0.40
2:C:463:GLN:HB3	2:C:501:ALA:O	2.21	0.40
2:C:850:ILE:HD13	2:C:1048:LYS:NZ	2.36	0.40
3:D:741:ALA:O	3:D:762:ASN:ND2	2.47	0.40
5:F:130:VAL:HG11	5:F:369:GLU:HG3	2.03	0.40
1:B:42:ALA:O	1:B:46:ILE:HG13	2.21	0.40
1:B:75:GLN:HE21	1:B:75:GLN:HB2	1.67	0.40
2:C:162:GLY:H	2:C:170:VAL:HG12	1.85	0.40
2:C:272:ARG:NH1	2:C:276:GLN:OE1	2.54	0.40
2:C:309:LEU:HD21	2:C:312:ALA:HB2	2.03	0.40
1:A:68:TYR:HE1	2:C:831:ILE:HD13	1.86	0.40
3:D:29:MET:O	3:D:32:SER:HB3	2.21	0.40
3:D:915:ILE:O	3:D:918:ILE:HG13	2.22	0.40
3:D:1172:LYS:O	3:D:1173:ARG:HB2	2.21	0.40
3:D:69:GLU:HG3	3:D:76:LYS:HG2	2.03	0.40
5:F:532:LEU:O	5:F:536:THR:HG23	2.22	0.40
1:B:56:VAL:HG22	1:B:144:ILE:HD11	2.04	0.40
1:B:219:ARG:HH11	1:B:219:ARG:HB2	1.86	0.40
2:C:88:ARG:NH1	2:C:88:ARG:HB2	2.36	0.40
3:D:1349:GLU:O	3:D:1353:VAL:HG22	2.21	0.40
3:D:224:LEU:O	3:D:228:VAL:HG23	2.22	0.40
3:D:327:LEU:HA	3:D:327:LEU:HD23	1.96	0.40
3:D:678:ARG:HA	3:D:681:LYS:HB2	2.03	0.40
3:D:735:ALA:O	3:D:738:ARG:HG2	2.21	0.40
5:F:319:ALA:HB1	5:F:326:TRP:CH2	2.56	0.40
2:C:79:VAL:HG11	5:F:476:ARG:HD3	2.03	0.40
6:N:26:DT:H2"	6:N:27:DA:C8	2.55	0.40
2:C:1243:MET:O	2:C:1243:MET:CE	2.70	0.40
2:C:1303:LYS:HD3	2:C:1303:LYS:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:PHE:O	2:C:57:PHE:HB2	2.22	0.40
3:D:36:GLY:HA3	3:D:61:ILE:HG23	2.03	0.40
4:E:26:ARG:HH22	4:E:38:LEU:HD13	1.87	0.40
5:F:586:ARG:O	5:F:590:ILE:HG13	2.22	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	
1	A	226/239 (95%)	193 (85%)	31 (14%)	2 (1%)	17	54
1	B	213/239 (89%)	183 (86%)	26 (12%)	4 (2%)	8	42
2	C	1333/1342 (99%)	1179 (88%)	140 (10%)	14 (1%)	14	51
3	D	1218/1409 (86%)	1093 (90%)	118 (10%)	7 (1%)	25	62
4	E	77/91 (85%)	69 (90%)	7 (9%)	1 (1%)	12	48
5	F	465/613 (76%)	426 (92%)	37 (8%)	2 (0%)	34	70
All	All	3532/3933 (90%)	3143 (89%)	359 (10%)	30 (1%)	19	57

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
2	C	399	ALA
2	C	573	ASN
2	C	1150	ASP
2	C	1151	LEU
3	D	1345	ARG
1	B	135	ASP
2	C	200	ARG

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Mol	Chain	Res	Type
2	C	485	ASP
2	C	625	GLU
2	C	1341	ASP
3	D	45	ASN
3	D	211	GLU
5	F	570	ASP
1	B	53	GLY
2	C	235	ASN
3	D	357	VAL
4	E	14	GLY
1	B	136	GLU
2	C	747	GLY
1	B	52	PRO
2	C	398	SER
3	D	518	VAL
2	C	1223	ARG
3	D	1173	ARG
5	F	310	GLU
2	C	1224	PRO
3	D	358	GLY
2	C	117	ILE
1	A	52	PRO

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	
1	A	191/206 (93%)	168 (88%)	23 (12%)	5	25
1	B	183/206 (89%)	163 (89%)	20 (11%)	6	29
2	C	1152/1157 (100%)	1027 (89%)	125 (11%)	6	29
3	D	1026/1170 (88%)	901 (88%)	125 (12%)	5	25
4	E	67/75 (89%)	55 (82%)	12 (18%)	2	12
5	F	420/540 (78%)	376 (90%)	44 (10%)	7	30
All	All	3039/3354 (91%)	2690 (88%)	349 (12%)	5	27

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	12	VAL
1	A	17	GLU
1	A	19	VAL
1	A	22	THR
1	A	51	MET
1	A	54	CYS
1	A	67	GLU
1	A	75	GLN
1	A	77	ASP
1	A	79	LEU
1	A	93	GLN
1	A	111	THR
1	A	114	ASP
1	A	117	HIS
1	A	124	VAL
1	A	140	ILE
1	A	159	ILE
1	A	162	GLU
1	A	185	TYR
1	A	197	ASP
1	A	207	THR
1	A	231	PHE
1	B	8	PHE
1	B	16	ILE
1	B	18	GLN
1	B	26	VAL
1	B	31	LEU
1	B	47	LEU
1	B	60	GLU
1	B	75	GLN
1	B	96	ASP
1	B	100	LEU
1	B	118	ASP
1	B	124	VAL
1	B	134	THR
1	B	136	GLU
1	B	144	ILE
1	B	146	VAL
1	B	148	ARG
1	B	186	ASN
1	B	219	ARG

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Mol	Chain	Res	Type
1	B	231	PHE
2	C	5	TYR
2	C	15	PHE
2	C	17	LYS
2	C	18	ARG
2	C	44	GLU
2	C	63	SER
2	C	66	SER
2	C	79	VAL
2	C	91	THR
2	C	96	LEU
2	C	99	LYS
2	C	105	TYR
2	C	113	THR
2	C	127	ILE
2	C	132	ASP
2	C	135	THR
2	C	152	SER
2	C	200	ARG
2	C	225	PHE
2	C	230	PHE
2	C	236	LYS
2	C	237	LEU
2	C	258	ASN
2	C	290	GLU
2	C	309	LEU
2	C	315	MET
2	C	321	LEU
2	C	322	LEU
2	C	354	ASP
2	C	377	THR
2	C	379	GLU
2	C	389	PHE
2	C	392	GLU
2	C	427	ASP
2	C	443	ASP
2	C	471	VAL
2	C	485	ASP
2	C	487	LEU
2	C	490	GLN
2	C	493	ILE
2	C	494	ASN

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Mol	Chain	Res	Type
2	C	510	GLN
2	C	522	SER
2	C	524	ILE
2	C	538	LEU
2	C	548	ARG
2	C	553	THR
2	C	555	TYR
2	C	558	VAL
2	C	562	GLU
2	C	569	ILE
2	C	573	ASN
2	C	582	ASN
2	C	596	ASP
2	C	609	ILE
2	C	623	LEU
2	C	626	GLU
2	C	635	THR
2	C	654	ASP
2	C	658	GLN
2	C	666	SER
2	C	674	ASP
2	C	681	MET
2	C	687	ARG
2	C	693	LEU
2	C	697	LYS
2	C	705	GLU
2	C	717	VAL
2	C	730	SER
2	C	731	ARG
2	C	748	ILE
2	C	754	THR
2	C	762	ASN
2	C	777	VAL
2	C	778	GLU
2	C	779	ARG
2	C	782	VAL
2	C	783	LEU
2	C	798	GLN
2	C	807	TRP
2	C	810	TYR
2	C	836	LEU
2	C	842	ASP

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Mol	Chain	Res	Type
2	C	876	GLU
2	C	888	THR
2	C	895	LEU
2	C	898	GLU
2	C	919	ARG
2	C	922	ASN
2	C	927	THR
2	C	941	LYS
2	C	951	MET
2	C	978	VAL
2	C	992	LEU
2	C	995	ASP
2	C	996	ARG
2	C	1011	LEU
2	C	1054	LEU
2	C	1060	ILE
2	C	1076	ILE
2	C	1082	ILE
2	C	1089	GLU
2	C	1092	THR
2	C	1106	ARG
2	C	1107	MET
2	C	1108	ASN
2	C	1146	GLN
2	C	1151	LEU
2	C	1161	LEU
2	C	1164	PHE
2	C	1165	SER
2	C	1166	ASP
2	C	1176	LEU
2	C	1191	LYS
2	C	1198	LEU
2	C	1222	GLU
2	C	1243	MET
2	C	1262	LYS
2	C	1264	GLN
2	C	1265	PHE
2	C	1291	LEU
2	C	1299	ASN
2	C	1312	ASN
2	C	1327	LEU
2	C	1341	ASP

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Mol	Chain	Res	Type
3	D	24	LEU
3	D	33	TRP
3	D	46	TYR
3	D	54	ASP
3	D	65	VAL
3	D	71	LEU
3	D	78	LEU
3	D	80	HIS
3	D	84	ILE
3	D	86	GLU
3	D	92	VAL
3	D	94	GLN
3	D	98	ARG
3	D	115	TRP
3	D	126	LEU
3	D	134	ASP
3	D	139	LEU
3	D	160	LEU
3	D	167	ASP
3	D	175	GLU
3	D	188	LEU
3	D	193	ASP
3	D	194	LEU
3	D	195	GLU
3	D	205	LEU
3	D	216	LYS
3	D	217	LEU
3	D	227	PHE
3	D	232	ASN
3	D	248	ASP
3	D	252	LEU
3	D	269	TYR
3	D	289	ASP
3	D	324	LEU
3	D	329	ASP
3	D	332	LYS
3	D	335	GLN
3	D	338	PHE
3	D	339	ARG
3	D	345	LYS
3	D	374	LEU
3	D	384	LYS

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Mol	Chain	Res	Type
3	D	390	LEU
3	D	394	ILE
3	D	413	ASP
3	D	418	GLU
3	D	425	ARG
3	D	430	HIS
3	D	442	ILE
3	D	452	LEU
3	D	453	VAL
3	D	460	ASP
3	D	474	LEU
3	D	506	VAL
3	D	544	LEU
3	D	552	ILE
3	D	567	THR
3	D	571	ASP
3	D	591	ILE
3	D	594	GLN
3	D	596	LEU
3	D	603	LYS
3	D	605	LEU
3	D	648	GLU
3	D	667	GLN
3	D	678	ARG
3	D	684	ASP
3	D	693	VAL
3	D	701	LEU
3	D	708	ASN
3	D	709	ARG
3	D	710	ASP
3	D	716	GLN
3	D	720	ASN
3	D	740	LEU
3	D	756	GLU
3	D	762	ASN
3	D	763	PHE
3	D	764	ARG
3	D	770	LEU
3	D	772	TYR
3	D	773	PHE
3	D	774	ILE
3	D	776	THR

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Mol	Chain	Res	Type
3	D	780	ARG
3	D	783	LEU
3	D	803	VAL
3	D	810	THR
3	D	812	ASP
3	D	823	THR
3	D	840	LEU
3	D	849	LEU
3	D	860	ARG
3	D	878	ASP
3	D	895	CYS
3	D	901	ARG
3	D	972	LYS
3	D	997	VAL
3	D	1011	VAL
3	D	1143	ASP
3	D	1144	LEU
3	D	1155	ILE
3	D	1168	GLU
3	D	1170	LYS
3	D	1186	TYR
3	D	1208	ASP
3	D	1209	VAL
3	D	1222	ARG
3	D	1238	GLN
3	D	1240	VAL
3	D	1244	GLN
3	D	1255	VAL
3	D	1258	ARG
3	D	1289	ASN
3	D	1291	GLU
3	D	1295	ASN
3	D	1305	ASP
3	D	1306	LEU
3	D	1325	PHE
3	D	1329	THR
3	D	1344	LEU
3	D	1353	VAL
3	D	1357	ILE
3	D	1366	HIS
3	D	1370	MET
4	E	3	ARG

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Mol	Chain	Res	Type
4	E	5	THR
4	E	8	ASP
4	E	13	ILE
4	E	16	ARG
4	E	25	ARG
4	E	36	ASP
4	E	42	GLU
4	E	43	ASN
4	E	46	THR
4	E	52	ARG
4	E	59	ILE
5	F	94	THR
5	F	99	ARG
5	F	113	ARG
5	F	118	ASP
5	F	131	GLN
5	F	213	ASP
5	F	223	GLU
5	F	231	THR
5	F	256	PHE
5	F	257	LYS
5	F	266	PHE
5	F	267	ASP
5	F	285	ARG
5	F	300	LYS
5	F	301	ASN
5	F	338	HIS
5	F	360	ASP
5	F	383	ASN
5	F	395	THR
5	F	417	ASP
5	F	421	TYR
5	F	423	ARG
5	F	428	SER
5	F	446	GLN
5	F	448	ARG
5	F	450	ILE
5	F	454	VAL
5	F	472	GLN
5	F	479	THR
5	F	481	GLU
5	F	485	GLU

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Mol	Chain	Res	Type
5	F	486	ARG
5	F	495	ARG
5	F	528	LEU
5	F	544	THR
5	F	559	LEU
5	F	566	ASP
5	F	568	ASN
5	F	569	THR
5	F	573	LEU
5	F	580	PHE
5	F	587	ILE
5	F	599	ARG
5	F	603	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	75	GLN
1	A	84	ASN
1	A	103	ASN
1	A	227	GLN
1	B	18	GLN
1	B	75	GLN
1	B	84	ASN
1	B	127	GLN
1	B	227	GLN
2	C	31	GLN
2	C	69	GLN
2	C	258	ASN
2	C	273	HIS
2	C	494	ASN
2	C	554	HIS
2	C	568	ASN
2	C	573	ASN
2	C	582	ASN
2	C	649	GLN
2	C	658	GLN
2	C	673	HIS
2	C	684	ASN
2	C	686	GLN
2	C	762	ASN

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Mol	Chain	Res	Type
2	C	798	GLN
2	C	834	GLN
2	C	922	ASN
2	C	1080	ASN
2	C	1108	ASN
2	C	1116	HIS
2	C	1134	GLN
2	C	1136	GLN
2	C	1220	GLN
2	C	1244	HIS
2	C	1268	GLN
2	C	1313	HIS
2	C	1314	GLN
3	D	200	GLN
3	D	232	ASN
3	D	294	ASN
3	D	335	GLN
3	D	341	ASN
3	D	365	GLN
3	D	495	ASN
3	D	545	HIS
3	D	560	ASN
3	D	594	GLN
3	D	667	GLN
3	D	669	GLN
3	D	716	GLN
3	D	771	GLN
3	D	777	HIS
3	D	792	ASN
3	D	861	ASN
3	D	875	ASN
3	D	910	ASN
3	D	1023	HIS
3	D	1197	ASN
3	D	1238	GLN
3	D	1244	GLN
3	D	1295	ASN
4	E	31	GLN
4	E	43	ASN
4	E	61	ASN
5	F	227	GLN
5	F	258	GLN

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Mol	Chain	Res	Type
5	F	331	HIS
5	F	342	GLN
5	F	345	GLN
5	F	383	ASN
5	F	464	ASN
5	F	589	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	228/239 (95%)	0.54	23 (10%) 7 6	144, 165, 185, 215	0
1	B	217/239 (90%)	0.07	8 (3%) 41 34	145, 167, 185, 189	0
2	C	1337/1342 (99%)	0.03	17 (1%) 77 70	30, 155, 181, 201	0
3	D	1226/1409 (87%)	0.25	50 (4%) 37 31	144, 160, 192, 206	0
4	E	79/91 (86%)	-0.07	2 (2%) 57 49	146, 154, 181, 188	0
5	F	471/613 (76%)	0.19	43 (9%) 9 7	144, 174, 195, 207	0
6	N	29/29 (100%)	-0.61	0 100 100	112, 180, 203, 205	0
7	T	24/24 (100%)	-0.56	0 100 100	108, 189, 204, 206	0
All	All	3611/3986 (90%)	0.15	143 (3%) 38 32	30, 161, 191, 215	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	GLU	9.2
1	A	89	ALA	8.7
1	A	194	GLN	7.8
5	F	259	PHE	7.2
1	A	90	VAL	6.5
1	A	131	CYS	5.9
1	A	13	ASP	5.2
1	A	88	LEU	5.1
5	F	136	GLU	5.0
3	D	1186	TYR	5.0
5	F	216	LEU	4.4
3	D	1136	GLY	4.4
1	A	143	ARG	4.3
5	F	149	ASN	4.3
3	D	747	MET	4.2
1	B	172	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	16	ILE	4.0
5	F	147	GLN	4.0
1	B	59	VAL	3.9
1	A	144	ILE	3.9
3	D	1204	VAL	3.7
3	D	522	GLY	3.6
5	F	226	ALA	3.6
5	F	256	PHE	3.6
1	A	130	ILE	3.6
2	C	258	ASN	3.6
1	A	142	MET	3.4
3	D	988	PHE	3.4
5	F	265	GLN	3.4
3	D	75	TYR	3.4
5	F	255	VAL	3.4
5	F	163	THR	3.4
1	A	100	LEU	3.3
3	D	732	GLY	3.3
3	D	641	ILE	3.3
3	D	707	ILE	3.3
5	F	213	ASP	3.3
5	F	165	PHE	3.3
2	C	1334	GLY	3.3
5	F	158	LEU	3.3
3	D	1300	ALA	3.2
3	D	1177	ILE	3.2
5	F	613	ASP	3.2
5	F	310	GLU	3.2
3	D	744	ARG	3.2
3	D	178	ALA	3.1
3	D	163	GLU	3.1
3	D	1168	GLU	3.1
3	D	1215	GLU	3.1
3	D	1017	VAL	3.1
3	D	204	GLU	3.1
2	C	232	ILE	3.0
3	D	731	ARG	3.0
2	C	224	PHE	3.0
3	D	217	LEU	2.9
3	D	853	THR	2.9
3	D	1166	GLY	2.9
5	F	162	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	1002	LEU	2.9
3	D	1241	TYR	2.9
3	D	216	LYS	2.9
2	C	1004	ASP	2.8
1	A	146	VAL	2.8
3	D	987	GLU	2.8
5	F	253	SER	2.8
5	F	160	ASP	2.8
3	D	290	ILE	2.7
5	F	254	GLU	2.7
3	D	1341	ARG	2.7
3	D	826	ILE	2.7
3	D	966	VAL	2.7
5	F	146	GLU	2.7
3	D	194	LEU	2.7
5	F	260	ARG	2.7
5	F	161	LEU	2.7
3	D	986	ASP	2.6
2	C	703	GLY	2.6
5	F	157	ARG	2.6
4	E	34	GLY	2.6
3	D	1299	GLY	2.6
3	D	958	ILE	2.6
3	D	1289	ASN	2.6
3	D	1187	GLU	2.6
1	A	110	VAL	2.6
1	A	87	GLY	2.6
3	D	596	LEU	2.5
3	D	1272	SER	2.5
5	F	137	TYR	2.5
2	C	186	PHE	2.5
3	D	1149	ARG	2.5
5	F	476	ARG	2.5
5	F	154	GLU	2.5
1	B	171	LEU	2.5
1	B	96	ASP	2.4
2	C	161	LYS	2.4
5	F	229	VAL	2.4
3	D	1196	LEU	2.4
5	F	145	LEU	2.4
3	D	1165	PHE	2.4
5	F	483	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
5	F	214	PRO	2.4
1	A	145	LYS	2.4
1	B	61	ILE	2.3
5	F	489	MET	2.3
5	F	258	GLN	2.3
5	F	153	ALA	2.3
5	F	143	TYR	2.3
1	A	98	VAL	2.3
3	D	1302	TYR	2.3
3	D	931	THR	2.3
3	D	1198	VAL	2.3
5	F	488	LEU	2.3
5	F	325	PRO	2.2
2	C	659	GLN	2.2
3	D	972	LYS	2.2
2	C	231	GLU	2.2
1	A	173	VAL	2.2
1	B	98	VAL	2.2
3	D	1193	TRP	2.2
1	A	192	VAL	2.2
2	C	172	TYR	2.1
5	F	548	LEU	2.1
2	C	910	ALA	2.1
2	C	783	LEU	2.1
5	F	257	LYS	2.1
1	A	102	LEU	2.1
5	F	284	GLU	2.1
4	E	38	LEU	2.1
1	A	184	ALA	2.1
5	F	148	TYR	2.1
3	D	767	LEU	2.1
1	B	142	MET	2.1
5	F	217	ALA	2.1
1	A	81	ILE	2.1
3	D	179	LYS	2.1
3	D	304	ASP	2.0
5	F	311	THR	2.0
1	B	14	VAL	2.0
3	D	1185	PRO	2.0
5	F	215	GLU	2.0
2	C	979	LEU	2.0
2	C	214	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	C	1149	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	ZN	D	1502	1/1	0.87	0.07	161,161,161,161	0
8	MG	D	1501	1/1	0.94	0.61	144,144,144,144	0
9	ZN	D	1503	1/1	0.95	0.14	160,160,160,160	0

6.5 Other polymers [i](#)

There are no such residues in this entry.