Full wwPDB X-ray Structure Validation Report ⓘ

Dec 23, 2024 – 04:19 PM JST

PDB ID	:	8Y09
Title	:	Crystal structure of LbCas12a in complex with crRNA and 15nt target DNA
Authors	:	Lin, X.; Chen, J.; Liu, L.
Deposited on	:	2024-01-22
Resolution	:	2.87 Å(reported)

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

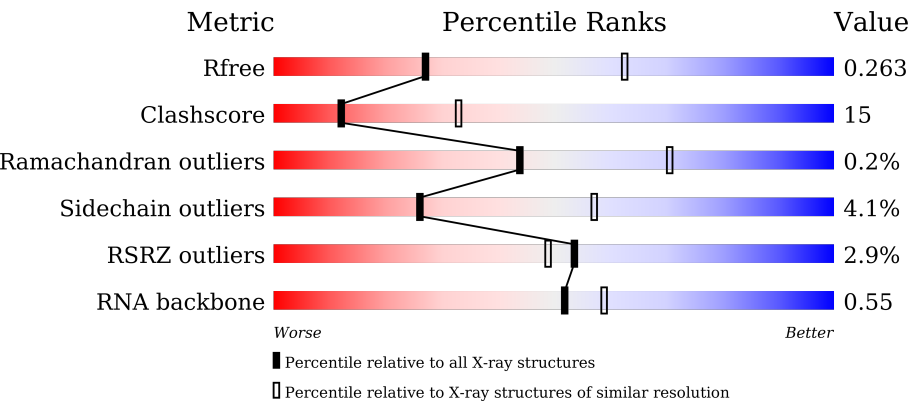|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.87 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	Percentile Ranks	Value
Rfree		0.263
Clashscore		15
Ramachandran outliers		0.2%
Sidechain outliers		4.1%
RSRZ outliers		2.9%
RNA backbone		0.55

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	3316 (2.90-2.86)
Clashscore	180529	3609 (2.90-2.86)
Ramachandran outliers	177936	3529 (2.90-2.86)
Sidechain outliers	177891	3532 (2.90-2.86)
RSRZ outliers	164620	3319 (2.90-2.86)
RNA backbone	3690	1088 (3.10-2.66)

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 <=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	1228	2% · 68% 29% ··
1	E	1228	4% · 66% 30% ··
2	B	40	2% · 28% 40% 15% · 15%
2	F	40	2% · 38% 30% 18% 15%

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Mol	Chain	Length	Quality of chain
3	C	24	8% / 54% / 42%
3	G	24	21% / 50% / 38% / 8%
4	D	11	82% / 18%
4	H	11	18% / 82% / 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	LI	A	1301	-	-	-	X
5	LI	A	1302	-	-	-	X
5	LI	B	101	-	-	-	X
5	LI	E	1301	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 22752 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 LbCas12a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1214	Total 9949	C 6402	N 1626	O 1892	S 29	0	0	0
1	E	1217	Total 9964	C 6409	N 1627	O 1899	S 29	0	0	0

- Molecule 2 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	34	Total 719	C 324	N 128	O 234	P 33	0	0	0
2	F	34	Total 719	C 324	N 128	O 234	P 33	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	23	Total 476	C 226	N 89	O 138	P 23	0	0	0
3	G	23	Total 476	C 226	N 89	O 138	P 23	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*AP*TP* T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total 217	C 107	N 31	O 69	P 10	0	0	0
4	H	11	Total 217	C 107	N 31	O 69	P 10	0	0	0

- Molecule 5 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Li 2	0	0
5	B	1	Total 1	Li 1	0	0
5	E	1	Total 1	Li 1	0	0
5	F	1	Total 1	Li 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total 8	O 8	0	0
6	E	2	Total 2	O 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.
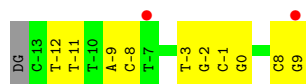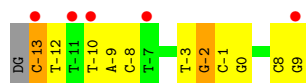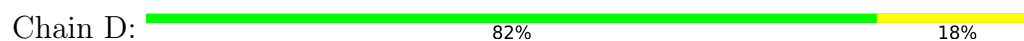
• Molecule 1: LbCas12a

L1135 Q1136 N1139 S1140 I1141 R1144 T1145 D1146 V1147 D1148 F1149 L1150 K1155 N1156 D1163 S1164 W1193 K1199 E1202 D1203 E1204 K1205 L1206 I1211 A1212 I1213 K1216 V1226 LYS HIS

● **Molecule 1: LbCas12a**

4%

Chain E:

66%　　　　30%

M1 S2 K3 L4 E5 K6 F7 L13 R18 I22 P23 V24 T27 R35 L36 L37 K52 Y58 I62 N63 D64 V65 S68 I69 K70 L71 K72 N73 L74 N75 N76 Y77 I78 S79 L80 F81 R82 K83 K84 T85 R86 T87 E88 K89 E90 N91 K92 E93 L94 E95

I99 N100 L101 R102 K103 K110 E113 G114 Y115 K116 S117 L118 F119 K120 K121 D122 I123 I124 E125 T126 I127 L128 P129 E130 F131 L132 D136 F147 F155 E159 F162 S163 K167 S170 I171 R174 R182 Y183 I184 S185 N186 M187 D188 I189 F190 E191 K192 V193

I196 F197 D198 K199 H200 E201 V202 Q203 E204 I205 K206 E207 K208 I209 I210 N211 S212 D213 Y214 D215 V216 E217 D218 G222 E223 F224 F225 N226 F244 V245 T246 E247 E250 K251 I252 K253 G254 L255 N256 E257 Y258 L261 Y262 N263 T266 K267 Q268 K269 L270 P271 K272 P275 L276 Y277

K278 S282 D283 R284 GLU SER LEU SER PHE TYR G291 Y294 T295 S296 D297 L301 E302 V303 F304 R305 N306 T307 L308 N309 I314 F315 I318 K319 F325 K326 N327 F328 D329 S332 S333 V338 K339 N340 S345 T346 I347 K349 D350 I351 F352 G353 E354 W355 N356 V357

I358 R359 D360 K361 W362 N363 A364 E365 Y366 D367 D368 I369 H370 L371 K372 K373 K374 A375 T378 E379 K380 Y381 E382 D383 D384 R385 R386 K387 S388 F389 K390 L397 E398 Q399 L400 Q401 E402 Y403 A406 D407 V410 V411 E412 K413 L414 K415 I419 V422 Y426 Y429 E433

D437 A438 D439 L442 E443 K444 S445 L446 K447 K448 K457 D458 L459 K464 S465 K471 A472 F473 G477 K478 Y487 F490 V491 Y494 L497 H502 N509 T512 Q513 Y516 K522 L523 Y524 F525 Q526 N527 F530 M531 K538 D541 Y542 R543

G550 M558 Y562 K568 K571 D572 D573 V574 N575 G576 N577 P587 K601 W602 Y606 N607 P608 S609 E610 D611 I612 Q613 K614 I615 D625 L629 H633 I636 K640 P647 S650 D654 E659 T660 E661 E675 S686 K687 K688 E689 V690

D691 K698 M701 F702 Y705 N706 S713 N718 T721 D729 E730 N731 G740 G741 A742 R748 L751 E755 H759 I765 T777 V783 V784 K785 D786 K787 E791 D792 P799 C805 P806 I809 T814 V818 L819 L820 K821 I829

R833 G834 E835 R836 N837 L838 V843 N857 E858 F863 D871 Y872 H873 S874 D877 K878 K879 E880 I881 E882 R883 F884 E885 A886 R887 Q888 N889 W890 T891 S892 I893 I896 K897 E898 Y903 I904 K917 Y918 D919 A923 L924 E925 F931 S934 R935 V936 K937 V938

E939 K940 Q941 F946 E947 D952 N955 Q975 F980 E981 S982 F983 K984 S985 M986 I996 W999 D1005 P1006 S1007 K1015 T1016 K1017 Y1018 T1019 S1020 I1021 A1022 D1023 F1027 F1031 D1032 R1033 I1034 M1035 E1039 E1040 D1041 L1042 F1052 A1057 K1064 N1070 R1071

I1072 R1073 I1074 F1075 R1076 N1077 PRO LYS LYS N1081 N1082 W1086 E1087 E1088 L1091 L1098 F1099 Y1102 G1103 I1104 Q1107 Q1118 K1121 A1122 F1123 Y1124 S1126 F1127 M1128 S1132 N1139 S1140 I1141 T1142 T1145 D1146 V1147 D1148 F1149 L1150 Y1162 D1163 S1164 R1165 E1168 A1169 Q1170

E1171 I1187 L1192 I1195 A1201 L1206 D1207 K1216 V1226 LYS HIS

● **Molecule 2: RNA (34-MER)**

Chain B:

• Molecule 2: RNA (34-MER)

Chain F:

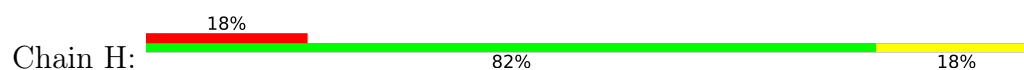• Molecule 3: DNA (5'-D(P*CP*TP*TP*TP*AP*CP*TP*GP*GP*AP*TP*GP*CP*GP*TP*A P*AP*AP*GP*GP*AP*CP*G)-3')

Chain C:

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

Chain G:

• Molecule 4: DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*AP*TP*T)-3')

Chain D:

• Molecule 4: DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*AP*TP*T)-3')

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.15Å 143.40Å 203.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 2.87 49.28 – 2.87	Depositor EDS
% Data completeness (in resolution range)	84.5 (49.28-2.87) 84.7 (49.28-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.204 , 0.267 0.203 , 0.263	Depositor DCC
R_{free} test set	4087 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	50.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.3	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	22752	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.56	4/10158 (0.0%)	0.74	21/13664 (0.2%)
1	E	0.60	5/10172 (0.0%)	0.80	28/13683 (0.2%)
2	B	0.78	0/804	1.39	11/1250 (0.9%)
2	F	0.77	0/804	1.32	7/1250 (0.6%)
3	C	1.04	1/534 (0.2%)	1.13	1/823 (0.1%)
3	G	1.06	2/534 (0.4%)	1.14	0/823
4	D	1.12	0/240	1.27	1/368 (0.3%)
4	H	1.21	0/240	1.22	0/368
All	All	0.64	12/23486 (0.1%)	0.86	69/32229 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	5
All	All	0	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	754	GLU	CB-CG	-8.68	1.35	1.52
1	E	985	SER	CA-C	-7.45	1.33	1.52
1	A	84	LYS	CD-CE	7.25	1.69	1.51
1	A	391	LYS	CD-CE	6.80	1.68	1.51
3	G	-13	DC	C1'-N1	6.72	1.57	1.49
1	E	1171	GLU	CG-CD	-6.29	1.42	1.51
1	E	568	LYS	CD-CE	6.15	1.66	1.51
1	E	359	ARG	CG-CD	5.80	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	-2	DG	C3'-O3'	-5.72	1.36	1.44
1	A	84	LYS	CG-CD	5.57	1.71	1.52
3	C	-3	DT	C3'-O3'	-5.40	1.36	1.44
1	E	354	GLU	CD-OE2	-5.12	1.20	1.25

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	754	GLU	CA-CB-CG	11.32	138.31	113.40
1	A	754	GLU	N-CA-CB	-11.29	90.28	110.60
1	E	381	TYR	CB-CG-CD2	-10.98	114.41	121.00
1	E	261	LEU	CA-CB-CG	9.86	137.97	115.30
1	E	359	ARG	CD-NE-CZ	9.27	136.57	123.60
2	B	-1	U	C5-C4-O4	-9.12	120.43	125.90
1	A	116	LYS	CA-CB-CG	-8.85	93.93	113.40
1	E	359	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	E	284	ARG	NE-CZ-NH1	-8.52	116.04	120.30
1	E	1170	GLN	C-N-CA	8.42	142.75	121.70
1	E	415	LYS	CD-CE-NZ	-7.92	93.47	111.70
1	A	754	GLU	CB-CG-CD	-7.79	93.17	114.20
1	E	937	LYS	CG-CD-CE	7.49	134.37	111.90
1	A	267	LYS	CD-CE-NZ	-7.41	94.65	111.70
2	B	-1	U	N3-C4-O4	7.37	124.56	119.40
2	B	0	C	O4'-C1'-N1	7.36	114.09	108.20
1	E	654	ASP	CB-CG-OD2	7.34	124.90	118.30
1	A	931	PHE	N-CA-CB	7.28	123.71	110.60
1	A	1146	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	E	381	TYR	CB-CG-CD1	7.26	125.36	121.00
1	E	863	PHE	CB-CG-CD2	-7.17	115.78	120.80
2	B	-5	U	O5'-P-OP2	-7.13	99.28	105.70
1	E	863	PHE	CB-CG-CD1	7.12	125.78	120.80
1	E	1171	GLU	N-CA-CB	-7.03	97.94	110.60
2	F	-1	U	N3-C4-O4	7.02	124.31	119.40
1	E	92	LYS	CD-CE-NZ	6.95	127.67	111.70
1	A	1104	ILE	CA-CB-CG1	6.75	123.83	111.00
1	E	383	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	940	LYS	CD-CE-NZ	6.56	126.78	111.70
2	F	-14	U	C5-C4-O4	-6.50	122.00	125.90
1	E	35	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	F	-19	A	N9-C4-C5	6.37	108.35	105.80
1	A	1141	ILE	CG1-CB-CG2	6.35	125.38	111.40
2	B	-20	A	O4'-C1'-N9	6.33	113.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	247	GLU	N-CA-CB	-6.03	99.75	110.60
1	E	389	PHE	CB-CG-CD1	5.97	124.98	120.80
1	A	267	LYS	CA-CB-CG	-5.96	100.29	113.40
1	E	661	GLU	CA-CB-CG	-5.94	100.32	113.40
2	B	0	C	N1-C2-O2	5.88	122.43	118.90
2	B	-6	G	N3-C4-N9	5.88	129.53	126.00
1	E	568	LYS	CD-CE-NZ	5.86	125.19	111.70
1	E	354	GLU	OE1-CD-OE2	5.84	130.31	123.30
1	A	450	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	754	GLU	CB-CA-C	5.81	122.01	110.40
2	F	-19	A	N1-C6-N6	-5.68	115.19	118.60
1	E	1074	ILE	CG1-CB-CG2	-5.68	98.91	111.40
2	F	-1	U	C5-C4-O4	-5.64	122.51	125.90
2	B	-6	G	C8-N9-C1'	-5.61	119.71	127.00
2	B	-6	G	C4-N9-C1'	5.60	133.78	126.50
1	A	26	LYS	CA-CB-CG	5.55	125.60	113.40
1	E	985	SER	CA-C-O	-5.44	108.68	120.10
1	A	931	PHE	CB-CA-C	-5.37	99.65	110.40
1	E	354	GLU	CA-CB-CG	-5.37	101.59	113.40
2	B	6	C	OP2-P-O3'	5.36	116.99	105.20
1	A	74	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	292	GLU	CG-CD-OE1	-5.32	107.66	118.30
1	A	931	PHE	CB-CG-CD2	-5.28	117.11	120.80
1	E	1146	ASP	CB-CG-OD2	-5.24	113.59	118.30
2	F	-4	A	C5-C6-N6	-5.15	119.58	123.70
1	E	661	GLU	N-CA-CB	-5.15	101.34	110.60
1	E	384	ASP	CB-CG-OD1	5.14	122.93	118.30
2	B	-20	A	C2-N3-C4	5.10	113.15	110.60
3	C	-3	DT	O4'-C4'-C3'	-5.08	102.47	104.50
2	F	0	C	N1-C2-O2	5.07	121.94	118.90
1	A	103	LYS	CD-CE-NZ	5.07	123.35	111.70
4	D	-6	DC	O4'-C1'-N1	5.07	111.55	108.00
1	A	762	ASN	C-N-CA	-5.04	109.09	121.70
1	E	985	SER	N-CA-CB	5.04	118.06	110.50
1	A	292	GLU	CA-CB-CG	-5.01	102.38	113.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	VAL	Peptide
1	E	1087	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	E	284	ARG	Sidechain
1	E	381	TYR	Sidechain
1	E	705	TYR	Peptide
1	E	93	GLU	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9949	0	9787	287	0
1	E	9964	0	9793	356	0
2	B	719	0	366	19	0
2	F	719	0	366	21	0
3	C	476	0	260	7	0
3	G	476	0	260	9	0
4	D	217	0	129	1	0
4	H	217	0	129	1	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	8	0	0	0	0
6	E	2	0	0	1	0
All	All	22752	0	21090	672	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 15.

All (672) 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:E:361:LYS:HD2	1:E:403:TYR:CD1	1.47	1.46
1:A:278:LYS:HE2	2:B:6:C:OP1	1.22	1.36
1:E:983:PHE:CE1	1:E:986:MET:HE2	1.75	1.22
1:E:370:HIS:HB3	1:E:381:TYR:OH	1.44	1.15
1:A:174:ARG:NH2	1:A:277:TYR:HB3	1.62	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:LYS:CD	1:E:403:TYR:CD1	2.37	1.08
1:E:387:LYS:HZ3	1:E:390:LYS:HE2	1.18	1.05
1:E:284:ARG:NH2	3:G:-10:DT:OP2	1.91	1.02
1:E:369:ILE:HD12	1:E:370:HIS:CD2	1.97	1.00
1:A:1193:TRP:CD2	1:A:1213:ILE:HD12	1.98	0.98
1:A:1193:TRP:CE3	1:A:1213:ILE:HD12	1.99	0.97
1:E:706:ASN:HD21	1:E:721:THR:HG22	1.30	0.95
1:A:174:ARG:NH1	2:B:6:C:O3'	1.99	0.95
1:E:387:LYS:HZ3	1:E:390:LYS:CE	1.79	0.94
1:A:1193:TRP:CD2	1:A:1213:ILE:CD1	2.50	0.94
1:A:278:LYS:CE	2:B:6:C:OP1	2.16	0.92
1:E:983:PHE:CE1	1:E:986:MET:CE	2.54	0.91
1:E:253:LYS:HG2	1:E:257:GLU:HG2	1.51	0.91
1:E:27:THR:HG21	1:E:701:MET:H	1.34	0.90
1:E:201:GLU:OE1	1:E:258:TYR:CZ	2.25	0.90
1:E:370:HIS:CB	1:E:381:TYR:OH	2.19	0.89
1:A:1026:LYS:HE2	1:A:1030:SER:OG	1.74	0.88
1:E:675:GLU:OE2	1:E:805:CYS:SG	2.32	0.87
1:A:930:GLY:O	1:A:940:LYS:NZ	2.08	0.86
1:E:369:ILE:CD1	1:E:370:HIS:CD2	2.59	0.86
1:A:256:ASN:HD21	1:A:273:PHE:H	1.20	0.85
1:A:174:ARG:NH2	1:A:278:LYS:O	2.10	0.84
1:A:1016:THR:OG1	1:A:1132:SER:OG	1.95	0.83
1:E:80:LEU:HB3	1:E:94:LEU:HD12	1.60	0.83
1:E:1040:GLU:O	1:E:1042:LEU:HD13	1.77	0.82
1:E:1150:LEU:H	1:E:1164:SER:HB3	1.43	0.82
1:A:1193:TRP:CE3	1:A:1213:ILE:CD1	2.61	0.82
1:A:752:LYS:HD3	1:A:754:GLU:OE1	1.81	0.81
1:E:361:LYS:HD2	1:E:403:TYR:CE1	2.15	0.81
1:A:988:THR:HB	1:A:1211:ILE:HD11	1.63	0.79
1:E:983:PHE:HE1	1:E:986:MET:HE2	1.45	0.79
1:A:525:PHE:O	1:A:543:ARG:NH2	2.16	0.78
1:E:182:ARG:NH1	1:E:275:PRO:O	2.16	0.78
1:E:1140:SER:HB3	1:E:1148:ASP:HA	1.66	0.78
1:E:806:PRO:O	6:E:1401:HOH:O	2.01	0.78
1:E:203:GLN:HA	1:E:206:LYS:HB3	1.65	0.78
1:E:1087:GLU:HG2	1:E:1088:GLU:H	1.47	0.78
1:E:361:LYS:HD2	1:E:403:TYR:CG	2.16	0.77
1:E:387:LYS:NZ	1:E:390:LYS:HE2	1.97	0.77
1:E:885:GLU:O	1:E:889:ASN:HB2	1.83	0.77
1:A:467:GLU:OE1	1:A:497:LEU:HB3	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:538:LYS:CE	1:E:541:ASP:OD2	2.34	0.76
1:A:27:THR:HG23	1:A:694:VAL:HG13	1.66	0.76
1:A:931:PHE:HA	1:A:940:LYS:HE3	1.66	0.76
1:A:1140:SER:OG	1:A:1148:ASP:HA	1.85	0.76
1:E:87:THR:OG1	1:E:89:LYS:HB2	1.86	0.75
1:E:675:GLU:OE2	1:E:805:CYS:CB	2.34	0.75
1:E:525:PHE:O	1:E:543:ARG:NH2	2.20	0.75
2:F:10:A:N6	3:G:-10:DT:O4	2.19	0.74
1:E:90:GLU:HA	1:E:93:GLU:HB2	1.68	0.74
1:A:577:ASN:HD22	1:A:687:LYS:H	1.35	0.74
1:A:182:ARG:HE	1:A:274:LYS:HB3	1.51	0.74
1:E:573:ASP:O	1:E:577:ASN:ND2	2.20	0.73
1:E:983:PHE:HE1	1:E:986:MET:CE	1.96	0.73
1:E:366:TYR:CE2	1:E:370:HIS:ND1	2.56	0.72
1:A:467:GLU:OE1	1:A:497:LEU:CG	2.37	0.72
1:E:1027:PHE:HD1	1:E:1128:MET:CE	2.02	0.72
1:E:471:LYS:HE3	1:E:494:TYR:OH	1.89	0.71
1:A:483:ASP:OD2	1:A:485:SER:HB3	1.90	0.71
1:E:882:GLU:HA	1:E:885:GLU:HB3	1.71	0.71
1:E:326:LYS:O	1:E:415:LYS:NZ	2.23	0.71
1:A:401:GLN:HG2	1:A:410:VAL:HG22	1.70	0.71
1:E:361:LYS:NZ	1:E:403:TYR:HD1	1.89	0.71
1:E:366:TYR:HE2	1:E:370:HIS:HD1	1.37	0.70
2:F:-10:A:H5'	2:F:-8:G:N1	2.07	0.70
1:A:576:GLY:O	1:A:577:ASN:ND2	2.25	0.69
1:E:198:ASP:O	1:E:201:GLU:HB3	1.91	0.69
1:E:314:ILE:HD12	1:E:314:ILE:H	1.58	0.69
1:E:1033:ARG:HH21	1:E:1035:MET:CE	2.05	0.69
1:E:263:ASN:ND2	1:E:270:LEU:H	1.90	0.69
1:E:359:ARG:NH2	1:E:386:ARG:HA	2.08	0.69
1:A:1104:ILE:HG12	1:A:1118:GLN:NE2	2.08	0.68
1:E:1033:ARG:HE	1:E:1035:MET:HE3	1.58	0.68
1:A:467:GLU:OE1	1:A:497:LEU:CB	2.41	0.68
1:A:1202:GLU:HB2	1:A:1205:LYS:HE3	1.76	0.68
1:E:675:GLU:OE2	1:E:805:CYS:HB2	1.93	0.68
1:E:361:LYS:NZ	1:E:403:TYR:CD1	2.62	0.67
1:A:577:ASN:ND2	1:A:687:LYS:H	1.91	0.67
1:E:448:LYS:HG3	1:E:755:GLU:HB3	1.76	0.67
1:E:538:LYS:HE3	1:E:541:ASP:OD2	1.95	0.67
1:E:897:LYS:HG3	1:E:898:GLU:HG3	1.77	0.67
1:A:1150:LEU:H	1:A:1164:SER:HB3	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:ASP:HB3	1:E:201:GLU:HB2	1.76	0.66
1:E:352:PHE:HB2	1:E:357:VAL:HG11	1.78	0.66
1:E:369:ILE:HD12	1:E:370:HIS:HD2	1.55	0.66
1:A:207:GLU:OE2	1:A:212:SER:OG	2.13	0.66
1:E:401:GLN:NE2	1:E:410:VAL:HG12	2.11	0.66
1:E:917:LYS:HD3	1:E:918:TYR:CE2	2.31	0.66
1:A:467:GLU:OE1	1:A:497:LEU:HG	1.96	0.66
1:E:1033:ARG:HE	1:E:1035:MET:CE	2.09	0.66
1:E:531:MET:HG2	1:E:742:ALA:HB3	1.78	0.66
1:E:401:GLN:HE21	1:E:410:VAL:HG12	1.60	0.66
1:E:301:LEU:HD11	1:E:442:LEU:CD1	2.26	0.66
1:E:361:LYS:HD2	1:E:403:TYR:HD1	1.50	0.65
1:E:379:GLU:O	1:E:383:ASP:HB2	1.96	0.65
1:E:937:LYS:O	1:E:941:GLN:HG3	1.96	0.65
1:A:1076:ARG:HH11	1:A:1076:ARG:HB2	1.61	0.65
1:A:1076:ARG:HB2	1:A:1076:ARG:NH1	2.11	0.65
1:E:370:HIS:C	1:E:381:TYR:OH	2.35	0.65
1:A:71:LEU:HB2	1:A:74:LEU:HB2	1.79	0.65
1:E:245:VAL:HA	1:E:250:GLU:O	1.97	0.65
1:E:205:ILE:HG23	1:E:209:ILE:HD12	1.78	0.64
1:E:387:LYS:NZ	1:E:390:LYS:NZ	2.46	0.64
1:E:202:VAL:HB	1:E:216:VAL:HG11	1.78	0.64
1:E:538:LYS:HE2	1:E:541:ASP:HB2	1.79	0.64
1:A:315:PHE:HA	1:A:318:ILE:HD12	1.78	0.64
1:E:58:TYR:O	1:E:62:ILE:HG13	1.98	0.64
1:E:74:LEU:HD21	1:E:225:PHE:HB3	1.78	0.64
1:A:301:LEU:HD11	1:A:442:LEU:HG	1.80	0.63
1:A:301:LEU:HD22	1:A:435:LEU:HD21	1.80	0.63
1:E:378:THR:HG22	1:E:380:LYS:H	1.63	0.63
1:E:263:ASN:HD21	1:E:270:LEU:H	1.44	0.63
1:A:833:ARG:NH1	1:A:940:LYS:HG3	2.14	0.63
1:E:419:ILE:HA	1:E:422:VAL:HG12	1.80	0.62
1:E:740:GLY:O	1:E:799:PRO:HG2	1.99	0.62
1:E:208:LYS:HD2	1:E:252:ILE:HD11	1.80	0.62
1:A:305:ARG:O	1:A:309:ASN:ND2	2.31	0.62
1:E:359:ARG:CG	1:E:363:ASN:HD21	2.12	0.62
1:E:1027:PHE:HD1	1:E:1128:MET:HE2	1.64	0.62
1:E:1168:GLU:HG3	1:E:1169:ALA:N	2.13	0.62
1:E:246:THR:HG22	1:E:247:GLU:H	1.63	0.62
1:A:350:ASP:HB3	1:A:417:ILE:HD13	1.81	0.62
1:E:262:TYR:O	1:E:266:THR:OG1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD21	1:A:240:ILE:HD11	1.82	0.61
1:E:78:ILE:HG12	1:E:184:ILE:HD11	1.82	0.61
1:E:718:ASN:HB2	1:E:721:THR:HG23	1.82	0.61
1:E:538:LYS:HE2	1:E:541:ASP:CB	2.31	0.61
1:E:1021:ILE:HD11	1:E:1121:LYS:HB3	1.83	0.61
1:E:359:ARG:HG2	1:E:363:ASN:HD21	1.66	0.61
1:A:174:ARG:HH21	1:A:277:TYR:HB3	1.60	0.61
1:A:314:ILE:HG23	1:A:497:LEU:HD12	1.83	0.61
1:E:380:LYS:O	1:E:383:ASP:HB3	2.00	0.61
1:E:387:LYS:HZ3	1:E:390:LYS:NZ	1.98	0.61
1:E:934:SER:HA	1:E:937:LYS:HB2	1.83	0.61
1:A:174:ARG:HH22	1:A:278:LYS:N	1.99	0.61
1:A:434:LYS:HA	1:A:437:ASP:OD1	2.00	0.61
1:A:336:ILE:CD1	1:A:486:PHE:CD2	2.84	0.61
2:F:9:U:H2'	2:F:10:A:H8	1.66	0.61
1:E:387:LYS:NZ	1:E:390:LYS:CE	2.59	0.60
1:A:882:GLU:OE1	1:A:894:GLU:HG3	2.00	0.60
1:E:1019:THR:OG1	1:E:1023:ASP:HB2	2.01	0.60
1:E:201:GLU:OE1	1:E:258:TYR:CE1	2.53	0.60
1:E:301:LEU:HD11	1:E:442:LEU:HD12	1.84	0.60
1:E:82:ARG:NH2	1:E:191:GLU:OE1	2.34	0.60
1:A:27:THR:CG2	1:A:694:VAL:HG13	2.32	0.60
1:A:886:ALA:HB1	1:A:891:THR:O	2.01	0.60
1:A:333:SER:HB2	1:A:398:GLU:HG2	1.83	0.60
1:E:371:LEU:HD22	1:E:372:LYS:N	2.17	0.60
1:A:268:GLN:OE1	1:A:269:LYS:HD2	2.01	0.59
1:E:821:LYS:HE2	1:E:1201:ALA:O	2.01	0.59
1:A:278:LYS:HE2	2:B:6:C:P	2.37	0.59
1:A:1193:TRP:CE2	1:A:1213:ILE:HD12	2.36	0.59
1:E:983:PHE:HB3	1:E:984:LYS:HA	1.83	0.59
1:E:538:LYS:CE	1:E:541:ASP:CG	2.71	0.59
1:E:319:LYS:HD3	1:E:426:TYR:OH	2.03	0.59
3:C:-12:DT:H2'	3:C:-11:DT:C6	2.38	0.59
1:E:349:LYS:HD2	1:E:355:TRP:HB3	1.85	0.59
1:E:706:ASN:ND2	1:E:721:THR:HG22	2.11	0.59
2:B:-10:A:H5'	2:B:-8:G:N1	2.18	0.59
1:E:80:LEU:HD22	1:E:94:LEU:HB2	1.85	0.59
1:A:444:LYS:HB2	1:A:449:ASN:HB2	1.85	0.58
1:E:1087:GLU:HG2	1:E:1088:GLU:N	2.15	0.58
1:A:1007:SER:O	1:A:1226:VAL:HG11	2.04	0.58
1:E:362:TRP:CH2	1:E:366:TYR:HD1	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:925:GLU:HG3	1:E:1187:ILE:HD11	1.85	0.58
1:E:1018:TYR:CD1	1:E:1125:SER:HA	2.39	0.58
1:E:174:ARG:NH2	1:E:278:LYS:O	2.36	0.58
1:E:904:ILE:HD12	1:E:946:PHE:HB2	1.85	0.58
1:A:374:LYS:HE2	1:A:374:LYS:N	2.18	0.58
1:E:367:ASP:OD1	1:E:385:ARG:NH1	2.37	0.58
1:A:522:LYS:HD3	1:A:524:TYR:CZ	2.39	0.58
1:E:1165:ARG:O	1:E:1168:GLU:HG2	2.04	0.57
1:E:113:GLU:HG3	1:E:114:GLY:N	2.19	0.57
1:E:361:LYS:CE	1:E:403:TYR:HD1	2.17	0.57
1:E:836:ARG:HD2	1:E:1148:ASP:OD1	2.04	0.57
1:A:467:GLU:CD	1:A:497:LEU:HB3	2.24	0.57
1:A:1193:TRP:CZ3	1:A:1213:ILE:HD12	2.37	0.57
1:A:606:TYR:O	1:A:608:PRO:HD3	2.04	0.57
1:E:359:ARG:NH1	1:E:389:PHE:CB	2.67	0.57
1:E:401:GLN:HE22	1:E:410:VAL:H	1.52	0.57
1:E:437:ASP:OD2	1:E:438:ALA:N	2.36	0.57
1:E:362:TRP:CZ3	1:E:389:PHE:HB2	2.40	0.57
1:E:345:SER:OG	1:E:355:TRP:HB2	2.03	0.57
1:E:538:LYS:HE2	1:E:541:ASP:OD2	2.04	0.57
1:E:606:TYR:O	1:E:608:PRO:HD3	2.04	0.57
1:E:879:LYS:HB3	1:E:896:ILE:CD1	2.34	0.57
1:E:80:LEU:HB3	1:E:94:LEU:CD1	2.33	0.57
1:A:291:GLY:HA3	1:A:502:HIS:CE1	2.40	0.57
1:A:292:GLU:HG3	1:A:293:GLY:H	1.69	0.57
1:E:62:ILE:HD13	1:E:171:ILE:HD11	1.87	0.57
1:E:326:LYS:HA	1:E:415:LYS:CD	2.35	0.57
1:E:601:LYS:HG2	1:E:602:TRP:CD1	2.39	0.57
1:A:27:THR:HG21	1:A:701:MET:H	1.70	0.56
1:A:336:ILE:HD12	1:A:486:PHE:CD2	2.40	0.56
1:A:442:LEU:HD11	1:A:446:LEU:HD13	1.87	0.56
3:G:-2:DG:H2'	3:G:-1:DC:C6	2.40	0.56
1:E:187:MET:CE	1:E:222:GLY:HA2	2.35	0.56
1:E:487:TYR:O	1:E:491:VAL:HG12	2.04	0.56
1:E:740:GLY:O	3:G:0:DG:H2''	2.05	0.56
1:E:879:LYS:HB3	1:E:896:ILE:HD11	1.88	0.56
2:F:-15:C:H2'	2:F:-14:U:C6	2.41	0.56
1:E:359:ARG:HH12	1:E:389:PHE:CB	2.18	0.56
1:E:207:GLU:HG3	1:E:208:LYS:HG3	1.87	0.56
1:E:291:GLY:HA3	1:E:502:HIS:CE1	2.40	0.56
1:E:304:PHE:CZ	1:E:459:LEU:HD23	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:GLU:O	1:E:402:GLU:HG3	2.06	0.56
1:E:3:LYS:HG2	1:E:819:LEU:HB3	1.87	0.56
1:E:307:THR:O	1:E:314:ILE:HD13	2.06	0.56
1:A:174:ARG:HH11	2:B:6:C:H4'	1.71	0.55
1:A:837:ASN:OD1	1:A:855:SER:OG	2.15	0.55
1:A:1:MET:HB3	1:E:2:SER:HA	1.89	0.55
1:A:576:GLY:N	2:F:-9:A:N1	2.40	0.55
1:A:639:PHE:O	1:A:643:ILE:HG13	2.05	0.55
1:A:328:PHE:CZ	1:A:397:LEU:HD11	2.42	0.55
1:E:361:LYS:CE	1:E:403:TYR:CD1	2.88	0.55
2:F:9:U:H2'	2:F:10:A:C8	2.42	0.55
1:E:353:GLY:C	1:E:354:GLU:HG3	2.21	0.55
1:E:187:MET:HE1	1:E:222:GLY:HA2	1.88	0.55
1:E:359:ARG:HH12	1:E:389:PHE:HB3	1.72	0.55
1:A:1024:SER:O	1:A:1028:ILE:HG13	2.07	0.55
1:A:498:LEU:HD11	2:B:13:G:H4'	1.89	0.54
1:A:686:SER:OG	1:A:689:GLU:HG3	2.08	0.54
1:A:65:VAL:O	1:A:69:ILE:HG13	2.07	0.54
1:E:95:GLU:O	1:E:99:ILE:HG13	2.07	0.54
1:E:359:ARG:NH1	1:E:389:PHE:HB3	2.23	0.54
1:E:759:HIS:HB2	1:E:783:VAL:HG22	1.90	0.54
1:A:904:ILE:HD12	1:A:946:PHE:HB2	1.90	0.54
1:A:1075:PHE:CD1	1:A:1085:ASP:HA	2.41	0.54
2:B:6:C:H2'	2:B:7:A:C8	2.42	0.54
1:A:1031:PHE:O	1:A:1112:ARG:NH1	2.40	0.54
1:E:196:ILE:HG23	1:E:262:TYR:CD1	2.42	0.54
1:E:883:ARG:HH11	1:E:893:ILE:HG22	1.72	0.54
1:A:171:ILE:HG23	1:A:279:GLN:HE22	1.71	0.54
1:A:305:ARG:NH1	1:A:437:ASP:O	2.41	0.54
1:A:428:VAL:HG11	1:A:459:LEU:HA	1.90	0.54
1:E:371:LEU:HD22	1:E:372:LYS:H	1.73	0.54
1:A:2:SER:HA	1:E:1:MET:HE2	1.90	0.54
1:A:512:THR:O	1:A:893:ILE:HG12	2.08	0.54
1:A:689:GLU:O	1:A:693:LEU:HG	2.08	0.54
1:E:278:LYS:HE2	2:F:6:C:OP1	2.06	0.54
2:F:-15:C:H2'	2:F:-14:U:H6	1.73	0.54
1:E:1071:ARG:O	1:E:1088:GLU:HB2	2.08	0.54
1:A:22:ILE:O	1:A:702:PHE:HA	2.08	0.53
1:E:1107:GLN:OE1	1:E:1107:GLN:N	2.33	0.53
1:A:467:GLU:OE2	1:A:497:LEU:HB3	2.08	0.53
1:E:512:THR:O	1:E:893:ILE:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LYS:HA	1:A:383:ASP:CB	2.38	0.53
1:A:543:ARG:HG2	1:A:558:MET:HB2	1.89	0.53
1:A:1193:TRP:CE3	1:A:1213:ILE:HD13	2.43	0.53
1:E:110:LYS:NZ	1:E:162:PHE:O	2.41	0.53
1:A:837:ASN:HA	1:A:857:ASN:HD21	1.72	0.53
1:E:1039:GLU:OE1	1:E:1039:GLU:N	2.35	0.53
1:E:1040:GLU:HB3	1:E:1042:LEU:HD22	1.91	0.53
1:E:325:PHE:HE1	1:E:473:PHE:CE2	2.27	0.53
1:E:328:PHE:CZ	1:E:397:LEU:HD11	2.44	0.53
1:A:1140:SER:OG	1:A:1147:VAL:O	2.27	0.53
1:E:301:LEU:O	1:E:305:ARG:HG3	2.09	0.53
1:E:522:LYS:HD3	1:E:524:TYR:CZ	2.43	0.53
1:A:514:LYS:HE3	1:A:517:SER:HA	1.91	0.52
1:E:22:ILE:O	1:E:702:PHE:HA	2.09	0.52
1:E:361:LYS:CD	1:E:403:TYR:HD1	2.14	0.52
1:E:609:SER:O	1:E:613:GLN:HG3	2.09	0.52
1:A:423:ASP:O	1:A:427:LYS:NZ	2.29	0.52
1:E:215:ASP:O	1:E:218:ASP:HB2	2.09	0.52
2:B:9:U:H2'	2:B:10:A:H8	1.74	0.52
1:E:131:PHE:HD2	1:E:132:LEU:HD23	1.74	0.52
1:E:1070:ASN:OD1	1:E:1070:ASN:N	2.42	0.52
1:A:836:ARG:HE	1:A:1145:THR:HA	1.75	0.52
1:A:246:THR:HG23	1:A:252:ILE:HD11	1.92	0.52
1:A:376:VAL:O	1:A:377:VAL:HG13	2.09	0.52
1:E:366:TYR:HE2	1:E:370:HIS:ND1	2.00	0.52
2:F:6:C:H2'	2:F:7:A:C8	2.44	0.52
1:A:119:PHE:HB3	1:A:155:PHE:HB3	1.90	0.52
1:A:253:LYS:HG2	1:A:257:GLU:HG2	1.89	0.52
1:A:1075:PHE:HB2	1:A:1085:ASP:HB2	1.92	0.52
1:E:253:LYS:HD3	1:E:258:TYR:CE1	2.45	0.52
1:E:359:ARG:HH22	1:E:386:ARG:HA	1.74	0.52
1:A:201:GLU:HG2	1:A:258:TYR:CZ	2.45	0.52
1:A:571:LYS:HD2	1:A:577:ASN:OD1	2.10	0.52
1:A:931:PHE:HA	1:A:940:LYS:CE	2.37	0.52
1:A:292:GLU:CG	1:A:293:GLY:H	2.23	0.51
1:A:372:LYS:HD2	1:A:373:LYS:H	1.74	0.51
1:E:155:PHE:O	1:E:159:GLU:HG3	2.09	0.51
1:E:538:LYS:HE2	1:E:541:ASP:CG	2.30	0.51
1:E:185:SER:O	1:E:189:ILE:HG13	2.10	0.51
4:H:-5:DC:H2'	4:H:-4:DT:H71	1.92	0.51
1:A:1075:PHE:HB2	1:A:1085:ASP:CA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:GLN:NE2	1:E:410:VAL:H	2.08	0.51
1:E:686:SER:HB3	1:E:689:GLU:HB2	1.93	0.51
1:E:809:ILE:HG13	1:E:809:ILE:O	2.11	0.51
1:E:457:LYS:HD2	1:E:890:TRP:CG	2.45	0.51
1:E:1139:ASN:HB2	1:E:1149:PHE:CE1	2.45	0.51
1:A:268:GLN:HG3	1:A:269:LYS:H	1.76	0.51
3:C:-2:DG:H2'	3:C:-1:DC:C6	2.46	0.51
1:A:457:LYS:HE3	1:A:461:ASP:OD2	2.11	0.51
1:E:121:LYS:NZ	1:E:125:GLU:OE1	2.43	0.51
1:E:208:LYS:NZ	1:E:250:GLU:OE1	2.28	0.51
1:A:1:MET:HE3	1:E:2:SER:HA	1.93	0.51
1:A:380:LYS:HA	1:A:383:ASP:HB2	1.93	0.51
1:A:933:ASN:OD1	1:A:934:SER:N	2.44	0.51
1:E:365:GLU:O	1:E:368:ASP:HB2	2.11	0.51
1:E:829:ILE:HG12	1:E:843:VAL:HG22	1.92	0.51
1:E:872:TYR:CD1	1:E:903:TYR:HB2	2.45	0.51
1:A:310:LYS:NZ	1:A:433:GLU:HG3	2.26	0.50
1:A:443:GLU:OE2	1:A:449:ASN:ND2	2.42	0.50
1:E:1027:PHE:HD1	1:E:1128:MET:HE1	1.74	0.50
1:A:527:ASN:HB3	1:A:530:PHE:HB2	1.92	0.50
1:A:785:LYS:HB2	2:B:-20:A:H5"	1.92	0.50
1:A:1021:ILE:H	1:A:1021:ILE:HD12	1.76	0.50
1:A:1075:PHE:HD1	1:A:1085:ASP:HA	1.76	0.50
1:A:579:GLU:HB3	1:A:682:PHE:HB3	1.92	0.50
2:B:9:U:H2'	2:B:10:A:C8	2.46	0.50
1:A:1066:TYR:CZ	1:A:1155:LYS:HE3	2.46	0.50
1:E:1104:ILE:HD11	1:E:1118:GLN:HG3	1.94	0.50
1:E:193:VAL:HG12	1:E:270:LEU:HD13	1.93	0.50
1:A:434:LYS:O	1:A:440:PHE:HB2	2.11	0.50
1:E:198:ASP:OD1	1:E:199:LYS:N	2.45	0.50
1:E:366:TYR:HD2	1:E:366:TYR:O	1.95	0.50
1:A:522:LYS:NZ	1:A:743:GLU:HG2	2.27	0.50
1:E:574:VAL:HA	1:E:577:ASN:HB2	1.94	0.50
1:A:7:PHE:HB3	1:A:975:GLN:O	2.12	0.50
1:A:74:LEU:O	1:A:78:ILE:HG13	2.12	0.50
1:A:322:GLU:HG3	1:A:422:VAL:HG21	1.94	0.50
1:A:477:GLY:CA	1:A:478:LYS:HB2	2.42	0.50
1:E:294:TYR:OH	1:E:303:VAL:HG11	2.12	0.50
1:E:188:ASP:O	1:E:192:LYS:HD3	2.11	0.49
1:A:578:TYR:CE2	1:A:687:LYS:HG3	2.47	0.49
1:A:753:LYS:HA	1:A:756:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:527:ASN:HB3	1:E:530:PHE:HB2	1.94	0.49
1:E:1141:ILE:HD12	1:E:1142:THR:H	1.77	0.49
1:E:429:TYR:O	1:E:433:GLU:HG2	2.12	0.49
1:A:566:LEU:HD11	1:A:699:LEU:HD13	1.95	0.49
1:A:570:ASP:OD1	1:A:571:LYS:N	2.45	0.49
1:E:362:TRP:CH2	1:E:389:PHE:HB2	2.48	0.49
1:A:325:PHE:HE1	1:A:473:PHE:HE2	1.61	0.49
1:E:935:ARG:O	1:E:938:VAL:HG22	2.13	0.49
1:A:256:ASN:ND2	1:A:272:LYS:HB2	2.28	0.49
1:A:295:THR:OG1	1:A:296:SER:N	2.46	0.49
1:A:299:GLU:O	1:A:303:VAL:HG12	2.13	0.49
1:E:163:SER:O	1:E:170:SER:OG	2.28	0.49
1:E:305:ARG:O	1:E:309:ASN:HB3	2.12	0.49
1:A:406:ALA:HA	1:A:407:ASP:HA	1.52	0.49
1:A:983:PHE:HB3	1:A:984:LYS:HA	1.94	0.49
1:E:328:PHE:CD1	1:E:411:VAL:HG23	2.47	0.49
1:E:349:LYS:HB3	1:E:355:TRP:N	2.27	0.49
1:A:339:LYS:HB2	1:A:475:GLY:HA2	1.95	0.48
1:A:496:ILE:O	1:A:499:LYS:HG3	2.13	0.48
1:A:821:LYS:O	1:A:1199:LYS:HE2	2.13	0.48
1:A:1026:LYS:O	1:A:1030:SER:OG	2.25	0.48
1:E:1033:ARG:HH21	1:E:1035:MET:HE3	1.75	0.48
1:E:406:ALA:HB1	1:E:407:ASP:OD2	2.13	0.48
1:E:748:ARG:NH1	1:E:792:ASP:OD2	2.41	0.48
1:E:838:LEU:HD23	1:E:939:GLU:HG3	1.95	0.48
1:A:740:GLY:O	3:C:0:DG:H2"	2.14	0.48
1:E:1016:THR:HB	1:E:1132:SER:OG	2.13	0.48
1:A:386:ARG:O	1:A:390:LYS:HG2	2.13	0.48
1:A:982:SER:HB2	1:A:983:PHE:CD2	2.48	0.48
1:E:326:LYS:HA	1:E:415:LYS:HD2	1.96	0.48
1:E:1005:ASP:OD1	1:E:1007:SER:N	2.47	0.48
2:F:-9:A:H4'	2:F:-8:G:C8	2.47	0.48
1:A:1193:TRP:CG	1:A:1213:ILE:CD1	2.97	0.48
1:E:1086:TRP:CD1	1:E:1141:ILE:HG12	2.48	0.48
1:A:580:LYS:HD3	1:A:685:ALA:HB2	1.95	0.48
1:E:349:LYS:HB2	1:E:353:GLY:C	2.33	0.48
1:E:365:GLU:HA	1:E:368:ASP:OD1	2.13	0.48
1:E:706:ASN:HB2	2:F:-17:U:OP1	2.14	0.48
1:A:540:THR:HG22	1:A:563:ALA:O	2.14	0.48
1:E:1027:PHE:CE2	1:E:1052:PHE:HE2	2.31	0.48
1:A:174:ARG:HH12	2:B:7:A:P	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:LYS:NZ	3:G:-2:DG:OP1	2.37	0.47
1:A:320:LYS:O	1:A:323:LYS:HG2	2.15	0.47
1:A:558:MET:SD	1:A:558:MET:N	2.87	0.47
1:E:207:GLU:HA	1:E:212:SER:OG	2.15	0.47
1:E:785:LYS:HB2	2:F:-20:A:H5"	1.96	0.47
1:A:245:VAL:HG22	1:A:246:THR:O	2.14	0.47
2:B:-10:A:H1'	1:E:550:GLY:HA2	1.96	0.47
1:E:3:LYS:N	1:E:919:ASP:OD2	2.42	0.47
1:E:82:ARG:HH22	1:E:191:GLU:CD	2.18	0.47
1:A:292:GLU:CG	1:A:293:GLY:N	2.78	0.47
1:E:611:ASP:O	1:E:615:ILE:HG12	2.15	0.47
3:G:-13:DC:H2"	3:G:-12:DT:C6	2.49	0.47
1:A:740:GLY:O	1:A:799:PRO:HG2	2.14	0.47
1:E:325:PHE:CZ	1:E:473:PHE:HD2	2.33	0.47
1:A:257:GLU:O	1:A:261:LEU:HD12	2.15	0.47
1:A:409:SER:OG	1:A:412:GLU:HB3	2.15	0.47
1:E:7:PHE:HB3	1:E:975:GLN:O	2.14	0.46
1:E:65:VAL:O	1:E:69:ILE:HG13	2.15	0.46
1:E:116:LYS:H	1:E:116:LYS:HD2	1.80	0.46
1:E:325:PHE:O	1:E:328:PHE:HB2	2.15	0.46
1:E:340:ASN:ND2	1:E:389:PHE:O	2.48	0.46
1:E:349:LYS:HB3	1:E:354:GLU:C	2.36	0.46
1:E:1140:SER:HB2	1:E:1147:VAL:O	2.14	0.46
1:A:121:LYS:NZ	1:A:125:GLU:OE1	2.39	0.46
1:A:514:LYS:HG3	1:A:516:TYR:O	2.15	0.46
1:E:338:VAL:HG12	1:E:473:PHE:CD1	2.50	0.46
1:E:487:TYR:HA	1:E:490:PHE:HB3	1.97	0.46
1:A:58:TYR:O	1:A:62:ILE:HG13	2.15	0.46
1:A:1091:LEU:HD11	1:A:1134:MET:HA	1.96	0.46
1:E:3:LYS:HE3	1:E:3:LYS:HB2	1.48	0.46
1:E:1027:PHE:CD1	1:E:1128:MET:HE2	2.47	0.46
1:A:1:MET:HG3	1:E:919:ASP:OD2	2.14	0.46
1:A:325:PHE:HE1	1:A:473:PHE:CE2	2.33	0.46
1:A:821:LYS:HG3	1:A:1199:LYS:HA	1.98	0.46
1:A:995:TYR:O	1:A:996:ILE:HD13	2.16	0.46
1:E:1015:LYS:HD3	1:E:1015:LYS:HA	1.77	0.46
1:E:1104:ILE:HD11	1:E:1118:GLN:CG	2.46	0.46
1:A:3:LYS:HB2	1:A:3:LYS:HE2	1.75	0.46
1:A:354:GLU:HB2	1:A:357:VAL:HG23	1.97	0.46
1:A:382:GLU:O	1:A:386:ARG:HG3	2.15	0.46
1:A:424:GLU:OE1	1:A:424:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:ASN:HB3	1:A:980:PHE:CE2	2.50	0.46
1:E:251:LYS:HB3	1:E:251:LYS:HE3	1.50	0.46
1:A:760:PRO:HA	1:A:782:ASP:OD1	2.15	0.46
1:A:813:ASN:O	1:A:817:ARG:HG3	2.16	0.46
1:E:362:TRP:CH2	1:E:366:TYR:CD1	3.03	0.46
1:E:636:ILE:HG22	1:E:640:LYS:HD2	1.96	0.46
1:E:1073:ARG:HD2	1:E:1075:PHE:HB3	1.97	0.46
1:A:297:ASP:OD2	1:A:446:LEU:HB2	2.16	0.46
1:A:1005:ASP:OD1	1:A:1007:SER:N	2.49	0.46
1:E:131:PHE:CD2	1:E:132:LEU:HD23	2.51	0.46
1:E:390:LYS:HE2	1:E:390:LYS:HB3	1.61	0.46
1:E:633:HIS:CE1	1:E:661:GLU:HA	2.51	0.46
2:F:-20:A:C2	2:F:-11:U:C2	3.04	0.46
1:A:752:LYS:O	1:A:755:GLU:HG2	2.15	0.46
3:C:-9:DA:H2"	3:C:-8:DC:H5"	1.97	0.46
1:E:64:ASP:O	1:E:68:SER:OG	2.30	0.46
1:E:326:LYS:HA	1:E:415:LYS:HD3	1.98	0.46
1:A:174:ARG:NH2	1:A:277:TYR:CB	2.54	0.46
1:A:187:MET:HG2	1:A:220:PHE:O	2.16	0.46
1:A:616:TYR:HA	1:A:621:PHE:HE2	1.80	0.46
3:G:-9:DA:H2"	3:G:-8:DC:H5"	1.98	0.46
1:A:325:PHE:CG	1:A:418:ILE:HG21	2.50	0.46
1:E:86:ARG:HH11	1:E:91:ASN:ND2	2.13	0.46
1:A:51:LYS:HG2	1:A:154:PHE:CE1	2.52	0.45
1:A:160:ASN:HD21	3:C:-2:DG:C4'	2.29	0.45
1:E:577:ASN:HA	1:E:687:LYS:HB2	1.97	0.45
1:A:268:GLN:CG	1:A:269:LYS:H	2.29	0.45
1:E:24:VAL:O	1:E:27:THR:HG23	2.15	0.45
1:E:359:ARG:O	1:E:363:ASN:ND2	2.49	0.45
1:E:983:PHE:CZ	1:E:986:MET:HE2	2.43	0.45
1:A:230:THR:O	1:A:234:ILE:HG13	2.16	0.45
1:A:600:LYS:N	1:A:600:LYS:HD2	2.31	0.45
1:E:325:PHE:HE1	1:E:473:PHE:HE2	1.64	0.45
1:A:102:ARG:NH1	1:A:177:ASN:OD1	2.49	0.45
1:A:1109:GLY:O	1:A:1111:ILE:HG23	2.16	0.45
1:A:1193:TRP:CD2	1:A:1213:ILE:HD13	2.48	0.45
1:E:314:ILE:HD12	1:E:314:ILE:N	2.30	0.45
1:A:821:LYS:HD3	1:A:822:HIS:NE2	2.32	0.45
1:E:201:GLU:O	1:E:204:GLU:HB3	2.15	0.45
1:A:756:LEU:HD11	1:A:790:SER:HB3	1.99	0.45
2:B:-20:A:N1	2:B:-11:U:O2'	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:THR:HG22	1:E:380:LYS:HB2	1.97	0.45
1:A:115:TYR:HB3	1:A:116:LYS:HD3	1.98	0.45
1:A:182:ARG:NH1	1:A:277:TYR:CZ	2.84	0.45
1:A:296:SER:OG	1:A:297:ASP:N	2.49	0.45
1:A:1075:PHE:HB2	1:A:1085:ASP:O	2.17	0.45
1:A:599:SER:O	1:A:603:MET:HB2	2.16	0.45
1:A:1089:VAL:HG21	1:A:1133:LEU:HD13	1.98	0.45
1:A:1206:LEU:HA	1:A:1206:LEU:HD23	1.81	0.45
1:E:101:LEU:HD12	1:E:101:LEU:HA	1.76	0.45
1:E:378:THR:CG2	1:E:380:LYS:HB2	2.47	0.45
1:A:415:LYS:O	1:A:419:ILE:HG12	2.16	0.45
1:A:562:TYR:CE2	1:A:698:LYS:HE2	2.52	0.45
1:A:1075:PHE:CB	1:A:1085:ASP:HB2	2.46	0.45
1:A:1216:LYS:HE3	1:A:1216:LYS:H	1.82	0.45
1:E:516:TYR:HB3	1:E:751:LEU:HD11	1.99	0.45
1:A:305:ARG:NH1	1:A:438:ALA:HA	2.32	0.45
1:A:611:ASP:O	1:A:615:ILE:HG23	2.18	0.45
1:A:880:GLU:OE2	1:A:938:VAL:HG11	2.16	0.45
1:E:76:ASN:HA	1:E:79:SER:HB3	1.98	0.45
1:E:784:TYR:HB2	1:E:787:LYS:HB2	1.98	0.45
1:A:264:GLN:O	1:A:267:LYS:HG2	2.17	0.44
1:E:196:ILE:HD12	1:E:262:TYR:CZ	2.51	0.44
1:E:210:LEU:O	1:E:211:ASN:HB2	2.17	0.44
1:A:837:ASN:HA	1:A:857:ASN:ND2	2.31	0.44
1:E:193:VAL:O	1:E:196:ILE:HG12	2.17	0.44
1:E:333:SER:HB2	1:E:398:GLU:HG2	2.00	0.44
1:E:442:LEU:HD11	1:E:446:LEU:HD13	1.99	0.44
1:A:595:LYS:NZ	4:D:-2:DT:O2	2.41	0.44
1:E:304:PHE:HZ	1:E:459:LEU:HD23	1.81	0.44
1:E:1150:LEU:HD23	1:E:1162:TYR:HE2	1.83	0.44
2:F:-10:A:H5'	2:F:-8:G:C2	2.52	0.44
1:E:348:SER:OG	1:E:354:GLU:O	2.33	0.44
1:E:361:LYS:CD	1:E:403:TYR:CE1	2.89	0.44
2:F:-10:A:H5'	2:F:-8:G:H1	1.81	0.44
1:A:278:LYS:HD3	1:A:279:GLN:O	2.17	0.44
1:E:363:ASN:OD1	1:E:385:ARG:NE	2.50	0.44
1:E:1033:ARG:NH2	1:E:1035:MET:CE	2.77	0.44
1:A:838:LEU:HD23	1:A:939:GLU:HG3	1.99	0.44
1:A:841:ILE:HD11	1:A:911:ILE:HD11	2.00	0.44
1:A:184:ILE:HA	1:A:187:MET:HB2	2.00	0.44
1:E:363:ASN:HB3	1:E:385:ARG:CZ	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:387:LYS:HA	1:E:387:LYS:HD2	1.60	0.44
1:E:818:VAL:HG12	1:E:1206:LEU:HD12	2.00	0.44
1:A:305:ARG:HD2	1:A:436:PHE:O	2.17	0.44
1:A:323:LYS:HG3	1:A:324:LEU:N	2.31	0.44
1:A:577:ASN:HA	1:A:687:LYS:HB2	1.99	0.44
1:A:664:LYS:HA	1:A:664:LYS:HD3	1.80	0.44
1:A:1019:THR:HG22	1:A:1020:SER:N	2.32	0.44
1:E:255:LEU:HA	1:E:258:TYR:HD2	1.82	0.44
1:E:315:PHE:HA	1:E:318:ILE:HD12	2.00	0.44
1:A:931:PHE:HB3	1:A:940:LYS:HD3	2.00	0.44
1:E:477:GLY:HA2	1:E:478:LYS:C	2.39	0.44
1:E:777:THR:HG23	2:F:-8:G:C6	2.53	0.44
1:E:877:ASP:O	1:E:880:GLU:HB3	2.18	0.44
1:A:630:ASN:O	1:A:634:LYS:HG3	2.18	0.43
1:A:668:GLY:O	1:A:672:GLU:HG3	2.18	0.43
1:A:369:ILE:H	1:A:369:ILE:HG13	1.67	0.43
1:A:380:LYS:O	1:A:384:ASP:N	2.51	0.43
2:B:-19:A:C8	2:B:-6:G:C6	3.06	0.43
1:E:1102:TYR:CD2	1:E:1123:PHE:HB2	2.54	0.43
1:A:359:ARG:HH22	1:A:386:ARG:HG2	1.83	0.43
1:A:1139:ASN:HB2	1:A:1149:PHE:CE1	2.53	0.43
1:A:202:VAL:HG13	1:A:216:VAL:HB	2.00	0.43
1:E:272:LYS:NZ	1:E:272:LYS:HB2	2.33	0.43
1:E:406:ALA:HA	1:E:407:ASP:HA	1.67	0.43
1:E:924:LEU:HD13	1:E:947:GLU:HG2	1.99	0.43
1:E:1150:LEU:H	1:E:1164:SER:CB	2.24	0.43
1:A:27:THR:HG21	1:A:700:TYR:HA	2.00	0.43
1:A:231:GLN:HA	1:A:234:ILE:HG13	2.01	0.43
1:A:600:LYS:HD2	1:A:600:LYS:H	1.84	0.43
1:A:705:TYR:OH	1:A:710:SER:HB2	2.18	0.43
1:A:1045:PHE:CD1	1:A:1045:PHE:N	2.85	0.43
1:A:1111:ILE:HD12	1:A:1115:LEU:HD21	1.99	0.43
1:E:268:GLN:HE21	1:E:270:LEU:HD21	1.83	0.43
1:E:369:ILE:HD12	1:E:370:HIS:CG	2.50	0.43
1:E:70:LYS:HA	1:E:226:ASN:OD1	2.19	0.43
1:E:83:LYS:HB3	1:E:86:ARG:HB3	1.98	0.43
1:A:205:ILE:HG23	1:A:209:ILE:HD12	2.00	0.43
1:A:522:LYS:HZ3	1:A:743:GLU:HG2	1.82	0.43
1:A:1136:GLN:NE2	1:A:1139:ASN:OD1	2.45	0.43
2:B:-15:C:H2'	2:B:-14:U:C6	2.54	0.43
1:E:325:PHE:HZ	1:E:473:PHE:HD2	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1027:PHE:CE2	1:E:1031:PHE:HE1	2.36	0.43
2:F:-20:A:N3	2:F:-11:U:C4	2.87	0.43
1:A:75:ASN:OD1	1:A:75:ASN:N	2.51	0.43
1:E:80:LEU:HD11	1:E:90:GLU:OE2	2.18	0.43
1:E:119:PHE:HB3	1:E:155:PHE:HB3	2.00	0.43
1:E:314:ILE:H	1:E:314:ILE:CD1	2.30	0.43
1:E:980:PHE:HD1	1:E:980:PHE:H	1.66	0.43
3:G:-3:DT:H2'	3:G:-2:DG:C8	2.53	0.43
1:A:351:ILE:O	1:A:413:LYS:HD3	2.19	0.43
1:A:455:ILE:HA	1:A:458:ASP:HB2	2.00	0.43
1:A:1110:ASP:OD2	1:A:1112:ARG:NH2	2.43	0.43
1:E:509:ASN:O	1:E:513:GLN:HG2	2.19	0.43
3:G:8:DC:H2"	3:G:9:DG:C8	2.54	0.43
1:A:2:SER:HA	1:E:1:MET:HB3	2.01	0.43
1:A:593:LEU:HB2	1:A:594:PRO:HD3	2.01	0.43
1:E:72:LYS:HD2	1:E:72:LYS:HA	1.87	0.43
1:E:325:PHE:CE1	1:E:473:PHE:CE2	3.07	0.43
1:E:1057:ALA:HA	1:E:1216:LYS:HG2	2.01	0.43
1:A:347:ILE:O	1:A:351:ILE:HG13	2.18	0.42
1:A:457:LYS:HG3	1:A:890:TRP:CE2	2.53	0.42
1:E:296:SER:OG	1:E:297:ASP:N	2.51	0.42
1:E:351:ILE:O	1:E:413:LYS:HD3	2.19	0.42
1:E:952:ASP:O	1:E:955:ASN:HB2	2.19	0.42
1:E:1033:ARG:NE	1:E:1035:MET:CE	2.81	0.42
1:A:27:THR:CG2	1:A:700:TYR:HA	2.49	0.42
1:A:193:VAL:HG11	1:A:270:LEU:HD13	2.00	0.42
1:A:645:ARG:HH21	1:A:645:ARG:HG3	1.83	0.42
1:A:833:ARG:HD3	1:A:927:LEU:HD11	2.01	0.42
1:E:729:ASP:OD2	1:E:731:ASN:HB2	2.18	0.42
1:E:986:MET:HE2	1:E:986:MET:HB3	1.75	0.42
1:A:257:GLU:HG3	1:A:261:LEU:HD11	2.01	0.42
1:A:314:ILE:O	1:A:318:ILE:HG13	2.20	0.42
1:A:823:ASP:O	1:A:826:PRO:HD3	2.19	0.42
1:A:1086:TRP:CG	1:A:1141:ILE:HD13	2.54	0.42
1:E:80:LEU:O	1:E:83:LYS:HB2	2.19	0.42
1:E:571:LYS:CG	1:E:577:ASN:HD21	2.33	0.42
1:A:262:TYR:CZ	1:A:266:THR:HG21	2.54	0.42
1:A:525:PHE:CD2	1:A:557:ILE:HG21	2.55	0.42
1:A:636:ILE:HG22	1:A:640:LYS:HD2	2.00	0.42
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.75	0.42
1:A:317:SER:HA	1:A:320:LYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:LYS:NZ	1:A:1203:ASP:OD1	2.48	0.42
1:A:1000:LEU:HD23	1:A:1000:LEU:H	1.84	0.42
1:E:37:LEU:HD23	1:E:37:LEU:HA	1.84	0.42
1:E:348:SER:OG	1:E:357:VAL:HG12	2.19	0.42
1:E:897:LYS:HG3	1:E:898:GLU:N	2.33	0.42
1:E:1192:LEU:HD23	1:E:1195:ILE:HD12	2.01	0.42
1:A:123:ILE:O	1:A:128:LEU:HB2	2.19	0.42
1:A:257:GLU:HG3	1:A:261:LEU:CD1	2.50	0.42
1:E:373:LYS:O	1:E:373:LYS:HG3	2.19	0.42
1:E:659:GLU:HB3	1:E:661:GLU:OE1	2.20	0.42
1:E:1040:GLU:CB	1:E:1042:LEU:HD22	2.50	0.42
1:A:900:LYS:O	1:A:904:ILE:HG12	2.20	0.42
2:B:-17:U:C4	2:B:-16:U:C4	3.07	0.42
1:E:123:ILE:HA	1:E:127:ILE:HB	2.01	0.42
1:E:562:TYR:CD2	1:E:698:LYS:HD3	2.54	0.42
1:E:837:ASN:HA	1:E:857:ASN:HD21	1.84	0.42
1:E:1098:LEU:HD21	1:E:1127:PHE:HB2	2.01	0.42
2:F:0:C:H1'	2:F:1:G:C8	2.53	0.42
1:A:476:GLU:C	1:A:478:LYS:HB2	2.40	0.42
1:E:982:SER:O	1:E:986:MET:HB2	2.19	0.42
1:A:193:VAL:CG1	1:A:270:LEU:HD13	2.50	0.42
1:A:301:LEU:HA	1:A:301:LEU:HD23	1.75	0.42
1:E:833:ARG:NH1	1:E:939:GLU:OE1	2.53	0.42
1:A:615:ILE:HB	1:A:620:THR:OG1	2.20	0.41
1:E:996:ILE:HD13	1:E:996:ILE:HA	1.63	0.41
1:E:1165:ARG:HA	1:E:1168:GLU:HG2	2.01	0.41
1:A:313:GLU:HG2	1:A:496:ILE:HG21	2.00	0.41
1:E:2:SER:OG	1:E:5:GLU:HG3	2.20	0.41
1:E:1086:TRP:O	1:E:1087:GLU:HB2	2.20	0.41
1:A:343:ALA:O	1:A:347:ILE:HD12	2.21	0.41
1:A:550:GLY:HA2	2:F:-10:A:N3	2.35	0.41
1:A:1086:TRP:CD1	1:A:1141:ILE:HD13	2.55	0.41
1:E:543:ARG:HG2	1:E:558:MET:HB2	2.02	0.41
1:E:814:THR:HG22	1:E:1207:ASP:HB3	2.02	0.41
1:E:879:LYS:HB3	1:E:896:ILE:HD12	2.02	0.41
1:E:1005:ASP:OD1	1:E:1005:ASP:C	2.59	0.41
1:A:301:LEU:CD2	1:A:435:LEU:HD21	2.49	0.41
1:A:744:LEU:HD12	1:A:795:GLU:O	2.21	0.41
1:E:923:ALA:HB1	1:E:1187:ILE:HG22	2.02	0.41
1:E:1071:ARG:CZ	1:E:1091:LEU:HD11	2.51	0.41
1:A:155:PHE:O	1:A:159:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ILE:HD12	1:A:196:ILE:H	1.86	0.41
1:A:196:ILE:HD12	1:A:196:ILE:N	2.36	0.41
1:A:982:SER:O	1:A:986:MET:HB2	2.19	0.41
1:A:73:ASN:HB3	1:A:76:ASN:HB3	2.03	0.41
3:C:8:DC:H2"	3:C:9:DG:C8	2.55	0.41
1:E:118:LEU:HA	1:E:123:ILE:HD12	2.03	0.41
1:E:198:ASP:HB3	1:E:201:GLU:CB	2.46	0.41
1:E:880:GLU:OE1	1:E:938:VAL:HG11	2.20	0.41
1:A:71:LEU:N	1:A:226:ASN:OD1	2.47	0.41
1:A:952:ASP:O	1:A:955:ASN:HB2	2.20	0.41
1:E:359:ARG:HG2	1:E:363:ASN:ND2	2.35	0.41
1:E:366:TYR:CD1	1:E:385:ARG:HG3	2.56	0.41
1:A:716:THR:HA	1:A:717:PRO:HD3	1.93	0.41
2:B:8:G:H1	3:C:-8:DC:H42	1.67	0.41
1:E:80:LEU:HD21	1:E:90:GLU:HB3	2.03	0.41
1:E:126:THR:C	1:E:129:PRO:HD2	2.41	0.41
1:A:18:ARG:HG2	1:A:797:HIS:CD2	2.56	0.41
1:A:514:LYS:CE	1:A:517:SER:HA	2.51	0.41
1:A:1202:GLU:HB2	1:A:1205:LYS:CE	2.49	0.41
1:E:327:ASN:HD22	1:E:327:ASN:HA	1.71	0.41
1:E:457:LYS:HG3	1:E:890:TRP:CE2	2.56	0.41
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.75	0.41
1:E:647:PRO:HA	1:E:650:SER:OG	2.21	0.41
1:E:687:LYS:O	1:E:691:ASP:HB2	2.20	0.41
1:E:1041:ASP:O	1:E:1042:LEU:HD12	2.21	0.41
1:E:1216:LYS:HE3	1:E:1216:LYS:HB3	1.82	0.41
2:F:6:C:H2'	2:F:7:A:H8	1.86	0.41
1:A:580:LYS:HE2	1:A:580:LYS:HB2	1.88	0.41
1:A:859:ILE:HG21	1:A:906:GLN:HB3	2.03	0.41
1:E:75:ASN:N	1:E:75:ASN:OD1	2.54	0.41
1:E:352:PHE:CB	1:E:357:VAL:HG11	2.50	0.41
1:A:719:LEU:HD21	1:A:723:TYR:OH	2.22	0.40
1:A:1091:LEU:HD23	1:A:1091:LEU:HA	1.84	0.40
1:E:347:ILE:O	1:E:351:ILE:HG13	2.20	0.40
1:A:339:LYS:CB	1:A:475:GLY:HA2	2.51	0.40
1:E:401:GLN:HE21	1:E:401:GLN:HB2	1.72	0.40
1:A:321:LEU:O	1:A:325:PHE:HD2	2.04	0.40
1:A:1075:PHE:HB2	1:A:1085:ASP:CB	2.52	0.40
1:E:308:LEU:O	1:E:429:TYR:OH	2.20	0.40
1:E:442:LEU:HD22	1:E:444:LYS:O	2.20	0.40
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:ILE:O	1:A:1213:ILE:HG23	2.21	0.40
1:E:198:ASP:C	1:E:201:GLU:HB3	2.40	0.40
1:E:278:LYS:NZ	1:E:282:SER:O	2.43	0.40
1:E:858:GLU:HG2	1:E:871:ASP:HA	2.02	0.40
1:E:1099:PHE:HB3	1:E:1104:ILE:HB	2.03	0.40
1:A:406:ALA:HB1	1:A:407:ASP:CG	2.42	0.40
1:A:807:LYS:HD3	1:A:807:LYS:HA	1.86	0.40
2:B:4:U:H2'	2:B:5:C:C6	2.56	0.40
1:E:18:ARG:HB3	2:F:-17:U:H1'	2.04	0.40
1:E:209:ILE:HG22	1:E:210:LEU:HD23	2.04	0.40
1:E:765:ILE:HD13	1:E:765:ILE:HG21	1.92	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	1208/1228 (98%)	1174 (97%)	30 (2%)	4 (0%)	37	63
1	E	1211/1228 (99%)	1177 (97%)	32 (3%)	2 (0%)	44	71
All	All	2419/2456 (98%)	2351 (97%)	62 (3%)	6 (0%)	44	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	89	LYS
1	A	588	GLY
1	A	89	LYS
1	A	1105	ASN
1	A	376	VAL
1	E	587	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1081/1115 (97%)	1037 (96%)	44 (4%)	26	57
1	E	1082/1115 (97%)	1037 (96%)	45 (4%)	25	56
All	All	2163/2230 (97%)	2074 (96%)	89 (4%)	26	57

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	52	LYS
1	A	84	LYS
1	A	86	ARG
1	A	116	LYS
1	A	147	PHE
1	A	174	ARG
1	A	199	LYS
1	A	203	GLN
1	A	213	ASP
1	A	224	PHE
1	A	244	PHE
1	A	256	ASN
1	A	269	LYS
1	A	272	LYS
1	A	278	LYS
1	A	283	ASP
1	A	296	SER
1	A	328	PHE
1	A	380	LYS
1	A	396	SER
1	A	439	ASP
1	A	458	ASP
1	A	465	SER
1	A	558	MET
1	A	573	ASP
1	A	633	HIS

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Mol	Chain	Res	Type
1	A	653	TYR
1	A	686	SER
1	A	711	ASP
1	A	713	SER
1	A	810	PHE
1	A	867	ARG
1	A	934	SER
1	A	984	LYS
1	A	1025	LYS
1	A	1049	TYR
1	A	1067	SER
1	A	1075	PHE
1	A	1125	SER
1	A	1156	ASN
1	A	1163	ASP
1	A	1164	SER
1	A	1216	LYS
1	E	13	LEU
1	E	52	LYS
1	E	79	SER
1	E	94	LEU
1	E	103	LYS
1	E	136	ASP
1	E	147	PHE
1	E	163	SER
1	E	185	SER
1	E	213	ASP
1	E	251	LYS
1	E	282	SER
1	E	328	PHE
1	E	329	ASP
1	E	332	SER
1	E	348	SER
1	E	366	TYR
1	E	373	LYS
1	E	380	LYS
1	E	413	LYS
1	E	439	ASP
1	E	464	LYS
1	E	465	SER
1	E	471	LYS
1	E	558	MET

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Mol	Chain	Res	Type
1	E	571	LYS
1	E	625	ASP
1	E	629	LEU
1	E	713	SER
1	E	833	ARG
1	E	836	ARG
1	E	874	SER
1	E	883	ARG
1	E	884	PHE
1	E	889	ASN
1	E	892	SER
1	E	931	PHE
1	E	980	PHE
1	E	986	MET
1	E	1035	MET
1	E	1064	LYS
1	E	1075	PHE
1	E	1146	ASP
1	E	1150	LEU
1	E	1171	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	96	ASN
1	A	160	ASN
1	A	256	ASN
1	A	577	ASN
1	A	941	GLN
1	E	91	ASN
1	E	268	GLN
1	E	327	ASN
1	E	401	GLN
1	E	1108	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	33/40 (82%)	7 (21%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	33/40 (82%)	7 (21%)	0
All	All	66/80 (82%)	14 (21%)	0

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-17	U
2	B	-10	A
2	B	-9	A
2	B	-8	G
2	B	-6	G
2	B	1	G
2	B	8	G
2	F	-17	U
2	F	-10	A
2	F	-9	A
2	F	-8	G
2	F	-6	G
2	F	1	G
2	F	8	G

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 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	1214/1228 (98%)	-0.23	19 (1%)	70	65	14, 44, 80, 138	0
1	E	1217/1228 (99%)	-0.09	44 (3%)	46	41	15, 47, 95, 130	1 (0%)
2	B	34/40 (85%)	-0.49	1 (2%)	54	49	18, 26, 157, 168	0
2	F	34/40 (85%)	-0.42	1 (2%)	54	49	20, 25, 196, 203	0
3	C	23/24 (95%)	0.15	2 (8%)	17	15	21, 68, 153, 161	0
3	G	23/24 (95%)	0.44	5 (21%)	3	3	27, 73, 180, 190	0
4	D	11/11 (100%)	-0.47	0	100	100	27, 30, 89, 105	0
4	H	11/11 (100%)	-0.04	2 (18%)	4	4	32, 35, 103, 118	0
All	All	2567/2606 (98%)	-0.16	74 (2%)	54	49	14, 45, 93, 203	1 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	999	TRP	5.5
1	A	1077	ASN	4.2
1	A	982	SER	4.0
1	E	381	TYR	3.7
1	A	291	GLY	3.6
1	E	403	TYR	3.5
1	E	374	LYS	3.5
1	E	884	PHE	3.2
1	A	179	ASN	3.2
1	A	277	TYR	3.2
1	E	397	LEU	3.2
1	A	983	PHE	3.2
1	E	886	ALA	3.1
1	E	361	LYS	3.1
1	E	73	ASN	3.1
1	E	889	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	223	GLU	3.0
1	A	863	PHE	3.0
1	E	277	TYR	3.0
1	A	981	GLU	2.9
1	E	982	SER	2.8
1	E	984	LYS	2.8
1	E	399	GLN	2.8
1	E	375	ALA	2.8
1	E	891	THR	2.8
1	E	1082	ASN	2.7
1	E	863	PHE	2.7
3	C	-7	DT	2.7
1	A	278	LYS	2.6
2	F	11	A	2.6
1	E	1145	THR	2.6
1	A	375	ALA	2.5
3	G	9	DG	2.5
1	E	276	LEU	2.5
1	E	244	PHE	2.5
3	G	-7	DT	2.5
1	E	888	GLN	2.4
3	G	-11	DT	2.4
1	A	980	PHE	2.4
1	A	576	GLY	2.4
1	A	73	ASN	2.4
1	E	373	LYS	2.4
1	E	378	THR	2.4
1	A	197	PHE	2.4
1	A	1144	ARG	2.3
1	E	88	GLU	2.3
1	E	934	SER	2.3
1	A	273	PHE	2.3
1	A	986	MET	2.3
1	E	1081	ASN	2.3
1	A	1075	PHE	2.3
4	H	-9	DC	2.3
1	E	85	THR	2.3
3	C	9	DG	2.2
3	G	-10	DT	2.2
4	H	-7	DT	2.2
1	E	1141	ILE	2.2
1	E	986	MET	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	13	G	2.2
1	E	328	PHE	2.1
1	E	791	GLU	2.1
1	E	364	ALA	2.1
1	E	834	GLY	2.1
1	E	1148	ASP	2.1
3	G	-13	DC	2.1
1	E	981	GLU	2.1
1	E	980	PHE	2.1
1	A	295	THR	2.0
1	E	898	GLU	2.0
1	E	372	LYS	2.0
1	E	389	PHE	2.0
1	E	200	HIS	2.0
1	E	400	LEU	2.0
1	E	575	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
5	LI	A	1302	1/1	0.09	0.97	8,8,8,8	0
5	LI	E	1301	1/1	0.36	0.75	10,10,10,10	0
5	LI	B	101	1/1	0.61	1.76	2,2,2,2	0
5	LI	A	1301	1/1	0.67	0.81	3,3,3,3	0
5	LI	F	101	1/1	0.86	0.79	5,5,5,5	0

6.5 Other polymers ⓘ

There are no such residues in this entry.