



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:32 AM GMT

PDB ID : 2XCR
Title : THE 3.5A CRYSTAL STRUCTURE OF THE CATALYTIC CORE (B'A' REGION) OF STAPHYLOCOCCUS AUREUS DNA GYRASE COMPLEXED WITH GSK299423 AND DNA
Authors : Bax, B.D.; Chan, P.F.; Eggleston, D.S.; Fosberry, A.; Gentry, D.R.; Gorrec, F.; Giordano, I.; Hann, M.M.; Hennessy, A.; Hibbs, M.; Huang, J.; Jones, E.; Jones, J.; Brown, K.K.; Lewis, C.J.; May, E.W.; Singh, O.; Spitzfaden, C.; Shen, C.; Shillings, A.; Theobald, A.F.; Wohlkonig, A.; Pearson, N.D.; Gwynn, M.N.
Deposited on : 2010-04-25
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

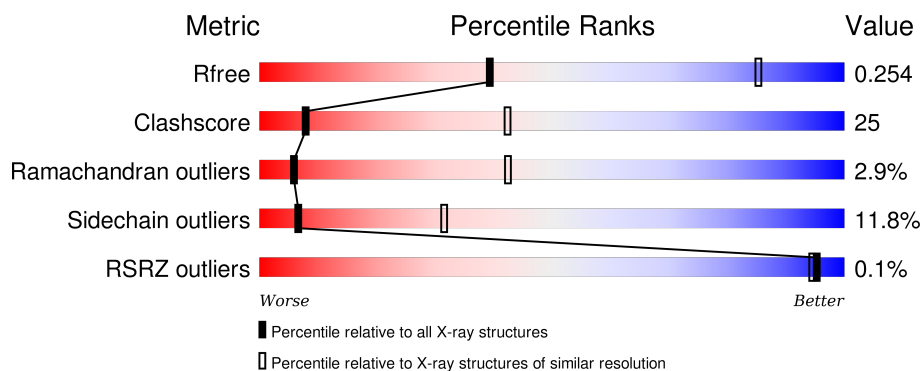
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	B	726	
1	D	726	
1	S	726	
1	U	726	
2	E	20	

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Mol	Chain	Length	Quality of chain
2	F	20	
3	V	20	
3	W	20	

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
4	RXV	E	1021[A]	-	-	-	X
4	RXV	E	1021[B]	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24495 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 GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	718	Total	C	N	O	S	0	0	0
			5689	3556	1018	1090	25			
1	D	719	Total	C	N	O	S	0	0	0
			5692	3556	1021	1090	25			
1	S	718	Total	C	N	O	S	0	0	0
			5694	3561	1022	1086	25			
1	U	717	Total	C	N	O	S	0	0	0
			5689	3558	1020	1086	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	EXPRESSION TAG	UNP Q99XG5
B	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5
D	409	MET	-	EXPRESSION TAG	UNP Q99XG5
D	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5
S	409	MET	-	EXPRESSION TAG	UNP Q99XG5
S	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5
U	409	MET	-	EXPRESSION TAG	UNP Q99XG5
U	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5

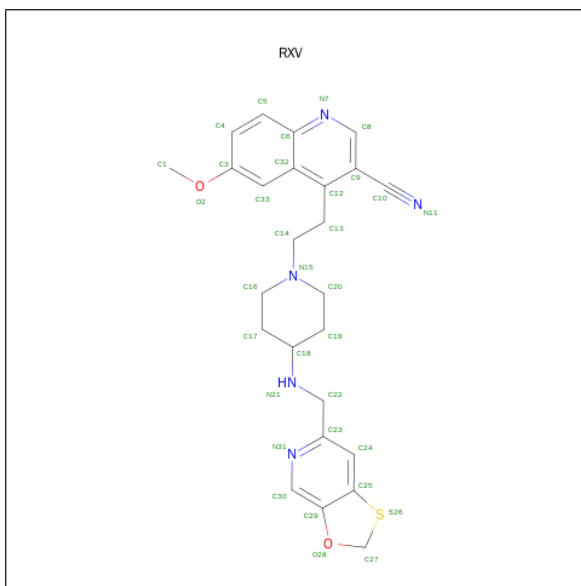
- Molecule 2 is a DNA chain called 5'-D(*5UA*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP *GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	20	Total	C	N	O	P	0	0	0
			410	194	77	120	19			
2	F	20	Total	C	N	O	P	0	0	0
			410	194	77	120	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	20	Total	C	N	O	P	0	0	0
			410	193	77	120	20			
3	W	18	Total	C	N	O	P	0	0	0
			369	173	70	108	18			

- Molecule 4 is 6-METHOXY-4-(2-{4-[(1,3]OXATHIOLO[5,4-C]PYRIDIN-6-YLMETHYL) AMINO]PIPERIDIN-1-YL}ETHYL)QUINOLINE-3-CARBONITRILE (three-letter code: RXV) (formula: C₂₅H₂₇N₅O₂S).

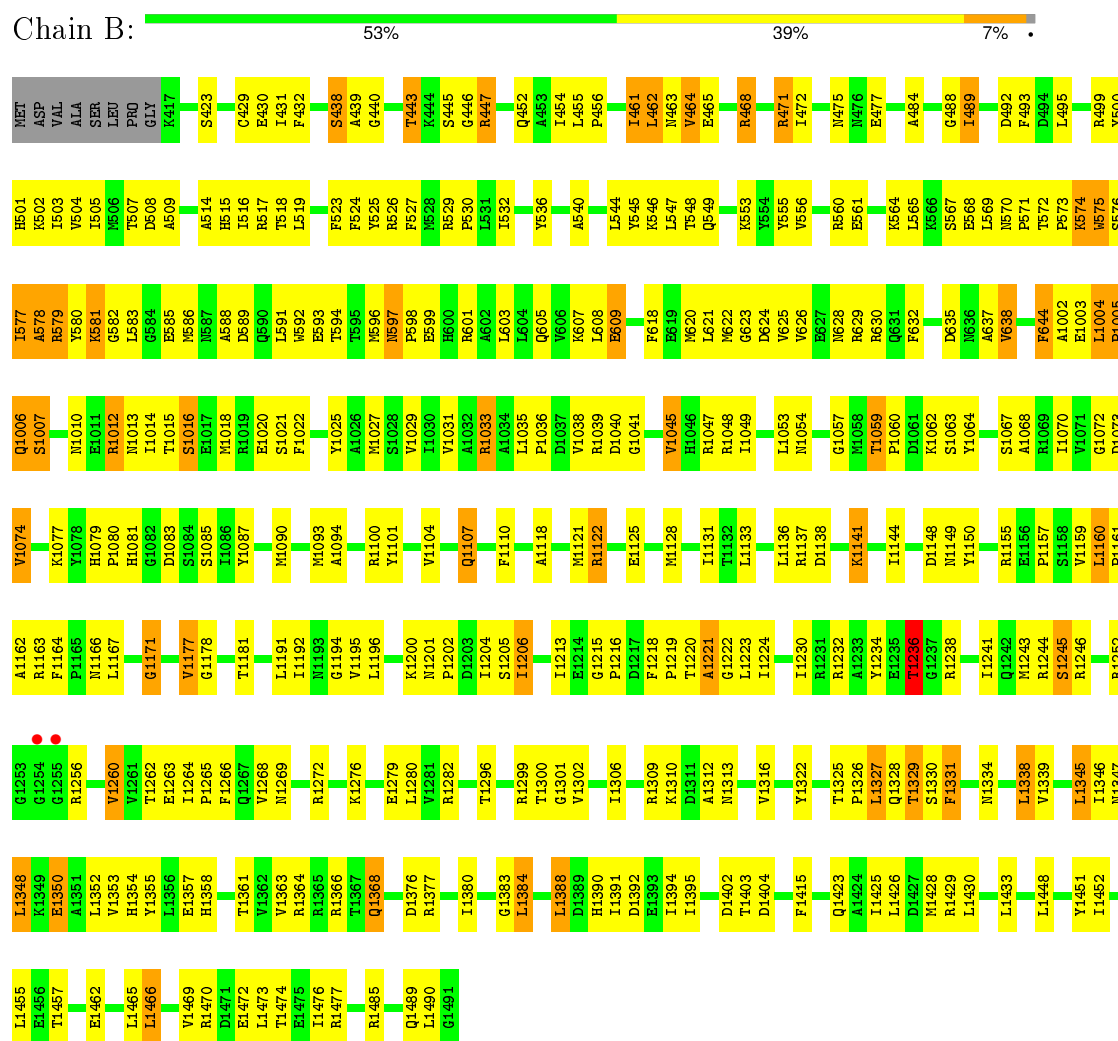


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	S	0	1
			66	50	10	4	2		
4	W	1	Total	C	N	O	S	0	1
			66	50	10	4	2		

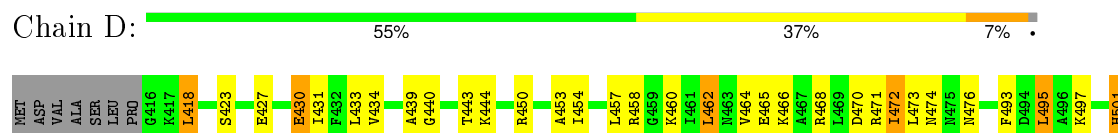
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A



• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

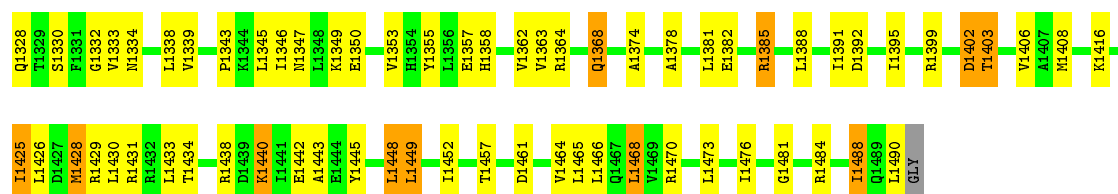


L1468	D1376	L1292	I1192	V1104	E1020	S576	K502
V1469	I1380	R1293	V1195	D1105	S1021	S577	I503
R1470	I1384	R1294	V1196	D1107	F1022	A578	I504
L1473	L1385	E1295	S1197	A1119	L1023	I579	I505
T1474	L1386	L1296	L1198	A1120	D1024	I580	I506
E1475	I1387	E1297	I1206	A1121	I1027	K581	T507
I1476	L1388	L1298	I1206	V1121	I1031	E582	D508
R1477	L1389	V1302	I1213	R1122	F1032	S583	A509
G1481	H1390	I1306	I1224	F1123	A1032	D590	V511
R1485	D1392	D1307	L1225	M1128	A1034	E592	A514
G1491	R1399	V1308	G1226	I1131	L1035	E593	E515
	L1411	R1309	K1227	T1132	P1036	T594	I516
	F1415	K1310	E1229	E1133	D1040	T595	E517
	L1416	A1311	L1230	E1134	G1041	L604	T518
	S1418	A1312	I1231	L1135	L1042	L604	I519
	E1419	H1313	R1231	L1136	K1043	E609	F523
	K1420	I1316	R1232	R1137	P1044	E609	F524
	Q1421	V1316	A1233	L1138	V1045	T617	I525
	A1422	L1317	E1234	I1139	R1046	F618	I528
	Q1423	L1318	E1235	I1144	R1047	E619	I529
	L1426	I1322	G1239	D1145	L1048	L621	K530
	R1429	L1327	M1243	F1146	L1050	R622	L531
	L1430	Q1328	R1244	Y1150	N1054	G623	I532
	R1431	T1329	R1244	D1151	E1055	V625	V536
	L1432	S1330	V1248	E1157	Q1056	I628	I537
	T1434	I1336	I1249	P1158	Q1057	R629	I539
	R1438	R1342	Q1257	V1159	T1059	F632	Q541
	I1441	P1343	R1258	L1160	P1060	I633	I544
	E1444	K1344	I1264	A1162	Y1064	N636	I545
	V1445	M1347	F1266	F1164	S1067	A637	E546
	M1446	L1348	V1268	M1165	A1068	V639	L547
	E1447	K1349	I1269	L1167	R1069	A640	I548
	L1448	L1352	K1270	L1171	V1074	N641	Q549
	L1449	V1353	I1271	I1175	H1079	A1002	V555
	M1450	L1356	A1272	A1176	P1080	E1003	V557
	Y1451	L1356	R1273	V1177	H1081	L1004	
	L1455	Q1359	I1274	M1179	D1082	P1005	L562
	E1456	K1360	I1277	A1180	D1083	Q1006	D563
	T1457	T1361	E1278	I1183	S1084	S1007	K564
	I1458	V1363	E1279	P1184	S1085	R1008	L565
	E1459	R1364	L1280	H1185	I1086	I1009	K566
	E1460	R1365	V1281	H1186	V1091	R1010	S567
	L1465	R1365	R1282	T1189	R1092	E1011	E568
	L1466	K1373	I1289	E1190	R1093	R1012	L569
	Q1467			E1191	M1093	I570	K570
				L1191	A1094	I1014	P571
					Q1095	T1015	T572
					Y1101	M1018	P573
						K574	K575
						R1019	

• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

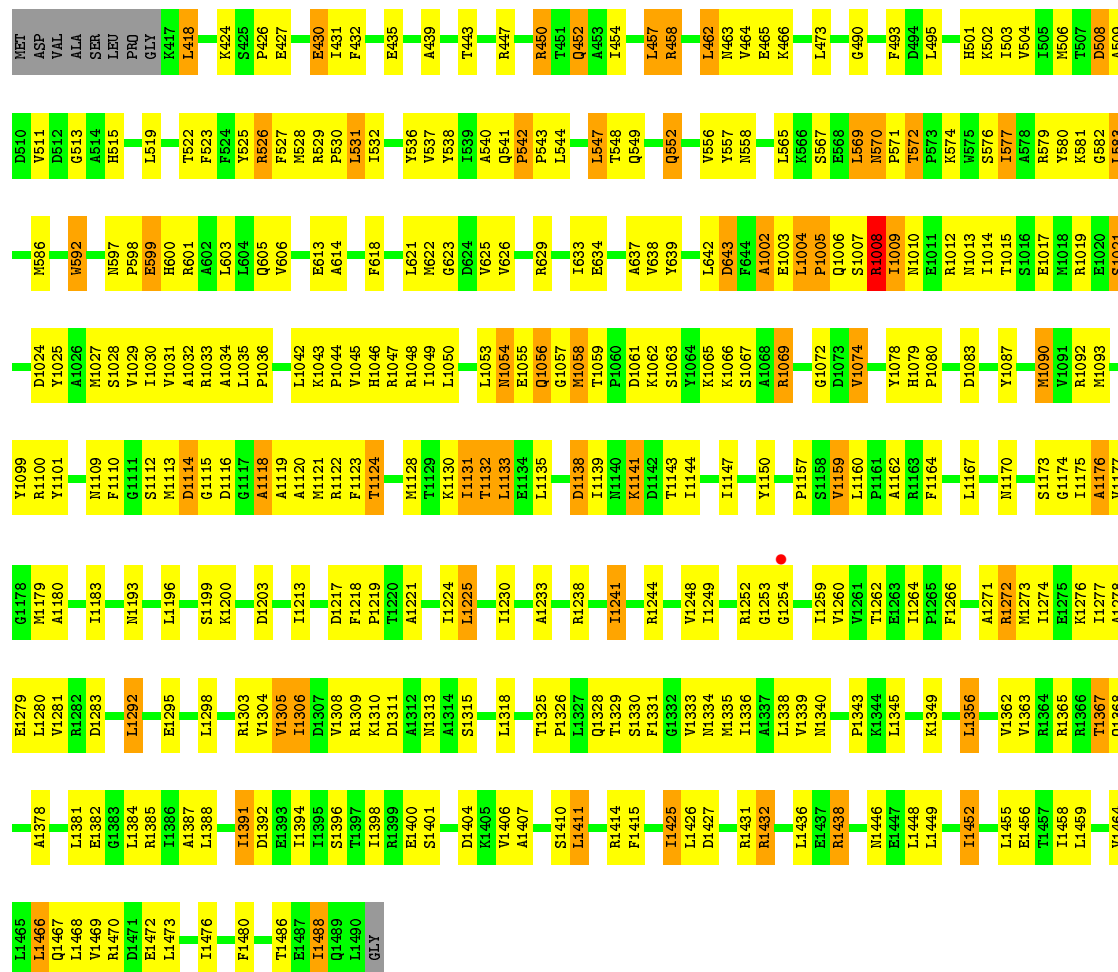
Chain S:  51% 40% 8% .

WET	I482	B560	V638	M1075	P1165	E1251	R1252
ASP	F485	L566	L642	G1076	L1168	R1256	R1257
VAL	F485	K566	D643	K1077	A1169	Q1257	Q1258
ALA	F493	S567	F644	P1080	S1173	T1261	T1262
SER	F493	E568	A1002	H1081	G1174	E1263	E1264
LEU	L495	L569	E1003	S1085	I1175	P1265	P1265
PRO	R499	P571	L1004	H1086	A1176	K1270	K1270
C416	Y500	T572	Q1006	Y1087	M1179	T1261	T1262
G417	H501	F573	S1007	E1088	A1180	E1263	E1264
L418	K502	K574	R1008	M1090	T1181	P1265	P1265
A419	I503	M575	I1009	Y1091	M1182	K1270	K1270
S425	V504	S576	R1012	V1091	I1183	M1273	M1273
P426	I505	A578	M1013	M1093	P1184	I1274	I1274
E427	M506	R579	I1014	Y1099	H1186	I1277	I1277
E428	T507	Y580	T1015	R1100	L1187	A1278	A1278
C429	D508	K581	R1019	Y1101	L1188	E1279	E1279
I431	V511	E582	D1024	Q1107	T1189	L1280	L1280
F432	H515	L516	Y1025	F1110	E1190	L1281	L1281
E435	R517	T518	M1027	F1111	L1191	R1282	R1282
S438	L519	L520	S1028	S1112	I1192	G1288	G1288
A439	L520	E592	Y1029	M1113	S1199	I1289	I1289
T443	L521	E593	D1026	D1114	I1204	L1292	L1292
K444	T522	T594	A1032	G1115	E1208	R1293	R1293
S445	F523	M596	R1033	D1116	L1209	D1294	D1294
G446	F524	R597	A1034	A1120	M1210	E1295	E1295
R447	Y525	P598	L1035	F1123	I1213	T1296	T1296
D448	R526	E599	P1036	T1124	F1218	S1297	S1297
S449	R529	H600	D1040	E1125	P1219	R1298	R1298
R450	L531	R601	G1041	L1131	T1300	G1301	G1301
Q452	I532	L603	L1042	L1132	T1220	V1302	V1302
A453	Y536	L604	V1045	L1133	G1222	R1303	R1303
L454	V537	Q605	H1046	E1134	V1304	I1305	I1305
L455	Y538	R607	R1047	L1135	L1224	T1306	T1306
	A540	L608	L1050	R1137	G1225	R1307	R1307
	Q541	T617	G1057	D1138	V1308	V1309	V1309
	L544	F618	M1058	K1141	R1309	K1310	K1310
	Y545	M622	T1059	D1142	D1311	A1312	A1312
	K546	V626	P1060	T1143	A1233	V1316	V1316
	L547	E627	S1063	I1144	R1238	M1320	M1320
	G550	R628	S1067	Y1150	G1239	L1321	L1321
	K551	R629	R1068	E1154	R1244	Y1322	Y1322
	Q552	R630	A1068	R1155	S1245	K1323	K1323
	K553	Q631	R1069	E1156	L1247	Q1324	Q1324
	Y554	F632	I1070	E1156	T1248	P1325	P1325
	E557	L633	V1071	A1162	I1249	L1327	L1327
	N558	E634	G1072	R1163			
	D559	A637	D1073	F1164			



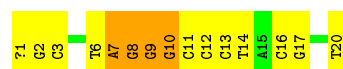
• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

Chain U: 53% 37% 8% .



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

Chain E: 25% 55% 20%



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

Chain F:  45% 30% 25%




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

Chain V:  5% 55% 40%



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

Chain W:  15% 55% 20% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.26Å 165.38Å 308.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.99 – 3.50 23.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	84.5 (23.99-3.50) 84.6 (23.99-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.208 , 0.258 0.191 , 0.254	Depositor DCC
R_{free} test set	2505 reflections (4.19%)	DCC
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	1.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 52.0	EDS
Estimated twinning fraction	None for NONE	Xtriage
Reported twinning fraction	None for NONE	Depositor
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	1 of 62227 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24495	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 5UA, RXV

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	B	0.40	0/5772	0.63	0/7784
1	D	0.42	0/5775	0.63	0/7792
1	S	0.43	0/5777	0.66	1/7789 (0.0%)
1	U	0.42	0/5772	0.64	0/7785
2	E	0.85	0/435	1.86	10/669 (1.5%)
2	F	0.84	0/435	1.70	9/669 (1.3%)
3	V	0.90	0/459	1.84	14/706 (2.0%)
3	W	0.94	1/413 (0.2%)	1.84	13/635 (2.0%)
All	All	0.47	1/24838 (0.0%)	0.80	47/33829 (0.1%)

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	S	0	1
1	U	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	14	DT	C1'-N1	5.28	1.56	1.49

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	DG	O4'-C1'-N9	-15.90	96.87	108.00
3	W	14	DT	O4'-C1'-N1	11.09	115.76	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	16	DC	O4'-C4'-C3'	-10.56	99.66	106.00
3	V	16	DC	O4'-C4'-C3'	-10.33	99.80	106.00
2	E	10	DG	O4'-C1'-N9	10.29	115.20	108.00
2	F	10	DG	O4'-C1'-N9	9.75	114.82	108.00
2	F	8	DG	O4'-C1'-N9	-9.37	101.44	108.00
2	E	7	DA	O4'-C4'-C3'	-9.13	100.52	106.00
3	V	16	DC	O4'-C1'-N1	8.98	114.29	108.00
3	V	14	DT	O4'-C1'-N1	8.96	114.27	108.00
3	W	9	DG	O4'-C4'-C3'	-8.86	100.69	106.00
3	V	6	DT	O4'-C1'-N1	8.74	114.12	108.00
3	V	17	DG	O4'-C1'-N9	-8.61	101.97	108.00
2	E	8	DG	P-O5'-C5'	-8.43	107.41	120.90
3	W	7	DA	O4'-C1'-N9	8.29	113.80	108.00
2	F	11	DC	O4'-C1'-N1	8.24	113.77	108.00
2	E	9	DG	O4'-C1'-N9	7.96	113.57	108.00
2	E	9	DG	C8-N9-C4	-7.93	103.23	106.40
2	F	19	DC	O4'-C1'-N1	7.55	113.29	108.00
3	V	12	DC	O4'-C1'-N1	7.51	113.26	108.00
2	E	9	DG	O4'-C4'-C3'	-7.23	101.61	104.50
2	F	9	DG	C4'-C3'-C2'	-7.12	96.69	103.10
3	W	13	DC	O4'-C1'-N1	6.88	112.82	108.00
3	V	1	DA	P-O3'-C3'	6.82	127.88	119.70
3	V	9	DG	O4'-C4'-C3'	-6.53	101.89	104.50
2	F	7	DA	O4'-C4'-C3'	-6.50	101.90	104.50
3	V	14	DT	N3-C4-O4	6.38	123.73	119.90
3	W	6	DT	N3-C4-O4	6.37	123.72	119.90
2	E	14	DT	C4'-C3'-C2'	-6.31	97.42	103.10
2	E	8	DG	C4'-C3'-C2'	-6.23	97.50	103.10
2	F	9	DG	O4'-C4'-C3'	-6.16	102.04	104.50
3	W	2	DG	P-O3'-C3'	6.07	126.98	119.70
3	W	5	DG	C3'-C2'-C1'	-5.92	95.40	102.50
3	V	15	DA	O4'-C1'-N9	5.79	112.05	108.00
3	V	11	DC	O4'-C4'-C3'	-5.67	102.23	104.50
3	V	11	DC	O4'-C1'-N1	5.60	111.92	108.00
3	V	16	DC	C1'-O4'-C4'	-5.60	104.50	110.10
1	S	1473	LEU	CA-CB-CG	5.54	128.05	115.30
3	W	17	DG	N1-C6-O6	5.36	123.11	119.90
3	W	14	DT	C6-N1-C2	-5.28	118.66	121.30
3	W	5	DG	O4'-C1'-N9	5.28	111.69	108.00
3	W	6	DT	C5-C4-O4	-5.25	121.22	124.90
2	E	14	DT	N3-C4-O4	5.14	122.98	119.90
3	V	12	DC	O4'-C1'-C2'	5.09	109.98	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	8	DG	P-O3'-C3'	5.07	125.78	119.70
2	F	19	DC	C1'-O4'-C4'	-5.04	105.06	110.10
3	W	5	DG	C1'-O4'-C4'	-5.00	105.10	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	572	THR	Peptide
1	U	572	THR	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	B	5689	0	5712	310	0
1	D	5692	0	5704	271	0
1	S	5694	0	5731	296	0
1	U	5689	0	5721	296	0
2	E	410	0	225	24	0
2	F	410	0	225	19	0
3	V	410	0	224	26	0
3	W	369	0	201	16	0
4	E	66	0	54	9	0
4	W	66	0	54	12	0
All	All	24495	0	23851	1204	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 25.

All (1204) 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:D:439:ALA:HB1	1:D:583:LEU:HB2	1.27	1.14
1:B:468:ARG:HG3	1:B:468:ARG:HH21	1.12	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ARG:HG2	1:B:471:ARG:HH11	0.92	1.08
1:S:1005:PRO:HA	1:S:1006:GLN:CB	1.85	1.07
1:S:1003:GLU:HA	1:S:1004:LEU:HB3	1.12	1.05
1:U:1002:ALA:HB3	1:U:1003:GLU:HA	1.38	1.04
1:D:1272:ARG:HH11	1:D:1272:ARG:HG2	1.13	1.04
1:U:1432:ARG:NH1	1:U:1432:ARG:HG3	1.61	1.04
1:B:630:ARG:HG2	1:B:630:ARG:HH11	1.14	1.03
1:U:1432:ARG:CG	1:U:1432:ARG:HH11	1.74	1.01
2:E:2:DG:H2''	2:E:3:DC:O5'	1.59	1.00
1:B:1122:ARG:HB3	1:B:1122:ARG:HH11	1.24	1.00
1:D:1279:GLU:HG2	1:D:1282:ARG:NH1	1.78	0.99
1:S:1003:GLU:HA	1:S:1004:LEU:CB	1.91	0.99
1:U:1432:ARG:HG3	1:U:1432:ARG:HH11	0.82	0.98
1:S:1003:GLU:CA	1:S:1004:LEU:HB3	1.93	0.98
1:B:471:ARG:CG	1:B:471:ARG:HH11	1.76	0.98
4:E:1021[A]:RXV:H141	4:E:1021[A]:RXV:H33	1.45	0.97
1:B:515:HIS:HD2	1:B:1025:TYR:CE2	1.82	0.96
1:B:468:ARG:HH21	1:B:468:ARG:CG	1.76	0.96
1:D:1388:LEU:HD13	1:D:1438:ARG:HG3	1.46	0.96
1:B:1325:THR:HB	1:B:1326:PRO:HD3	1.48	0.95
4:W:1020[B]:RXV:H33	4:W:1020[B]:RXV:H142	1.46	0.95
1:B:439:ALA:HB1	1:B:583:LEU:HB2	1.46	0.95
1:B:1243:MET:CE	1:B:1331:PHE:HB2	1.98	0.94
1:S:1247:ALA:HB2	1:S:1261:VAL:HG13	1.47	0.94
1:D:1139:ILE:HD12	1:D:1161:PRO:HD3	1.50	0.93
1:B:471:ARG:NH1	1:B:471:ARG:HG2	1.72	0.93
1:S:1002:ALA:HA	1:S:1003:GLU:O	1.68	0.93
1:S:1299:ARG:HD2	1:S:1299:ARG:H	1.34	0.93
1:S:1245:SER:HB3	1:S:1264:ILE:HA	1.47	0.93
1:B:580:TYR:HD2	1:B:586:MET:HG2	1.34	0.93
1:S:1273:MET:HG3	1:S:1326:PRO:HG2	1.51	0.91
1:D:1079:HIS:CD2	1:D:1081:HIS:HD2	1.89	0.91
1:S:1325:THR:HB	1:S:1326:PRO:HD2	1.53	0.89
1:U:1200:LYS:HG3	1:U:1470:ARG:HH21	1.34	0.89
1:D:1184:PRO:HG3	1:D:1331:PHE:CE2	2.08	0.88
2:E:12:DC:H2''	2:E:13:DC:H5''	1.55	0.88
1:U:548:THR:HB	1:U:576:SER:HB3	1.54	0.87
1:B:1309:ARG:NH2	1:B:1312:ALA:HB2	1.89	0.87
1:B:1054:ASN:HB2	1:B:1136:LEU:HD13	1.53	0.87
1:D:1080:PRO:HG3	1:D:1150:TYR:CG	2.09	0.86
2:E:12:DC:C2'	2:E:13:DC:H5''	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1230:ILE:HG13	1:U:1241:ILE:HD11	1.57	0.86
1:U:1272:ARG:CG	1:U:1272:ARG:HH11	1.89	0.86
1:B:630:ARG:HG2	1:B:630:ARG:NH1	1.90	0.85
1:D:622:MET:HE2	1:D:622:MET:HA	1.59	0.85
1:D:1272:ARG:HG2	1:D:1272:ARG:NH1	1.92	0.84
1:S:1325:THR:HB	1:S:1326:PRO:CD	2.06	0.84
1:S:1067:SER:HA	1:S:1070:ILE:HD12	1.58	0.84
1:B:1122:ARG:HH11	1:B:1122:ARG:CB	1.91	0.84
1:B:1361:THR:HG23	1:B:1364:ARG:HH12	1.42	0.84
1:B:1040:ASP:O	1:B:1166:ASN:HB3	1.78	0.83
1:U:1394:ILE:O	1:U:1398:ILE:HD12	1.78	0.83
1:D:1279:GLU:HG2	1:D:1282:ARG:HH11	1.40	0.83
1:U:1002:ALA:CB	1:U:1003:GLU:HA	2.07	0.83
1:B:1122:ARG:HB3	1:B:1122:ARG:NH1	1.93	0.83
4:W:1020[B]:RXV:C33	4:W:1020[B]:RXV:H142	2.08	0.83
1:D:1119:ALA:HB1	1:D:1123:PHE:HD1	1.44	0.83
1:U:1003:GLU:O	1:U:1004:LEU:HB2	1.79	0.82
1:U:1144:ILE:HD12	1:U:1157:PRO:HB3	1.62	0.81
1:B:1218:PHE:HD1	1:B:1266:PHE:HB2	1.44	0.81
1:U:515:HIS:CE1	1:U:519:LEU:HD11	2.15	0.81
1:S:1143:THR:HB	1:S:1362:VAL:HG13	1.61	0.81
1:B:1309:ARG:HH22	1:B:1312:ALA:HB2	1.42	0.81
1:U:1175:ILE:HD12	3:W:5:DG:C2	2.16	0.81
1:D:564:LYS:O	1:D:568:GLU:HG3	1.81	0.81
1:D:547:LEU:CD1	1:D:575:TRP:HB3	2.11	0.80
1:S:540:ALA:HA	1:S:603:LEU:CD2	2.10	0.80
1:D:1049:ILE:HA	1:D:1074:VAL:HG21	1.63	0.80
1:U:1048:ARG:HD3	1:U:1078:TYR:HB3	1.63	0.80
1:B:438:SER:HB2	2:E:10:DG:OP1	1.82	0.80
1:B:1243:MET:HE2	1:B:1331:PHE:HB2	1.62	0.80
1:B:1325:THR:HB	1:B:1326:PRO:CD	2.11	0.79
1:S:499:ARG:HH11	1:S:499:ARG:HG3	1.46	0.79
1:B:464:VAL:HG21	1:B:527:PHE:HE1	1.46	0.79
1:B:580:TYR:CD2	1:B:586:MET:HG2	2.18	0.79
1:B:1010:ASN:ND2	1:U:1010:ASN:HD21	1.81	0.79
1:D:1119:ALA:HB1	1:D:1123:PHE:CD1	2.17	0.78
1:B:468:ARG:HG3	1:B:468:ARG:NH2	1.88	0.78
1:U:1144:ILE:CD1	1:U:1157:PRO:HB3	2.14	0.78
1:B:565:LEU:HB2	1:U:1004:LEU:HD12	1.64	0.78
1:B:515:HIS:CD2	1:B:1025:TYR:CE2	2.69	0.78
1:B:1047:ARG:HG3	1:B:1160:LEU:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1090:MET:HA	1:B:1093:MET:HE3	1.66	0.77
1:B:1206:ILE:HD13	1:B:1206:ILE:H	1.49	0.77
1:U:450:ARG:HG3	1:U:450:ARG:HH21	1.48	0.77
1:D:1206:ILE:HG21	1:D:1235:GLU:HG2	1.66	0.77
1:U:509:ALA:O	1:U:544:LEU:HD13	1.85	0.77
1:U:1200:LYS:HG3	1:U:1470:ARG:NH2	2.00	0.77
1:D:1206:ILE:HG21	1:D:1235:GLU:CG	2.15	0.76
1:D:544:LEU:HD23	1:D:545:TYR:CE1	2.21	0.76
1:S:552:GLN:HB3	1:S:554:TYR:HE1	1.50	0.76
1:D:591:LEU:O	1:D:591:LEU:HG	1.86	0.76
1:S:1093:MET:HA	1:S:1099:TYR:CD1	2.20	0.75
1:D:1386:ILE:O	1:D:1390:HIS:HB2	1.87	0.75
1:S:552:GLN:HB3	1:S:554:TYR:CE1	2.20	0.75
1:S:1002:ALA:HA	1:S:1003:GLU:C	2.08	0.75
1:B:525:TYR:HA	1:B:532:ILE:HD11	1.69	0.74
1:U:1446:ASN:HA	1:U:1449:LEU:HD12	1.67	0.74
1:U:1388:LEU:HD13	1:U:1438:ARG:HG2	1.69	0.74
1:U:439:ALA:HB1	1:U:583:LEU:HD12	1.67	0.74
1:U:538:TYR:CE2	1:U:605:GLN:HG3	2.23	0.74
1:S:1035:LEU:CD2	1:S:1036:PRO:HD3	2.17	0.74
1:D:495:LEU:HG	1:D:495:LEU:O	1.87	0.74
2:E:6:DT:H2"	2:E:7:DA:O5'	1.87	0.73
1:U:1005:PRO:HA	1:U:1006:GLN:C	2.09	0.73
1:D:466:LYS:HE2	1:D:623:GLY:O	1.87	0.73
1:S:1402:ASP:O	1:U:1436:LEU:HB2	1.89	0.73
1:D:458:ARG:NH2	2:F:11:DC:H5"	2.04	0.73
1:B:1469:VAL:O	1:B:1473:LEU:HG	1.88	0.72
1:D:1079:HIS:CD2	1:D:1081:HIS:CD2	2.74	0.72
1:S:1363:VAL:HG12	1:S:1465:LEU:HD11	1.70	0.72
1:S:1107:GLN:HG2	1:S:1125:GLU:HG3	1.72	0.72
1:B:556:VAL:HG13	1:B:561:GLU:HB2	1.70	0.72
1:D:549:GLN:HG2	1:D:573:PRO:HB2	1.72	0.72
1:U:1004:LEU:O	1:U:1006:GLN:HB3	1.89	0.72
1:U:447:ARG:HD3	1:U:454:ILE:HD11	1.71	0.72
1:D:1027:MET:O	1:D:1031:VAL:HG22	1.89	0.72
1:B:1448:LEU:O	1:B:1452:ILE:HG13	1.89	0.72
1:D:1296:THR:HG23	1:D:1302:VAL:HA	1.70	0.71
1:D:547:LEU:HD11	1:D:575:TRP:HB3	1.72	0.71
1:U:1356:LEU:O	1:U:1356:LEU:HD12	1.90	0.71
1:D:640:ALA:HB3	1:D:641:ASN:HA	1.70	0.71
1:B:1243:MET:HE3	1:B:1331:PHE:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1042:LEU:HB3	1:U:1046:HIS:HB2	1.72	0.71
1:S:455:LEU:O	1:S:455:LEU:HG	1.90	0.71
1:D:1195:VAL:CG2	1:D:1352:LEU:HD22	2.20	0.71
3:V:10:DG:H2"	3:V:11:DC:H5"	1.71	0.71
1:B:1013:ASN:HB3	1:B:1016:SER:HB2	1.73	0.71
4:E:1021[A]:RXV:H141	4:E:1021[A]:RXV:C33	2.21	0.70
1:S:1135:LEU:HG	1:S:1164:PHE:CE2	2.27	0.70
1:S:1199:SER:HB2	1:S:1466:LEU:HD11	1.73	0.70
1:U:1042:LEU:HD12	1:U:1047:ARG:HG3	1.74	0.70
1:B:626:VAL:HG21	2:F:17:DG:H3'	1.73	0.70
1:B:430:GLU:OE2	1:B:452:GLN:HG2	1.92	0.70
1:U:1272:ARG:HH11	1:U:1272:ARG:HG2	1.56	0.70
1:B:1469:VAL:HG12	1:B:1473:LEU:HD11	1.73	0.70
1:S:522:THR:HA	1:S:618:PHE:HE2	1.56	0.70
1:U:1048:ARG:HD2	1:U:1079:HIS:HB2	1.72	0.69
1:B:1178:GLY:H	2:F:17:DG:H5"	1.56	0.69
1:S:1273:MET:HG3	1:S:1326:PRO:CG	2.19	0.69
1:D:1011:GLU:HG2	1:D:1012:ARG:H	1.56	0.69
1:U:1090:MET:HA	1:U:1093:MET:CE	2.22	0.69
1:U:450:ARG:HH21	1:U:450:ARG:CG	2.05	0.69
1:B:575:TRP:N	1:B:575:TRP:CD1	2.59	0.69
1:U:1310:LYS:O	1:U:1311:ASP:HB2	1.93	0.69
1:B:1004:LEU:CB	1:B:1005:PRO:CD	2.71	0.69
1:B:1218:PHE:CD1	1:B:1266:PHE:HB2	2.28	0.69
1:D:1179:MET:O	2:E:17:DG:H4'	1.91	0.69
1:B:630:ARG:CG	1:B:630:ARG:HH11	2.00	0.69
1:S:1218:PHE:HE2	1:S:1224:ILE:HD11	1.56	0.68
1:S:1326:PRO:O	1:S:1328:GLN:N	2.27	0.68
1:U:565:LEU:O	1:U:569:LEU:HD12	1.93	0.68
1:B:1004:LEU:O	1:B:1006:GLN:HG3	1.94	0.68
1:D:1050:LEU:HD21	1:D:1093:MET:SD	2.34	0.68
1:S:1026:ALA:O	1:S:1030:ILE:HG12	1.94	0.68
1:S:1274:ILE:HG22	1:S:1292:LEU:HD21	1.75	0.68
1:B:1325:THR:CB	1:B:1326:PRO:HD3	2.24	0.68
1:D:1232:ARG:HD2	1:D:1239:GLY:HA2	1.76	0.68
1:S:418:LEU:HD12	1:S:454:ILE:O	1.94	0.68
1:D:622:MET:CE	1:D:622:MET:HA	2.23	0.67
1:D:524:PHE:O	1:D:528:MET:HB2	1.94	0.67
1:B:1010:ASN:HD21	1:U:1010:ASN:HD21	1.41	0.67
1:D:1363:VAL:HG21	1:D:1469:VAL:HG22	1.76	0.67
1:D:565:LEU:O	1:D:565:LEU:HD12	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1381:LEU:O	1:U:1385:ARG:HG3	1.94	0.67
2:E:2:DG:C2'	2:E:3:DC:O5'	2.40	0.67
1:U:515:HIS:O	1:U:519:LEU:HD12	1.95	0.67
1:B:505:ILE:HD11	1:B:524:PHE:HE1	1.60	0.67
1:B:1264:ILE:HB	1:B:1265:PRO:CD	2.25	0.67
4:W:1020[A]:RXV:H142	4:W:1020[A]:RXV:H33	1.77	0.66
1:U:1008:ARG:O	1:U:1009:ILE:HG13	1.95	0.66
1:U:1199:SER:HB2	1:U:1466:LEU:HD11	1.74	0.66
1:U:1045:VAL:HG12	1:U:1079:HIS:HE1	1.60	0.66
2:E:8:DG:C2'	2:E:9:DG:O5'	2.44	0.66
1:D:1274:ILE:CG2	1:D:1292:LEU:HD21	2.25	0.66
1:D:1094:ALA:HB2	1:D:1104:VAL:HB	1.75	0.66
1:D:1139:ILE:HD12	1:D:1161:PRO:CD	2.24	0.66
1:B:1390:HIS:O	1:B:1394:ILE:HG12	1.96	0.66
1:B:1426:LEU:HB3	1:D:1431:ARG:HB3	1.76	0.66
1:S:1252:ARG:NH2	1:S:1256:ARG:HE	1.94	0.66
1:D:1056:GLN:HB2	1:D:1058:MET:HG3	1.77	0.66
1:D:1059:THR:HB	1:D:1060:PRO:CD	2.26	0.66
1:S:606:VAL:CG1	1:S:1014:ILE:HG13	2.26	0.66
1:U:1120:ALA:HB3	1:U:1123:PHE:CD1	2.31	0.66
1:S:495:LEU:HG	1:S:495:LEU:O	1.94	0.66
1:B:1053:LEU:HD21	1:B:1070:ILE:HD13	1.77	0.65
1:U:1090:MET:HA	1:U:1093:MET:HE2	1.79	0.65
1:B:1054:ASN:HB2	1:B:1136:LEU:CD1	2.27	0.65
1:D:579:ARG:HG2	1:D:580:TYR:H	1.61	0.65
1:B:1313:ASN:O	1:B:1316:VAL:HG12	1.97	0.65
1:B:1094:ALA:HB2	1:B:1104:VAL:CG1	2.27	0.65
1:S:1120:ALA:HB3	1:S:1123:PHE:HD1	1.60	0.65
1:B:556:VAL:HG22	1:U:1004:LEU:HD13	1.79	0.65
1:S:570:ASN:N	1:S:571:PRO:CD	2.60	0.65
1:B:556:VAL:HG13	1:B:561:GLU:CB	2.27	0.65
1:S:1218:PHE:CE2	1:S:1224:ILE:HD11	2.32	0.65
1:B:1402:ASP:O	1:D:1434:THR:HB	1.97	0.65
1:D:1189:THR:HG23	1:D:1477:ARG:HD2	1.78	0.65
1:U:570:ASN:CB	1:U:571:PRO:HD3	2.27	0.65
1:S:1042:LEU:HD22	1:S:1046:HIS:HB2	1.78	0.64
1:B:1325:THR:CB	1:B:1326:PRO:CD	2.73	0.64
3:V:11:DC:H1'	3:V:12:DC:H5'	1.80	0.64
1:S:1238:ARG:HA	1:S:1333:VAL:O	1.97	0.64
1:U:1048:ARG:HD3	1:U:1078:TYR:CB	2.27	0.64
1:B:489:ILE:HD13	1:B:489:ILE:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ARG:NH2	1:B:468:ARG:CG	2.46	0.64
1:U:443:THR:HG22	1:U:454:ILE:HD13	1.79	0.64
1:B:1141:LYS:N	1:B:1141:LYS:HD2	2.12	0.64
1:D:464:VAL:HG21	1:D:523:PHE:HA	1.79	0.64
1:D:1270:LYS:O	1:D:1274:ILE:HG13	1.98	0.64
1:S:590:GLN:O	1:S:594:THR:HG23	1.97	0.64
1:U:1177:VAL:HG22	3:V:16:DC:H4'	1.80	0.64
1:S:601:ARG:HH12	1:S:603:LEU:HD12	1.63	0.64
1:B:1391:ILE:HG21	1:D:1399:ARG:CZ	2.27	0.64
1:S:1135:LEU:CD2	1:S:1162:ALA:HA	2.28	0.64
1:S:505:ILE:HG21	1:S:517:ARG:HG2	1.80	0.64
1:U:579:ARG:HG3	1:U:580:TYR:N	2.13	0.64
1:D:1272:ARG:CG	1:D:1272:ARG:HH11	1.98	0.63
1:U:1241:ILE:HG22	1:U:1331:PHE:HB3	1.80	0.63
1:S:1135:LEU:HD23	1:S:1162:ALA:HA	1.79	0.63
2:E:8:DG:H2'	2:E:9:DG:O5'	1.98	0.63
1:D:1059:THR:HG22	1:D:1133:LEU:HD21	1.80	0.63
1:S:1445:TYR:CD1	1:S:1449:LEU:HD11	2.34	0.63
1:S:461:ILE:HG23	1:S:462:LEU:N	2.13	0.63
1:B:1068:ALA:HB1	4:E:1021[A]:RXV:S26	2.38	0.63
1:D:1080:PRO:HG3	1:D:1150:TYR:CD1	2.32	0.63
1:S:1035:LEU:HD23	1:S:1036:PRO:HD3	1.80	0.63
1:D:1104:VAL:HG12	1:D:1105:ASP:N	2.12	0.63
3:V:18:DG:H2''	3:V:19:DC:O5'	1.97	0.63
1:D:572:THR:N	1:D:573:PRO:CD	2.62	0.63
1:U:1054:ASN:HB2	1:U:1128:MET:CE	2.29	0.63
1:S:525:TYR:CE1	1:S:529:ARG:HD2	2.33	0.63
1:B:1191:LEU:O	1:B:1195:VAL:HG23	1.98	0.63
1:S:606:VAL:HG11	1:S:1014:ILE:HG13	1.80	0.63
1:B:1178:GLY:N	2:F:17:DG:H5''	2.13	0.63
1:S:1347:ASN:OD1	1:S:1350:GLU:HG3	1.98	0.63
1:B:1361:THR:HG23	1:B:1364:ARG:NH1	2.13	0.63
1:U:447:ARG:HD3	1:U:454:ILE:CD1	2.29	0.63
1:S:1252:ARG:HH22	1:S:1256:ARG:HE	1.45	0.63
1:B:439:ALA:CB	1:B:583:LEU:HB2	2.25	0.62
1:S:1134:GLU:O	1:S:1163:ARG:HG2	1.99	0.62
1:U:1143:THR:HB	1:U:1362:VAL:HG13	1.80	0.62
1:S:597:ASN:HD22	1:S:598:PRO:N	1.97	0.62
1:S:643:ASP:O	1:S:1002:ALA:N	2.32	0.62
1:U:1384:LEU:HD23	1:U:1425:ILE:HD12	1.82	0.62
1:B:501:HIS:HA	1:B:536:TYR:CD1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1130:LYS:O	1:U:1133:LEU:HB2	1.99	0.62
1:B:1005:PRO:HG2	1:U:565:LEU:HD13	1.81	0.62
1:D:1225:LEU:HD21	1:D:1244:ARG:HG3	1.81	0.62
1:S:1005:PRO:CA	1:S:1006:GLN:CB	2.70	0.62
1:S:597:ASN:HD22	1:S:598:PRO:CD	2.13	0.62
1:D:458:ARG:NH2	2:F:11:DC:C5'	2.62	0.62
1:B:430:GLU:HB3	1:B:502:LYS:HB2	1.82	0.62
1:B:488:GLY:C	1:B:489:ILE:HD13	2.20	0.62
1:D:1014:ILE:HG23	1:D:1015:THR:N	2.15	0.62
1:U:1368:GLN:HG3	1:U:1459:LEU:HD21	1.81	0.62
1:S:604:LEU:N	1:S:604:LEU:HD23	2.14	0.62
1:U:1174:GLY:O	1:U:1180:ALA:HB1	2.00	0.62
1:B:515:HIS:CD2	1:B:1025:TYR:CZ	2.88	0.62
1:S:447:ARG:HD3	1:S:454:ILE:HD11	1.80	0.62
1:U:1219:PRO:HD2	1:U:1266:PHE:CE1	2.35	0.62
1:U:1313:ASN:ND2	1:U:1315:SER:HB2	2.15	0.62
1:D:1074:VAL:HG12	1:D:1086:ILE:HD13	1.82	0.62
1:S:1388:LEU:HD23	1:S:1391:ILE:HD13	1.82	0.62
1:D:622:MET:HE1	1:D:1022:PHE:HE1	1.63	0.61
1:D:547:LEU:HD11	1:D:575:TRP:CG	2.34	0.61
1:B:589:ASP:HB3	1:D:1298:LEU:HD21	1.81	0.61
1:U:431:ILE:HG23	1:U:503:ILE:HA	1.81	0.61
1:S:1468:LEU:HD12	1:S:1468:LEU:O	1.99	0.61
2:F:8:DG:H2'	2:F:9:DG:O4'	1.99	0.61
1:U:511:VAL:HG11	1:U:1028:SER:HB2	1.82	0.61
1:B:509:ALA:HB3	1:B:544:LEU:HD13	1.81	0.61
1:D:1272:ARG:CG	1:D:1272:ARG:NH1	2.61	0.61
1:B:1148:ASP:OD1	1:B:1155:ARG:NH1	2.34	0.61
1:S:502:LYS:HG2	1:S:538:TYR:HE1	1.64	0.61
1:S:1080:PRO:HB3	1:S:1150:TYR:CD1	2.35	0.61
1:U:1031:VAL:HG23	1:U:1032:ALA:H	1.66	0.61
1:U:1278:ALA:HB2	1:U:1292:LEU:HD22	1.83	0.61
1:S:540:ALA:HA	1:S:603:LEU:HD23	1.82	0.61
1:S:499:ARG:CG	1:S:499:ARG:HH11	2.14	0.61
1:B:1366:ARG:O	1:B:1366:ARG:HG2	2.00	0.61
1:U:1388:LEU:CD1	1:U:1438:ARG:HG2	2.30	0.60
1:U:1055:GLU:HG3	1:U:1078:TYR:OH	2.01	0.60
1:B:464:VAL:HG21	1:B:527:PHE:CE1	2.32	0.60
1:U:1054:ASN:HB2	1:U:1128:MET:HE1	1.82	0.60
1:U:1058:MET:CE	1:U:1065:LYS:HG3	2.31	0.60
1:D:1092:ARG:HA	1:D:1095:GLN:HE21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:ALA:CB	1:D:583:LEU:HB2	2.18	0.60
1:S:1448:LEU:O	1:S:1452:ILE:HG13	2.01	0.60
1:S:1175:ILE:HD12	3:V:5:DG:C2	2.36	0.60
1:B:1430:LEU:HA	1:B:1433:LEU:HD12	1.83	0.60
1:S:1035:LEU:HD22	1:S:1036:PRO:HD3	1.83	0.60
1:S:1438:ARG:HD2	1:S:1438:ARG:O	2.02	0.60
1:S:522:THR:HA	1:S:618:PHE:CE2	2.37	0.60
1:U:457:LEU:HD23	1:U:457:LEU:N	2.15	0.60
1:S:592:TRP:HA	1:S:596:MET:HB2	1.84	0.59
1:S:1385:ARG:NH2	1:S:1442:GLU:OE1	2.34	0.59
1:B:1346:ILE:HB	1:B:1350:GLU:HG3	1.84	0.59
1:U:1176:ALA:HB3	1:U:1179:MET:O	2.01	0.59
2:E:11:DC:C2	4:E:1021[A]:RXV:N7	2.71	0.59
1:D:1177:VAL:HG22	2:E:16:DC:H4'	1.84	0.59
1:B:555:TYR:HE1	1:B:594:THR:HG21	1.66	0.59
1:B:556:VAL:CG1	1:B:561:GLU:HB2	2.33	0.59
1:D:572:THR:H	1:D:573:PRO:HD3	1.66	0.59
1:D:1175:ILE:HD12	2:E:17:DG:N3	2.17	0.59
1:B:1054:ASN:CB	1:B:1136:LEU:HD13	2.29	0.59
1:B:1138:ASP:HA	1:B:1141:LYS:HD3	1.84	0.59
1:B:1230:ILE:HG12	1:B:1241:ILE:HD12	1.84	0.59
1:D:431:ILE:HA	1:D:453:ALA:O	2.02	0.59
1:S:502:LYS:HG2	1:S:538:TYR:CE1	2.37	0.59
1:D:562:LEU:HD23	1:D:566:LYS:HG3	1.85	0.59
1:S:1227:LYS:HA	1:S:1230:ILE:HD13	1.85	0.59
1:S:1075:MET:HE1	4:W:1020[A]:RXV:H30	1.84	0.59
1:D:1101:TYR:HB3	1:D:1131:ILE:HD13	1.84	0.59
1:B:1027:MET:O	1:B:1031:VAL:HG22	2.02	0.59
3:V:10:DG:H2''	3:V:11:DC:C5'	2.33	0.59
1:D:544:LEU:HD23	1:D:545:TYR:HE1	1.66	0.59
1:B:547:LEU:HD21	1:B:575:TRP:CE3	2.38	0.59
1:D:493:PHE:CE2	1:D:530:PRO:HB2	2.38	0.59
1:U:1272:ARG:HG3	1:U:1272:ARG:HH11	1.65	0.59
1:B:1053:LEU:HD21	1:B:1070:ILE:HG21	1.85	0.59
1:B:1245:SER:OG	1:B:1327:LEU:HD12	2.02	0.59
1:B:1353:VAL:O	1:B:1357:GLU:HG2	2.03	0.58
1:D:557:TYR:CD1	1:D:557:TYR:N	2.70	0.58
1:D:1256:ARG:HB3	1:D:1310:LYS:HB3	1.85	0.58
1:S:1262:THR:O	1:S:1302:VAL:HB	2.03	0.58
1:U:601:ARG:HD2	1:U:603:LEU:HG	1.85	0.58
1:B:529:ARG:N	1:B:530:PRO:HD2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1045:VAL:HG23	1:D:1079:HIS:CE1	2.39	0.58
1:D:621:LEU:HD21	1:D:632:PHE:CE1	2.38	0.58
1:U:1407:ALA:O	1:U:1411:LEU:HD12	2.02	0.58
1:D:427:GLU:HG3	1:D:501:HIS:CD2	2.39	0.58
1:D:1167:LEU:HD11	1:D:1183:ILE:HD12	1.84	0.58
1:S:1187:ASN:HD22	1:S:1484:ARG:HA	1.69	0.58
1:B:1079:HIS:NE2	1:B:1081:HIS:HD2	2.02	0.58
1:U:1003:GLU:O	1:U:1004:LEU:CB	2.50	0.57
1:D:1195:VAL:HG23	1:D:1352:LEU:HD22	1.84	0.57
1:U:1131:ILE:HB	1:U:1480:PHE:CE1	2.39	0.57
1:U:457:LEU:O	1:U:458:ARG:HG2	2.04	0.57
1:B:1160:LEU:HD12	1:B:1160:LEU:N	2.19	0.57
1:S:416:GLY:O	1:S:417:LYS:HB3	2.03	0.57
3:V:11:DC:C2	4:W:1020[A]:RXV:N7	2.72	0.57
1:B:1329:THR:HG22	1:B:1330:SER:H	1.70	0.57
1:U:1448:LEU:O	1:U:1452:ILE:HG12	2.04	0.57
3:W:10:DG:H2"	3:W:11:DC:H5"	1.85	0.57
1:B:1347:ASN:OD1	1:B:1350:GLU:HG2	2.05	0.57
1:U:435:GLU:OE2	1:U:508:ASP:HB2	2.04	0.57
1:B:1161:PRO:O	1:B:1163:ARG:HD2	2.05	0.57
1:U:528:MET:HB3	1:U:531:LEU:HB2	1.86	0.57
4:W:1020[B]:RXV:H33	4:W:1020[B]:RXV:C14	2.21	0.57
1:S:1279:GLU:HG3	1:S:1282:ARG:HH22	1.70	0.57
1:U:1049:ILE:HG12	1:U:1074:VAL:HG11	1.87	0.57
1:U:1025:TYR:HE2	1:U:1177:VAL:HG21	1.68	0.57
1:S:1080:PRO:HB3	1:S:1150:TYR:CE1	2.40	0.57
1:S:439:ALA:HB1	1:S:583:LEU:HD12	1.86	0.57
1:U:522:THR:OG1	1:U:622:MET:HG3	2.04	0.57
1:S:544:LEU:HD23	1:S:558:ASN:HA	1.86	0.57
1:S:1251:GLU:H	1:S:1251:GLU:CD	2.05	0.57
1:D:1265:PRO:O	1:D:1268:VAL:HG22	2.05	0.57
1:S:1107:GLN:O	1:S:1107:GLN:HG3	2.05	0.56
1:D:1232:ARG:HG2	1:D:1238:ARG:O	2.05	0.56
1:U:1277:ILE:O	1:U:1281:VAL:HG23	2.05	0.56
1:U:556:VAL:HG12	1:U:557:TYR:N	2.20	0.56
1:S:1143:THR:HB	1:S:1362:VAL:CG1	2.35	0.56
1:B:1090:MET:HA	1:B:1093:MET:CE	2.36	0.56
1:D:509:ALA:HB1	1:D:544:LEU:HB2	1.86	0.56
1:D:1186:HIS:HB2	1:D:1191:LEU:HD11	1.85	0.56
1:S:1402:ASP:HB2	1:U:1436:LEU:HD13	1.87	0.56
3:V:18:DG:H1	3:W:3:DC:H42	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1131:ILE:HD13	1:U:1132:THR:N	2.20	0.56
1:U:431:ILE:CG2	1:U:503:ILE:HG13	2.35	0.56
3:W:14:DT:H2"	3:W:15:DA:H5'	1.86	0.56
1:B:462:LEU:HD21	1:B:472:ILE:HG12	1.86	0.56
1:U:1114:ASP:OD2	1:U:1271:ALA:HB2	2.05	0.56
1:B:1083:ASP:C	1:B:1085:SER:H	2.08	0.56
1:U:1295:GLU:HB2	1:U:1303:ARG:HG2	1.88	0.56
1:B:580:TYR:HD2	1:B:586:MET:CG	2.10	0.56
1:B:1035:LEU:HB2	1:B:1338:LEU:CD1	2.35	0.56
1:B:638:VAL:O	1:B:638:VAL:HG12	2.03	0.56
1:S:1074:VAL:O	1:S:1074:VAL:CG1	2.54	0.56
1:D:547:LEU:HD11	1:D:575:TRP:CB	2.35	0.56
1:S:1073:ASP:OD2	1:S:1077:LYS:HD2	2.05	0.56
1:B:465:GLU:HG3	1:B:622:MET:HB2	1.87	0.56
1:U:463:ASN:ND2	1:U:466:LYS:HE3	2.21	0.56
1:B:585:GLU:HG2	1:B:585:GLU:O	2.05	0.56
1:S:1007:SER:O	1:S:1009:ILE:N	2.39	0.56
1:B:630:ARG:CG	1:B:630:ARG:NH1	2.64	0.56
1:S:1107:GLN:HG2	1:S:1125:GLU:CG	2.35	0.56
1:U:642:LEU:O	1:U:643:ASP:HB2	2.05	0.56
1:B:1064:TYR:CE2	1:B:1107:GLN:HB2	2.41	0.56
1:U:1109:ASN:O	1:U:1118:ALA:HB1	2.06	0.56
1:S:1042:LEU:HD22	1:S:1046:HIS:CB	2.36	0.56
1:B:1230:ILE:HG12	1:B:1241:ILE:CD1	2.35	0.56
1:S:450:ARG:HG3	1:S:451:THR:HG22	1.88	0.56
1:S:541:GLN:CD	1:S:604:LEU:HD21	2.26	0.56
1:D:1438:ARG:HA	1:D:1441:ILE:HD11	1.88	0.56
1:U:1087:TYR:CG	1:U:1121:MET:HE2	2.41	0.56
1:U:1029:VAL:HG22	1:U:1033:ARG:HD2	1.88	0.56
1:S:637:ALA:HB1	1:S:1027:MET:SD	2.46	0.56
1:S:1110:PHE:HE1	1:S:1124:THR:HB	1.70	0.56
1:B:1216:PRO:HB2	1:B:1218:PHE:HE2	1.71	0.55
1:B:505:ILE:HD11	1:B:524:PHE:CE1	2.41	0.55
1:S:1252:ARG:HB2	1:S:1258:ARG:HH11	1.71	0.55
1:D:1249:ILE:HG23	1:D:1259:ILE:HG12	1.88	0.55
1:U:1313:ASN:HD21	1:U:1315:SER:HB2	1.70	0.55
1:U:1183:ILE:N	1:U:1183:ILE:HD12	2.21	0.55
1:B:578:ALA:O	1:B:579:ARG:HB3	2.06	0.55
1:U:1025:TYR:CE2	1:U:1177:VAL:HG21	2.41	0.55
1:D:1274:ILE:HG22	1:D:1292:LEU:HD21	1.87	0.55
1:S:1292:LEU:CD1	1:S:1306:ILE:HG23	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1007:SER:O	1:D:1009:ILE:N	2.38	0.55
1:S:1188:LEU:O	1:S:1192:ILE:HG12	2.06	0.55
1:U:1339:VAL:O	1:U:1340:ASN:HB3	2.06	0.55
3:V:1:DA:H2"	3:V:2:DG:O5'	2.05	0.55
1:D:640:ALA:HB3	1:D:641:ASN:CA	2.34	0.55
1:B:461:ILE:HD11	1:B:477:GLU:OE1	2.06	0.55
1:B:1064:TYR:HB3	1:B:1125:GLU:HB3	1.87	0.55
1:U:1135:LEU:CD2	1:U:1162:ALA:HA	2.36	0.55
1:D:1388:LEU:HD12	1:D:1441:ILE:HD11	1.86	0.55
1:B:1309:ARG:HG2	1:B:1310:LYS:H	1.70	0.55
1:D:511:VAL:O	1:D:514:ALA:HB3	2.06	0.55
1:U:511:VAL:HG11	1:U:1028:SER:CB	2.36	0.55
1:U:1401:SER:HB3	1:U:1406:VAL:HG13	1.88	0.55
1:B:1238:ARG:HH22	2:F:19:DC:P	2.29	0.55
1:B:1472:GLU:O	1:B:1476:ILE:HG12	2.06	0.55
1:D:1422:ALA:O	1:D:1426:LEU:HG	2.07	0.55
1:D:1054:ASN:HA	1:D:1128:MET:CE	2.37	0.55
1:U:1120:ALA:HB3	1:U:1123:PHE:HD1	1.67	0.55
1:S:517:ARG:O	1:S:521:LEU:HG	2.07	0.55
1:S:617:THR:HG21	1:S:1015:THR:HG23	1.89	0.55
1:S:1210:MET:HA	1:S:1213:ILE:O	2.07	0.55
1:U:1183:ILE:HG13	1:U:1335:MET:HG2	1.89	0.54
1:S:1277:ILE:CD1	1:S:1321:LEU:HD22	2.37	0.54
2:E:11:DC:H2"	2:E:12:DC:H5"	1.88	0.54
3:V:14:DT:H2'	3:V:15:DA:H8	1.72	0.54
1:U:1049:ILE:HD13	1:U:1090:MET:HB3	1.89	0.54
1:B:464:VAL:CG2	1:B:527:PHE:HE1	2.16	0.54
1:B:1049:ILE:HD13	1:B:1090:MET:HB2	1.88	0.54
1:S:570:ASN:N	1:S:571:PRO:HD3	2.21	0.54
1:U:1218:PHE:HB3	1:U:1266:PHE:HD1	1.73	0.54
1:B:1234:TYR:CD1	1:B:1348:LEU:HD22	2.42	0.54
1:S:1316:VAL:O	1:S:1320:ASN:HB2	2.06	0.54
1:S:554:TYR:N	1:S:554:TYR:CD1	2.72	0.54
1:B:1264:ILE:HB	1:B:1265:PRO:HD2	1.89	0.54
1:S:1031:VAL:HA	1:S:1338:LEU:HD11	1.89	0.54
1:S:501:HIS:HA	1:S:536:TYR:CD1	2.42	0.54
1:D:549:GLN:OE1	1:D:569:LEU:HD22	2.08	0.54
1:B:447:ARG:NH2	1:B:452:GLN:O	2.40	0.54
1:S:467:ALA:HB3	1:S:472:ILE:HD11	1.89	0.54
1:S:1281:VAL:HG21	1:S:1289:ILE:HG21	1.89	0.54
1:U:1446:ASN:HA	1:U:1449:LEU:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:529:ARG:N	1:S:530:PRO:HD2	2.22	0.54
1:S:544:LEU:HD12	1:S:544:LEU:O	2.07	0.54
1:U:1045:VAL:HG12	1:U:1079:HIS:CE1	2.42	0.54
1:S:525:TYR:CD1	1:S:529:ARG:HD2	2.42	0.54
1:U:1110:PHE:CE1	1:U:1124:THR:HB	2.43	0.54
2:E:13:DC:H6	2:E:13:DC:C5'	2.21	0.54
1:D:458:ARG:HH22	2:F:11:DC:C5'	2.20	0.54
1:D:1011:GLU:HG2	1:D:1012:ARG:N	2.22	0.54
1:U:1414:ARG:HB3	1:U:1415:PHE:CD1	2.42	0.54
1:U:1391:ILE:HG23	1:U:1392:ASP:H	1.72	0.54
1:B:547:LEU:CD2	1:B:577:ILE:HB	2.38	0.54
1:U:1425:ILE:HG22	1:U:1426:LEU:HD23	1.90	0.54
1:B:1230:ILE:HA	1:B:1241:ILE:HD11	1.90	0.54
1:B:644:PHE:CG	1:B:1002:ALA:N	2.76	0.54
1:S:1144:ILE:HD12	1:S:1144:ILE:O	2.07	0.54
1:S:1292:LEU:HD12	1:S:1306:ILE:HG23	1.90	0.54
1:D:1373:LYS:HD3	1:D:1373:LYS:N	2.22	0.54
1:U:529:ARG:N	1:U:530:PRO:CD	2.71	0.53
1:S:1168:LEU:O	1:S:1185:PRO:HA	2.09	0.53
1:U:1080:PRO:HG3	1:U:1150:TYR:CD1	2.43	0.53
1:B:564:LYS:O	1:B:568:GLU:HG2	2.08	0.53
1:B:1260:VAL:O	1:B:1260:VAL:HG12	2.07	0.53
1:D:619:GLU:HG2	1:D:619:GLU:O	2.07	0.53
1:U:1175:ILE:HD12	3:W:5:DG:N1	2.24	0.53
1:S:1169:ALA:O	1:S:1185:PRO:HB3	2.09	0.53
1:U:1090:MET:HA	1:U:1093:MET:HE3	1.89	0.53
1:S:1042:LEU:HD13	1:S:1047:ARG:HB2	1.90	0.53
1:S:1430:LEU:HD23	1:S:1433:LEU:HD12	1.91	0.53
1:U:1002:ALA:CB	1:U:1003:GLU:CA	2.84	0.53
1:D:470:ASP:HA	1:D:473:LEU:HD12	1.91	0.53
1:U:432:PHE:CE2	1:U:504:VAL:HG11	2.44	0.53
3:W:8:DG:H2'	3:W:9:DG:O4'	2.08	0.53
1:S:581:LYS:HB3	1:S:585:GLU:OE2	2.08	0.53
1:U:457:LEU:C	1:U:458:ARG:HG2	2.29	0.53
1:B:465:GLU:HG3	1:B:622:MET:CB	2.39	0.53
1:B:1040:ASP:OD2	1:B:1159:VAL:HG23	2.09	0.53
3:W:14:DT:C2'	3:W:15:DA:H5'	2.39	0.53
1:D:1259:ILE:HB	1:D:1306:ILE:HD12	1.91	0.53
1:U:1224:ILE:HG13	1:U:1488:ILE:HG22	1.91	0.53
1:U:1113:MET:SD	1:U:1264:ILE:HD11	2.49	0.53
1:D:622:MET:HE1	1:D:1022:PHE:CE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1431:ARG:HH12	1:D:1432:ARG:HD3	1.74	0.53
1:S:417:LYS:HG2	1:S:480:GLN:OE1	2.09	0.53
1:U:418:LEU:C	1:U:418:LEU:HD23	2.29	0.53
1:B:547:LEU:HD22	1:B:577:ILE:HB	1.91	0.53
1:U:431:ILE:HG21	1:U:503:ILE:HG13	1.91	0.53
1:D:1376:ASP:O	1:D:1380:ILE:HG12	2.08	0.53
1:U:430:GLU:HB3	1:U:502:LYS:HB2	1.91	0.53
1:D:625:VAL:HB	1:D:628:ASN:HB2	1.90	0.53
1:B:1363:VAL:HG21	1:B:1469:VAL:HG22	1.91	0.52
1:U:1042:LEU:CD1	1:U:1160:LEU:HD12	2.39	0.52
1:B:1204:ILE:HG13	1:B:1205:SER:N	2.25	0.52
1:S:1299:ARG:NH1	1:U:592:TRP:CD2	2.77	0.52
1:U:493:PHE:HE1	1:U:528:MET:HG2	1.74	0.52
2:E:11:DC:N4	4:E:1021[B]:RXV:H13C	2.25	0.52
1:D:465:GLU:HB3	1:D:622:MET:O	2.10	0.52
1:S:505:ILE:CG2	1:S:517:ARG:HG2	2.39	0.52
1:S:464:VAL:HG21	1:S:523:PHE:HA	1.90	0.52
1:D:503:ILE:HD13	1:D:531:LEU:HD11	1.90	0.52
1:D:1451:TYR:CE1	1:D:1455:LEU:HD21	2.45	0.52
1:S:1006:GLN:O	1:S:1007:SER:C	2.48	0.52
1:S:1299:ARG:NH1	1:U:592:TRP:CD1	2.78	0.52
1:D:1167:LEU:O	1:D:1171:GLY:HA2	2.10	0.52
1:U:1043:LYS:HG3	1:U:1046:HIS:CE1	2.45	0.52
1:S:443:THR:HG22	1:S:454:ILE:CD1	2.40	0.52
1:B:464:VAL:HG11	1:B:523:PHE:HB2	1.92	0.52
1:S:1249:ILE:HD12	1:S:1249:ILE:N	2.25	0.52
1:D:434:VAL:HG21	1:D:440:GLY:CA	2.39	0.52
1:U:1027:MET:O	1:U:1031:VAL:HG22	2.10	0.52
1:D:549:GLN:HG2	1:D:573:PRO:CB	2.40	0.52
1:S:1015:THR:O	1:S:1019:ARG:HG3	2.09	0.52
1:D:1281:VAL:HG13	1:D:1289:ILE:HG13	1.91	0.52
1:U:1043:LYS:HE2	3:W:6:DT:O5'	2.09	0.52
1:B:501:HIS:CD2	1:B:536:TYR:HE1	2.28	0.52
1:U:537:VAL:HG12	1:U:606:VAL:CG2	2.40	0.52
1:B:565:LEU:HD12	1:B:565:LEU:O	2.09	0.52
1:U:493:PHE:CE2	1:U:530:PRO:HB2	2.45	0.52
1:D:1234:TYR:CD1	1:D:1348:LEU:HB2	2.45	0.52
1:D:1419:GLU:O	1:D:1423:GLN:HB2	2.09	0.52
1:S:1137:ARG:O	1:S:1138:ASP:HB2	2.10	0.52
1:S:1256:ARG:HG2	1:S:1310:LYS:HG2	1.92	0.52
1:S:1233:ALA:HB2	1:S:1239:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1264:ILE:HB	1:D:1265:PRO:CD	2.40	0.52
1:B:516:ILE:O	1:B:517:ARG:C	2.47	0.52
1:U:1378:ALA:O	1:U:1382:GLU:HG3	2.10	0.52
1:S:644:PHE:N	1:S:644:PHE:CD1	2.77	0.52
1:U:1100:ARG:HG3	1:U:1101:TYR:CE2	2.45	0.52
1:B:461:ILE:O	1:B:519:LEU:HD13	2.10	0.51
1:B:1269:ASN:HB3	1:B:1272:ARG:HB3	1.91	0.51
1:U:1367:THR:HB	1:U:1459:LEU:HD23	1.91	0.51
1:U:1452:ILE:O	1:U:1456:GLU:HB2	2.11	0.51
1:S:579:ARG:HG3	1:S:580:TYR:N	2.25	0.51
1:S:1057:GLY:O	1:S:1059:THR:HG23	2.10	0.51
1:D:1079:HIS:CE1	2:F:7:DA:OP1	2.63	0.51
1:S:1030:ILE:HG22	1:S:1343:PRO:HG3	1.92	0.51
1:U:1414:ARG:HB3	1:U:1415:PHE:HD1	1.75	0.51
1:B:1079:HIS:CD2	1:B:1081:HIS:HD2	2.28	0.51
1:S:644:PHE:HD1	1:S:644:PHE:N	2.08	0.51
1:U:1336:ILE:HG13	1:U:1345:LEU:HD13	1.93	0.51
1:D:622:MET:CE	1:D:622:MET:CA	2.89	0.51
1:S:1120:ALA:HB3	1:S:1123:PHE:CD1	2.44	0.51
1:B:462:LEU:HB3	1:B:475:ASN:HD22	1.75	0.51
1:B:607:LYS:HE3	1:U:600:HIS:CE1	2.46	0.51
1:B:1059:THR:HB	1:B:1060:PRO:CD	2.41	0.51
1:S:1252:ARG:HB2	1:S:1258:ARG:NH1	2.25	0.51
1:B:1110:PHE:HA	1:B:1118:ALA:CB	2.41	0.51
3:V:13:DC:H42	3:W:8:DG:H1	1.57	0.51
1:B:1276:LYS:O	1:B:1280:LEU:HG	2.10	0.51
3:W:10:DG:H2'	4:W:1020[B]:RXV:N11	2.26	0.51
1:B:1094:ALA:HB2	1:B:1104:VAL:HG12	1.92	0.51
1:S:432:PHE:CE2	1:S:504:VAL:HG11	2.46	0.51
1:B:569:LEU:HD23	1:B:569:LEU:N	2.24	0.51
1:U:1055:GLU:C	1:U:1057:GLY:H	2.14	0.51
1:S:1385:ARG:HB3	1:S:1438:ARG:HH12	1.76	0.51
1:U:1219:PRO:HD2	1:U:1266:PHE:HE1	1.76	0.51
1:B:1004:LEU:O	1:B:1006:GLN:N	2.44	0.50
1:U:1238:ARG:HA	1:U:1333:VAL:O	2.11	0.50
1:U:1013:ASN:HD22	1:U:1014:ILE:N	2.10	0.50
1:B:1059:THR:HG22	1:B:1133:LEU:HD21	1.93	0.50
1:B:569:LEU:C	1:B:571:PRO:HD2	2.31	0.50
1:D:1081:HIS:HB3	2:F:8:DG:P	2.51	0.50
1:B:1068:ALA:HB1	4:E:1021[B]:RXV:O28	2.12	0.50
1:U:1384:LEU:HD23	1:U:1425:ILE:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:VAL:HG21	1:D:440:GLY:HA2	1.92	0.50
1:U:1034:ALA:C	1:U:1035:LEU:HD23	2.31	0.50
1:S:554:TYR:HD2	1:S:565:LEU:HD21	1.77	0.50
1:U:1014:ILE:O	1:U:1014:ILE:HG13	2.10	0.50
1:U:626:VAL:HG11	3:V:18:DG:OP2	2.12	0.50
1:U:1100:ARG:NH1	1:U:1101:TYR:CZ	2.80	0.50
1:D:430:GLU:HB3	1:D:502:LYS:HB2	1.92	0.50
1:B:592:TRP:HA	1:B:596:MET:HB2	1.93	0.50
1:D:1161:PRO:O	1:D:1163:ARG:HD2	2.11	0.50
1:S:1349:LYS:O	1:S:1353:VAL:HG23	2.11	0.50
1:S:1220:THR:O	1:S:1221:ALA:HB3	2.11	0.50
1:B:581:LYS:HG3	1:B:581:LYS:O	2.11	0.50
1:U:1093:MET:HA	1:U:1099:TYR:CD1	2.46	0.50
1:S:1430:LEU:HD23	1:S:1433:LEU:CD1	2.42	0.50
1:B:1246:ARG:HH11	1:B:1246:ARG:HG3	1.76	0.50
1:B:1376:ASP:O	1:B:1380:ILE:HG12	2.11	0.50
1:B:570:ASN:N	1:B:571:PRO:HD2	2.27	0.50
1:D:544:LEU:O	1:D:545:TYR:CG	2.65	0.50
1:S:1449:LEU:H	1:S:1449:LEU:HD12	1.76	0.50
1:U:1135:LEU:HD22	1:U:1162:ALA:HA	1.94	0.50
1:D:1184:PRO:HG3	1:D:1331:PHE:HE2	1.74	0.50
1:S:525:TYR:O	1:S:525:TYR:CG	2.65	0.50
1:U:1472:GLU:O	1:U:1476:ILE:HG13	2.11	0.50
1:D:629:ARG:O	1:D:633:ILE:HD12	2.12	0.50
1:D:418:LEU:O	1:D:418:LEU:HD13	2.12	0.50
1:D:1278:ALA:O	1:D:1282:ARG:HG3	2.11	0.50
1:S:1245:SER:CB	1:S:1264:ILE:HA	2.31	0.50
1:U:1143:THR:CB	1:U:1362:VAL:HG13	2.42	0.50
1:B:443:THR:HB	1:B:454:ILE:HD13	1.93	0.50
1:D:1180:ALA:O	1:D:1336:ILE:HD12	2.12	0.50
1:U:638:VAL:HG12	1:U:638:VAL:O	2.12	0.50
1:D:1380:ILE:O	1:D:1384:LEU:HG	2.12	0.49
1:U:464:VAL:HG21	1:U:523:PHE:HA	1.94	0.49
1:U:1017:GLU:O	1:U:1021:SER:HB2	2.12	0.49
1:D:1274:ILE:HG23	1:D:1292:LEU:HD21	1.93	0.49
1:B:1110:PHE:HA	1:B:1118:ALA:HB2	1.94	0.49
1:S:515:HIS:HB2	1:S:1025:TYR:CD1	2.47	0.49
1:S:1112:SER:OG	1:S:1116:ASP:HB2	2.11	0.49
1:U:1469:VAL:O	1:U:1473:LEU:HG	2.12	0.49
2:F:1:5UA:C6'	2:F:1:5UA:H3'	2.42	0.49
1:B:1384:LEU:O	1:B:1388:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1045:VAL:CG1	1:D:1046:HIS:N	2.75	0.49
1:D:1195:VAL:HG22	1:D:1352:LEU:HD22	1.93	0.49
1:D:1006:GLN:O	1:D:1007:SER:C	2.50	0.49
1:B:609:GLU:OE1	1:B:609:GLU:HA	2.11	0.49
1:B:546:LYS:O	1:B:546:LYS:HG2	2.12	0.49
1:B:578:ALA:O	1:B:579:ARG:CB	2.61	0.49
1:U:1279:GLU:O	1:U:1283:ASP:HB2	2.13	0.49
1:S:426:PRO:O	1:S:501:HIS:CD2	2.66	0.49
1:B:1101:TYR:HB3	1:B:1131:ILE:CD1	2.42	0.49
1:B:471:ARG:NH1	1:B:471:ARG:CG	2.46	0.49
1:D:1388:LEU:HD12	1:D:1441:ILE:CD1	2.43	0.49
1:U:579:ARG:HG3	1:U:580:TYR:H	1.77	0.49
1:B:440:GLY:HA2	1:B:443:THR:OG1	2.12	0.49
1:B:572:THR:N	1:B:573:PRO:HD3	2.28	0.49
1:U:1005:PRO:HA	1:U:1007:SER:N	2.27	0.49
1:S:554:TYR:N	1:S:554:TYR:HD1	2.11	0.49
1:S:499:ARG:NH1	1:S:499:ARG:CG	2.76	0.49
1:U:1058:MET:HE1	1:U:1065:LYS:HG3	1.95	0.49
1:S:1299:ARG:NH1	1:U:592:TRP:CG	2.81	0.48
1:U:1387:ALA:HB3	1:U:1425:ILE:HD11	1.94	0.48
1:S:1442:GLU:HA	1:S:1445:TYR:CB	2.43	0.48
1:D:556:VAL:C	1:D:557:TYR:CD1	2.87	0.48
1:B:1246:ARG:HB3	1:B:1263:GLU:HB2	1.95	0.48
1:U:621:LEU:O	1:U:629:ARG:HD3	2.12	0.48
1:D:1388:LEU:CD1	1:D:1438:ARG:HG3	2.32	0.48
1:U:1047:ARG:HD3	1:U:1159:VAL:HA	1.95	0.48
1:D:1104:VAL:CG1	1:D:1105:ASP:N	2.76	0.48
1:D:1144:ILE:HD13	1:D:1159:VAL:O	2.12	0.48
1:B:1296:THR:HG23	1:B:1301:GLY:O	2.13	0.48
2:E:13:DC:C2	2:F:9:DG:N2	2.81	0.48
3:W:11:DC:C2	4:W:1020[B]:RXV:C8	2.97	0.48
1:U:463:ASN:HD21	1:U:466:LYS:HE3	1.78	0.48
1:D:531:LEU:O	1:D:536:TYR:HB2	2.14	0.48
1:S:1131:ILE:O	1:S:1131:ILE:HG13	2.12	0.48
1:S:1035:LEU:HD22	1:S:1036:PRO:CD	2.43	0.48
3:W:11:DC:C2	4:W:1020[A]:RXV:C4	2.97	0.48
1:U:1092:ARG:NH1	3:W:5:DG:OP1	2.46	0.48
1:D:1159:VAL:HG22	1:D:1160:LEU:N	2.29	0.48
1:D:1277:ILE:O	1:D:1281:VAL:HG23	2.14	0.48
1:B:605:GLN:HE22	1:U:599:GLU:HB3	1.78	0.48
1:D:1055:GLU:OE2	1:D:1055:GLU:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1123:PHE:HE2	1:U:582:GLY:HA3	1.77	0.48
1:D:1361:THR:O	1:D:1365:ARG:HG2	2.14	0.48
1:U:519:LEU:HD21	3:V:15:DA:H4'	1.96	0.48
1:S:1176:ALA:HB3	1:S:1179:MET:O	2.13	0.48
1:B:1391:ILE:O	1:B:1395:ILE:HD13	2.13	0.48
1:S:1382:GLU:HA	1:S:1385:ARG:HD2	1.95	0.48
1:B:493:PHE:HE2	1:B:495:LEU:HB2	1.78	0.48
1:D:503:ILE:HD12	1:D:503:ILE:N	2.28	0.48
1:S:1280:LEU:HD11	1:S:1324:GLN:HB3	1.96	0.48
1:D:468:ARG:HH21	1:D:471:ARG:HD3	1.79	0.48
1:D:549:GLN:HE22	1:D:569:LEU:HB3	1.79	0.48
1:D:1023:LEU:O	1:D:1027:MET:HG2	2.14	0.48
1:D:1091:VAL:HG12	1:D:1095:GLN:NE2	2.29	0.48
1:B:555:TYR:CE1	1:B:594:THR:HG21	2.47	0.48
1:S:1226:GLY:O	1:S:1230:ILE:HD13	2.14	0.48
1:B:1059:THR:HB	1:B:1060:PRO:HD2	1.95	0.48
1:D:525:TYR:HA	1:D:532:ILE:HD11	1.95	0.48
4:E:1021[B]:RXV:H202	4:E:1021[B]:RXV:H131	1.28	0.47
1:U:1123:PHE:HZ	3:V:9:DG:OP1	1.96	0.47
1:S:1239:GLY:O	1:S:1333:VAL:HB	2.14	0.47
1:S:1445:TYR:CE1	1:S:1449:LEU:HD11	2.49	0.47
1:U:431:ILE:CG2	1:U:503:ILE:HA	2.44	0.47
1:S:466:LYS:HG3	1:S:622:MET:O	2.14	0.47
1:S:626:VAL:O	1:S:629:ARG:N	2.44	0.47
1:D:639:TYR:CD1	1:D:1342:ARG:HG2	2.49	0.47
1:D:565:LEU:HD11	1:D:569:LEU:CD1	2.44	0.47
1:D:1160:LEU:C	1:D:1162:ALA:H	2.17	0.47
1:S:501:HIS:HA	1:S:536:TYR:CE1	2.50	0.47
1:U:1113:MET:O	1:U:1115:GLY:N	2.47	0.47
1:U:424:LYS:O	1:U:426:PRO:HD3	2.15	0.47
1:S:575:TRP:CD1	1:S:575:TRP:N	2.80	0.47
1:U:1009:ILE:O	1:U:1009:ILE:HG22	2.13	0.47
1:S:1426:LEU:HB3	1:U:1431:ARG:HB3	1.96	0.47
1:D:507:THR:HG21	1:D:516:ILE:CG2	2.44	0.47
1:U:1467:GLN:O	1:U:1470:ARG:HB2	2.15	0.47
1:D:622:MET:CE	1:D:1022:PHE:CE1	2.98	0.47
1:U:450:ARG:NH2	1:U:450:ARG:CG	2.69	0.47
1:D:1388:LEU:HD13	1:D:1438:ARG:CG	2.31	0.47
1:D:1014:ILE:CG2	1:D:1015:THR:N	2.76	0.47
1:S:1080:PRO:HD2	1:S:1081:HIS:CD2	2.50	0.47
1:D:1234:TYR:HD1	1:D:1348:LEU:HB2	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1260:VAL:HG22	1:U:1305:VAL:CG2	2.44	0.47
1:B:1167:LEU:O	1:B:1171:GLY:HA2	2.14	0.47
1:S:1346:ILE:O	1:S:1346:ILE:HG13	2.13	0.47
1:D:458:ARG:HH21	2:F:11:DC:H5"	1.76	0.47
3:V:11:DC:C2	4:W:1020[A]:RXV:C8	2.98	0.47
1:D:1074:VAL:CG1	1:D:1086:ILE:HD13	2.45	0.47
1:U:570:ASN:O	1:U:572:THR:N	2.47	0.47
1:B:544:LEU:O	1:B:545:TYR:CD1	2.67	0.47
1:U:529:ARG:N	1:U:530:PRO:HD3	2.30	0.47
1:B:1222:GLY:C	1:B:1223:LEU:HD12	2.35	0.47
1:B:1029:VAL:HA	1:B:1033:ARG:HB3	1.96	0.47
1:B:514:ALA:O	1:B:518:THR:HG23	2.15	0.47
1:U:549:GLN:OE1	1:U:569:LEU:HD22	2.15	0.47
1:S:1030:ILE:HG21	1:S:1343:PRO:HG2	1.96	0.47
1:U:557:TYR:O	1:U:558:ASN:HB3	2.14	0.47
1:B:462:LEU:HB3	1:B:475:ASN:ND2	2.30	0.47
1:D:1040:ASP:CG	1:D:1047:ARG:HH21	2.19	0.47
1:U:537:VAL:HG12	1:U:606:VAL:HG21	1.97	0.47
1:S:1245:SER:HB2	1:S:1263:GLU:O	2.15	0.47
3:V:15:DA:H2"	3:V:16:DC:C6	2.49	0.47
1:S:1378:ALA:O	1:S:1382:GLU:HG3	2.15	0.47
1:S:557:TYR:O	1:S:558:ASN:HB3	2.15	0.47
1:U:1100:ARG:HH11	1:U:1100:ARG:HG3	1.80	0.47
1:B:597:ASN:HD22	1:B:598:PRO:HD2	1.80	0.47
1:U:1225:LEU:HD21	1:U:1244:ARG:HD2	1.97	0.47
1:U:465:GLU:HG2	1:U:623:GLY:HA2	1.95	0.47
1:U:1292:LEU:HB2	1:U:1306:ILE:HG22	1.97	0.47
1:S:1072:GLY:O	1:U:1069:ARG:HB2	2.15	0.47
1:B:608:LEU:HD13	1:B:1014:ILE:HG21	1.96	0.47
1:D:1164:PHE:O	1:D:1166:ASN:N	2.47	0.47
1:D:1080:PRO:HG3	1:D:1150:TYR:CD2	2.47	0.46
1:B:515:HIS:HB2	1:B:1025:TYR:CD1	2.50	0.46
1:U:1173:SER:OG	3:W:5:DG:H5'	2.14	0.46
1:S:1040:ASP:HB3	1:S:1162:ALA:HB2	1.96	0.46
1:D:505:ILE:HD11	1:D:524:PHE:HE2	1.80	0.46
1:B:1053:LEU:CD2	1:B:1070:ILE:HG21	2.46	0.46
1:S:1238:ARG:HG3	1:S:1345:LEU:HD21	1.97	0.46
1:D:1310:LYS:O	1:D:1311:ASP:HB3	2.14	0.46
1:U:1410:SER:O	1:U:1414:ARG:HB2	2.15	0.46
1:S:1168:LEU:HB2	1:S:1191:LEU:HD11	1.96	0.46
1:B:1164:PHE:HA	1:B:1355:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1458:ILE:HG12	1:U:1464:VAL:CG1	2.46	0.46
1:B:1040:ASP:OD1	1:B:1041:GLY:N	2.48	0.46
1:S:540:ALA:HB1	1:S:595:THR:CG2	2.45	0.46
1:S:431:ILE:HA	1:S:453:ALA:O	2.16	0.46
1:D:1040:ASP:HB2	1:D:1162:ALA:HB2	1.97	0.46
1:B:632:PHE:CD2	1:B:632:PHE:C	2.88	0.46
1:S:1445:TYR:O	1:S:1448:LEU:HB2	2.15	0.46
1:D:427:GLU:HG3	1:D:501:HIS:NE2	2.30	0.46
1:U:1183:ILE:HD11	1:U:1335:MET:HA	1.97	0.46
1:U:1363:VAL:HG21	1:U:1469:VAL:HG22	1.97	0.46
1:D:516:ILE:HG22	1:D:517:ARG:N	2.30	0.46
1:S:1100:ARG:NH1	1:S:1101:TYR:CE1	2.83	0.46
1:D:1064:TYR:CD1	1:D:1107:GLN:HB2	2.51	0.46
1:S:1204:ILE:HG13	1:S:1208:GLU:CD	2.36	0.46
1:D:1137:ARG:HG2	1:D:1163:ARG:HG3	1.98	0.46
1:U:1144:ILE:HD11	1:U:1157:PRO:HB3	1.92	0.46
1:B:1049:ILE:HA	1:B:1074:VAL:HG21	1.97	0.46
1:S:1445:TYR:CE1	1:S:1449:LEU:HD21	2.50	0.46
1:U:1128:MET:HG2	1:U:1132:THR:HG21	1.97	0.46
1:B:509:ALA:CB	1:B:544:LEU:HD13	2.45	0.46
1:S:1182:ASN:HB3	1:S:1332:GLY:O	2.15	0.46
1:S:435:GLU:OE1	1:S:508:ASP:OD2	2.32	0.46
1:D:518:THR:HB	1:D:1018:MET:CE	2.46	0.46
3:V:13:DC:N4	3:W:8:DG:H1	2.13	0.46
1:S:1358:HIS:O	1:S:1362:VAL:HG23	2.16	0.46
1:B:1031:VAL:HA	1:B:1338:LEU:HD21	1.98	0.46
1:D:555:TYR:HE1	1:D:594:THR:HG21	1.81	0.46
1:U:527:PHE:O	1:U:528:MET:HG3	2.13	0.46
1:S:1190:GLU:O	1:S:1213:ILE:HG12	2.15	0.46
1:D:1318:LEU:HG	1:D:1322:TYR:CE2	2.50	0.46
1:D:1448:LEU:HD12	1:D:1448:LEU:HA	1.76	0.46
1:S:1488:ILE:H	1:S:1488:ILE:HD12	1.80	0.46
1:B:1391:ILE:HG23	1:B:1392:ASP:H	1.80	0.46
1:S:1442:GLU:HA	1:S:1445:TYR:HB3	1.97	0.46
1:U:511:VAL:HG21	1:U:1028:SER:OG	2.16	0.46
1:U:1056:GLN:HB3	1:U:1058:MET:HE3	1.96	0.46
1:U:556:VAL:CG1	1:U:557:TYR:N	2.79	0.46
1:U:1113:MET:C	1:U:1115:GLY:H	2.18	0.46
1:U:1273:MET:HG3	1:U:1326:PRO:HB2	1.97	0.46
1:B:1451:TYR:O	1:B:1455:LEU:HG	2.15	0.46
1:S:1113:MET:C	1:S:1115:GLY:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:627:GLU:HA	1:S:627:GLU:OE1	2.16	0.46
1:D:1458:ILE:HD13	1:D:1468:LEU:HD22	1.97	0.46
1:D:1137:ARG:O	1:D:1138:ASP:HB2	2.16	0.46
3:V:14:DT:H2'	3:V:15:DA:C8	2.50	0.46
1:D:1477:ARG:O	1:D:1481:GLY:HA3	2.15	0.46
1:B:445:SER:HB3	1:B:588:ALA:HB1	1.97	0.46
1:B:565:LEU:C	1:B:567:SER:H	2.18	0.46
1:S:601:ARG:NH1	1:S:603:LEU:HD12	2.30	0.46
1:S:581:LYS:NZ	3:V:8:DG:OP1	2.48	0.46
1:S:571:PRO:C	1:S:573:PRO:HD3	2.35	0.46
1:S:462:LEU:HD12	1:S:463:ASN:N	2.31	0.46
1:D:632:PHE:CD2	1:D:632:PHE:C	2.89	0.46
1:D:1234:TYR:O	1:D:1347:ASN:HB2	2.16	0.46
1:S:1288:GLY:HA2	1:S:1309:ARG:HB2	1.96	0.46
1:U:577:ILE:HG12	1:U:577:ILE:O	2.15	0.46
1:B:1062:LYS:HD3	1:B:1062:LYS:HA	1.68	0.46
1:D:549:GLN:HG2	1:D:573:PRO:HG2	1.98	0.46
1:D:1313:ASN:OD1	1:D:1316:VAL:HG23	2.16	0.46
1:D:1146:PHE:CE2	1:D:1157:PRO:HB3	2.50	0.46
1:S:1395:ILE:O	1:S:1399:ARG:HG3	2.15	0.46
1:S:526:ARG:HD3	1:S:526:ARG:HA	1.58	0.46
3:V:11:DC:H2''	3:V:12:DC:OP2	2.16	0.46
1:S:1270:LYS:O	1:S:1274:ILE:HG13	2.16	0.46
1:S:1274:ILE:HG22	1:S:1292:LEU:CD2	2.45	0.46
1:B:505:ILE:HG22	1:B:505:ILE:O	2.16	0.46
1:B:465:GLU:OE2	1:B:526:ARG:NH2	2.49	0.46
1:B:1073:ASP:O	1:B:1077:LYS:HB2	2.15	0.46
1:D:541:GLN:CD	1:D:604:LEU:HD11	2.37	0.46
1:U:547:LEU:C	1:U:547:LEU:HD12	2.36	0.46
1:S:1381:LEU:HA	1:S:1381:LEU:HD23	1.61	0.45
1:S:475:ASN:C	1:S:475:ASN:OD1	2.53	0.45
1:B:1201:ASN:HD21	1:B:1204:ILE:HA	1.81	0.45
1:S:515:HIS:HB2	1:S:1025:TYR:CG	2.50	0.45
1:D:1444:GLU:HA	1:D:1447:GLU:HB2	1.97	0.45
1:B:1196:LEU:O	1:B:1200:LYS:HG3	2.16	0.45
1:D:1068:ALA:HB1	4:E:1021[B]:RXV:S26	2.56	0.45
4:W:1020[A]:RXV:H142	4:W:1020[A]:RXV:C33	2.45	0.45
1:U:597:ASN:OD1	1:U:598:PRO:HD2	2.15	0.45
1:B:1107:GLN:HG2	1:B:1125:GLU:OE1	2.16	0.45
1:D:1281:VAL:CG1	1:D:1289:ILE:HG13	2.46	0.45
1:S:1322:TYR:O	1:S:1328:GLN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:LYS:HE3	2:E:16:DC:OP2	2.16	0.45
1:D:565:LEU:HD11	1:D:569:LEU:HD12	1.99	0.45
1:B:547:LEU:HD21	1:B:575:TRP:HE3	1.80	0.45
1:U:1277:ILE:HG12	1:U:1325:THR:HG21	1.98	0.45
1:U:1034:ALA:O	1:U:1035:LEU:HD23	2.17	0.45
1:D:516:ILE:HA	1:D:519:LEU:HD12	1.99	0.45
1:U:525:TYR:HD2	1:U:526:ARG:HG2	1.80	0.45
1:S:506:MET:HG3	1:S:540:ALA:HB3	1.99	0.45
1:U:570:ASN:CB	1:U:571:PRO:CD	2.94	0.45
1:U:540:ALA:HA	1:U:603:LEU:HD23	1.98	0.45
1:S:1187:ASN:ND2	1:S:1484:ARG:HA	2.32	0.45
1:U:556:VAL:HG12	1:U:557:TYR:H	1.81	0.45
1:S:1068:ALA:O	1:U:1072:GLY:HA3	2.16	0.45
1:S:481:MET:O	1:S:482:ILE:C	2.54	0.45
1:D:569:LEU:O	1:D:571:PRO:HD3	2.16	0.45
1:D:1027:MET:HE2	1:D:1027:MET:HB3	1.78	0.45
1:S:493:PHE:CE2	1:S:495:LEU:HB2	2.51	0.45
1:B:1048:ARG:HD2	1:B:1079:HIS:ND1	2.31	0.45
1:B:1234:TYR:CE1	1:B:1348:LEU:HD22	2.52	0.45
1:D:1467:GLN:O	1:D:1470:ARG:HB2	2.16	0.45
1:D:1445:TYR:CE2	1:D:1449:LEU:HD11	2.51	0.45
1:B:1080:PRO:HG3	1:B:1150:TYR:CG	2.52	0.45
1:S:469:LEU:HD22	1:S:469:LEU:O	2.17	0.45
1:D:1042:LEU:HA	1:D:1042:LEU:HD23	1.72	0.45
1:D:624:ASP:OD1	1:D:624:ASP:N	2.50	0.45
1:U:1112:SER:OG	1:U:1116:ASP:HB2	2.16	0.45
1:D:1163:ARG:HA	1:D:1359:GLN:HE22	1.82	0.45
1:B:574:LYS:C	1:B:575:TRP:HD1	2.19	0.45
1:U:1143:THR:HA	1:U:1365:ARG:HE	1.81	0.45
1:U:1193:ASN:HA	1:U:1196:LEU:HD12	1.99	0.45
1:B:565:LEU:HB2	1:U:1004:LEU:CD1	2.41	0.45
1:B:1244:ARG:HD2	1:B:1322:TYR:CZ	2.52	0.45
1:S:1174:GLY:O	1:S:1180:ALA:HB1	2.17	0.45
1:U:1066:LYS:O	1:U:1067:SER:C	2.54	0.45
1:B:1279:GLU:HA	1:B:1282:ARG:NH1	2.32	0.45
1:B:1216:PRO:HB2	1:B:1218:PHE:CE2	2.52	0.45
1:B:1045:VAL:HG11	2:E:6:DT:O3'	2.17	0.45
1:U:1219:PRO:HD2	1:U:1266:PHE:CD1	2.52	0.45
1:S:1165:PRO:HG3	1:S:1355:TYR:CE1	2.52	0.45
1:D:1243:MET:HB2	1:D:1329:THR:O	2.17	0.45
1:U:493:PHE:CE1	1:U:528:MET:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1177:VAL:HG13	2:F:16:DC:H4'	1.98	0.45
1:B:561:GLU:HB3	1:U:1004:LEU:HD21	1.97	0.45
1:B:1243:MET:O	1:B:1328:GLN:HA	2.17	0.45
1:B:1035:LEU:HB2	1:B:1338:LEU:HD11	1.99	0.45
1:D:1191:LEU:HD23	1:D:1213:ILE:HD12	1.99	0.45
1:B:1236:THR:HB	1:B:1238:ARG:H	1.83	0.45
1:B:601:ARG:HG3	1:B:603:LEU:HG	1.99	0.45
1:U:1253:GLY:HA2	1:U:1254:GLY:HA2	1.54	0.45
1:S:1326:PRO:HB2	1:S:1327:LEU:H	1.57	0.44
1:S:1030:ILE:CG2	1:S:1343:PRO:HG3	2.47	0.44
1:S:461:ILE:HG22	1:S:519:LEU:HB3	1.98	0.44
1:D:555:TYR:CE1	1:D:594:THR:HG21	2.52	0.44
1:U:1135:LEU:HA	1:U:1162:ALA:HA	1.99	0.44
1:D:1333:VAL:HG12	1:D:1334:ASN:N	2.33	0.44
1:D:1334:ASN:O	1:D:1336:ILE:N	2.50	0.44
1:B:597:ASN:O	1:B:599:GLU:N	2.50	0.44
1:S:1403:THR:OG1	1:S:1406:VAL:HG23	2.17	0.44
1:D:1060:PRO:CG	1:D:1133:LEU:HD11	2.48	0.44
1:S:538:TYR:CE2	1:S:605:GLN:HB2	2.52	0.44
1:U:1458:ILE:HG12	1:U:1464:VAL:HG12	1.98	0.44
1:S:438:SER:HB3	1:U:1119:ALA:HB1	1.99	0.44
1:B:1402:ASP:CG	1:B:1403:THR:H	2.21	0.44
1:U:597:ASN:O	1:U:601:ARG:HG2	2.17	0.44
1:D:1020:GLU:O	1:D:1024:ASP:HB3	2.17	0.44
1:S:1364:ARG:HG2	1:S:1368:GLN:HE22	1.82	0.44
1:S:1429:ARG:NH1	1:U:1427:ASP:O	2.49	0.44
1:B:1012:ARG:NH2	1:B:1020:GLU:OE2	2.50	0.44
1:B:579:ARG:C	1:B:580:TYR:CD1	2.90	0.44
1:B:1345:LEU:HD12	1:B:1346:ILE:N	2.33	0.44
1:S:426:PRO:C	1:S:501:HIS:CD2	2.91	0.44
1:D:1423:GLN:C	1:D:1425:ILE:H	2.21	0.44
1:D:1196:LEU:HA	1:D:1196:LEU:HD23	1.69	0.44
1:U:1298:LEU:HD12	1:U:1298:LEU:HA	1.73	0.44
1:D:1349:LYS:O	1:D:1353:VAL:HG23	2.18	0.44
1:B:624:ASP:N	1:B:624:ASP:OD1	2.49	0.44
1:D:1167:LEU:HD12	1:D:1167:LEU:O	2.17	0.44
1:S:1045:VAL:HG13	1:S:1046:HIS:H	1.81	0.44
1:B:445:SER:HB3	1:B:588:ALA:CB	2.47	0.44
1:S:1223:LEU:HB2	1:S:1244:ARG:O	2.17	0.44
1:B:621:LEU:HA	1:B:629:ARG:HD3	1.98	0.44
1:B:432:PHE:N	1:B:432:PHE:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:549:GLN:HB3	1:U:552:GLN:HG3	1.99	0.44
1:U:579:ARG:CG	1:U:580:TYR:N	2.79	0.44
1:D:1054:ASN:HB2	1:D:1136:LEU:CD1	2.48	0.44
1:D:1415:PHE:O	1:D:1417:LEU:HG	2.17	0.44
1:S:1003:GLU:CB	1:S:1004:LEU:HB3	2.47	0.44
1:B:1206:ILE:HD13	1:B:1206:ILE:N	2.26	0.44
1:D:640:ALA:CB	1:D:641:ASN:HA	2.38	0.44
1:U:1274:ILE:HG23	1:U:1292:LEU:HD21	2.00	0.44
1:S:432:PHE:HE1	1:S:452:GLN:HB3	1.83	0.44
1:S:469:LEU:HD13	1:S:469:LEU:C	2.38	0.44
1:B:423:SER:HB3	1:B:429:CYS:SG	2.58	0.44
1:U:1329:THR:HG22	1:U:1330:SER:N	2.33	0.44
1:S:1308:VAL:HG12	1:S:1312:ALA:HB3	2.00	0.44
4:E:1021[A]:RXV:C4	2:F:11:DC:C2	3.01	0.44
1:B:1022:PHE:O	1:B:1025:TYR:HB3	2.17	0.44
1:U:1272:ARG:NH1	1:U:1272:ARG:HG2	2.25	0.44
1:S:1135:LEU:HD22	1:S:1162:ALA:HA	2.00	0.44
1:D:1179:MET:C	2:E:17:DG:H4'	2.38	0.44
1:S:418:LEU:HD11	1:S:453:ALA:HB1	2.00	0.44
1:U:1131:ILE:HD13	1:U:1131:ILE:C	2.38	0.44
1:S:1353:VAL:O	1:S:1357:GLU:HB2	2.17	0.44
1:U:633:ILE:HG22	1:U:634:GLU:N	2.32	0.44
1:D:1045:VAL:HG13	1:D:1046:HIS:N	2.33	0.44
1:S:1298:LEU:H	1:S:1299:ARG:HH21	1.66	0.44
2:E:10:DG:O5'	2:E:10:DG:H2'	2.18	0.44
1:U:447:ARG:HD2	1:U:452:GLN:O	2.18	0.44
1:D:505:ILE:HD11	1:D:524:PHE:CE2	2.53	0.44
1:U:1391:ILE:HG23	1:U:1392:ASP:N	2.33	0.44
1:S:1425:ILE:HG22	1:S:1426:LEU:N	2.33	0.44
1:B:1428:MET:HG2	1:B:1429:ARG:N	2.33	0.44
2:E:6:DT:C2	2:E:7:DA:C8	3.05	0.43
1:S:1381:LEU:O	1:S:1385:ARG:HG2	2.18	0.43
1:B:1350:GLU:HG2	1:B:1350:GLU:H	1.62	0.43
1:B:1339:VAL:HG11	1:B:1354:HIS:CE1	2.53	0.43
1:U:1349:LYS:O	1:U:1349:LYS:HG2	2.16	0.43
1:D:549:GLN:CG	1:D:573:PRO:HG2	2.48	0.43
1:U:1042:LEU:HD22	1:U:1046:HIS:HB3	1.99	0.43
1:D:1196:LEU:HD22	1:D:1470:ARG:HG2	2.00	0.43
1:U:1213:ILE:HD12	1:U:1213:ILE:N	2.33	0.43
1:S:553:LYS:C	1:S:554:TYR:HD1	2.21	0.43
1:S:1030:ILE:HD13	1:S:1176:ALA:HB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1035:LEU:HA	1:B:1036:PRO:HD3	1.71	0.43
1:D:1136:LEU:HD22	1:D:1160:LEU:HD22	1.99	0.43
1:U:418:LEU:O	1:U:418:LEU:HD23	2.18	0.43
1:B:1059:THR:CB	1:B:1060:PRO:CD	2.96	0.43
1:B:446:GLY:O	1:B:592:TRP:CE3	2.71	0.43
1:S:1071:VAL:HG22	1:S:1086:ILE:HG22	2.00	0.43
1:U:542:PRO:HA	1:U:543:PRO:HD3	1.83	0.43
1:B:1466:LEU:HD11	1:B:1470:ARG:NH2	2.33	0.43
1:S:1245:SER:OG	1:S:1327:LEU:HG	2.17	0.43
1:B:464:VAL:HG23	1:B:464:VAL:O	2.18	0.43
1:S:462:LEU:HD23	1:S:475:ASN:HD22	1.83	0.43
1:U:462:LEU:HD12	1:U:462:LEU:HA	1.57	0.43
1:S:1246:ARG:HB3	1:S:1263:GLU:HB2	1.99	0.43
1:U:1042:LEU:HD11	1:U:1160:LEU:HD12	2.00	0.43
1:S:1042:LEU:HA	1:S:1042:LEU:HD23	1.79	0.43
1:D:1004:LEU:HG	1:D:1005:PRO:HA	2.01	0.43
1:D:1032:ALA:C	1:D:1044:PRO:HG2	2.38	0.43
1:B:484:ALA:O	1:B:499:ARG:HG3	2.19	0.43
1:U:1015:THR:HG22	1:U:1019:ARG:HG3	2.00	0.43
1:B:586:MET:SD	1:B:591:LEU:CD1	3.07	0.43
1:U:1308:VAL:HG12	1:U:1309:ARG:O	2.19	0.43
1:B:1220:THR:O	1:B:1221:ALA:HB3	2.18	0.43
1:S:1087:TYR:O	1:S:1090:MET:N	2.52	0.43
1:S:1173:SER:HA	1:S:1181:THR:O	2.19	0.43
1:S:431:ILE:HD13	1:S:485:PHE:HE1	1.84	0.43
1:D:1252:ARG:NH1	1:D:1256:ARG:HE	2.16	0.43
1:U:597:ASN:HA	1:U:598:PRO:HD3	1.87	0.43
1:U:556:VAL:CG1	1:U:557:TYR:H	2.31	0.43
1:D:1411:LEU:HD12	1:D:1422:ALA:CB	2.48	0.43
1:U:606:VAL:HG11	1:U:1014:ILE:CD1	2.48	0.43
1:B:1038:VAL:O	1:B:1038:VAL:HG22	2.17	0.43
1:D:1134:GLU:O	1:D:1163:ARG:HG2	2.19	0.43
1:D:1230:ILE:O	1:D:1233:ALA:HB3	2.19	0.43
1:D:431:ILE:O	1:D:431:ILE:HG23	2.17	0.43
1:S:1428:MET:HG2	1:S:1429:ARG:N	2.34	0.43
1:S:429:CYS:HB3	1:S:500:TYR:HD2	1.83	0.43
1:B:508:ASP:OD2	1:B:582:GLY:HA2	2.19	0.43
1:B:1039:ARG:HB3	1:B:1358:HIS:CD2	2.54	0.43
1:B:1144:ILE:C	1:B:1144:ILE:HD12	2.39	0.43
1:U:1466:LEU:O	1:U:1470:ARG:HG3	2.18	0.43
1:S:1093:MET:CA	1:S:1099:TYR:CD1	2.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:LEU:HD13	1:B:548:THR:N	2.34	0.43
1:B:1137:ARG:O	1:B:1138:ASP:HB2	2.18	0.43
1:B:509:ALA:C	1:B:544:LEU:HD13	2.38	0.43
1:D:555:TYR:O	1:D:556:VAL:HG23	2.19	0.43
1:U:1099:TYR:HD2	1:U:1170:ASN:ND2	2.17	0.43
1:D:545:TYR:HD2	1:D:577:ILE:HD11	1.82	0.43
1:B:1072:GLY:O	1:D:1069:ARG:HA	2.19	0.43
1:S:1141:LYS:O	1:S:1142:ASP:C	2.56	0.43
1:D:1080:PRO:O	1:D:1081:HIS:CG	2.72	0.42
1:D:1359:GLN:O	1:D:1362:VAL:HG12	2.19	0.42
1:B:1364:ARG:HG2	1:B:1368:GLN:HE22	1.84	0.42
3:V:17:DG:H2''	3:V:18:DG:O5'	2.19	0.42
1:U:1135:LEU:HD23	1:U:1162:ALA:HA	2.00	0.42
1:D:1079:HIS:NE2	1:D:1081:HIS:CD2	2.87	0.42
1:S:1107:GLN:CG	1:S:1125:GLU:HG3	2.46	0.42
1:D:1270:LYS:HE2	1:D:1296:THR:OG1	2.19	0.42
1:B:1345:LEU:C	1:B:1345:LEU:HD12	2.39	0.42
1:B:1064:TYR:CD2	1:B:1107:GLN:HB2	2.54	0.42
1:B:1201:ASN:HA	1:B:1202:PRO:HD3	1.91	0.42
1:B:443:THR:HG22	1:B:596:MET:HE1	2.00	0.42
1:B:1246:ARG:NH1	1:B:1246:ARG:HG3	2.34	0.42
1:S:1461:ASP:HB3	1:S:1464:VAL:HG23	2.00	0.42
1:B:503:ILE:HD12	1:B:503:ILE:N	2.34	0.42
1:D:1457:THR:HG22	1:D:1464:VAL:HG11	2.01	0.42
1:B:579:ARG:C	1:B:580:TYR:HD1	2.22	0.42
1:D:544:LEU:O	1:D:545:TYR:CD1	2.72	0.42
1:B:1035:LEU:HB2	1:B:1338:LEU:HD12	2.01	0.42
1:U:1110:PHE:HA	1:U:1118:ALA:CB	2.49	0.42
1:B:1057:GLY:O	1:B:1059:THR:N	2.51	0.42
1:U:1276:LYS:O	1:U:1280:LEU:HG	2.19	0.42
1:B:1194:GLY:HA3	1:B:1213:ILE:HD11	2.00	0.42
1:S:444:LYS:HA	1:S:454:ILE:CD1	2.49	0.42
1:S:450:ARG:CG	1:S:451:THR:HG22	2.50	0.42
1:B:504:VAL:CG1	1:B:540:ALA:HB2	2.49	0.42
1:S:1042:LEU:HB2	1:S:1047:ARG:NH2	2.34	0.42
1:S:1382:GLU:HG2	1:S:1445:TYR:HE2	1.84	0.42
1:D:555:TYR:N	1:D:555:TYR:CD2	2.87	0.42
1:B:461:ILE:HA	1:B:461:ILE:HD13	1.63	0.42
1:U:1249:ILE:HD11	1:U:1318:LEU:HD22	2.02	0.42
1:S:532:ILE:HA	1:S:537:VAL:HG23	2.01	0.42
1:B:1159:VAL:HG22	1:B:1160:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:565:LEU:O	1:S:569:LEU:HD12	2.20	0.42
1:S:1035:LEU:HA	1:S:1035:LEU:HD23	1.71	0.42
1:U:443:THR:HG22	1:U:454:ILE:CD1	2.47	0.42
1:D:1417:LEU:HB3	1:D:1421:GLN:HB3	2.01	0.42
2:F:13:DC:C2'	2:F:14:DT:O5'	2.68	0.42
1:U:1004:LEU:N	1:U:1005:PRO:CD	2.83	0.42
1:B:1368:GLN:HE21	1:B:1368:GLN:HB2	1.65	0.42
1:D:1233:ALA:HA	1:D:1238:ARG:O	2.20	0.42
1:U:1233:ALA:HB1	1:U:1333:VAL:HG11	2.01	0.42
1:S:608:LEU:HA	1:S:608:LEU:HD13	1.78	0.42
1:B:1087:TYR:CD1	1:B:1090:MET:HE2	2.55	0.42
1:D:1060:PRO:HG2	1:D:1133:LEU:HD11	2.01	0.42
1:S:597:ASN:HD22	1:S:598:PRO:HD2	1.84	0.42
3:V:4:DC:C2'	3:V:5:DG:H5'	2.49	0.42
1:B:493:PHE:CE2	1:B:530:PRO:HG2	2.54	0.42
1:U:1100:ARG:NH2	1:U:1217:ASP:OD2	2.43	0.42
1:B:443:THR:HG22	1:B:454:ILE:CD1	2.50	0.42
1:D:1004:LEU:HA	1:D:1005:PRO:HA	1.76	0.42
1:B:1192:ILE:HD12	1:B:1477:ARG:HB2	2.01	0.42
1:D:1465:LEU:C	1:D:1465:LEU:HD23	2.40	0.42
1:B:553:LYS:HB3	1:B:553:LYS:HE2	1.91	0.42
1:U:515:HIS:ND1	1:U:519:LEU:HD11	2.34	0.42
1:D:572:THR:H	1:D:573:PRO:CD	2.25	0.42
1:S:522:THR:O	1:S:522:THR:HG22	2.20	0.42
1:B:1391:ILE:HG23	1:B:1392:ASP:N	2.34	0.42
1:D:1040:ASP:OD1	1:D:1047:ARG:NH2	2.53	0.42
1:D:440:GLY:O	1:D:444:LYS:HG3	2.20	0.42
1:B:499:ARG:HH11	1:B:499:ARG:HG3	1.84	0.42
1:B:618:PHE:CE2	1:B:1018:MET:CE	3.03	0.42
3:V:20:DT:H6	3:V:20:DT:H5''	1.85	0.42
3:V:8:DG:H2'	3:V:9:DG:O4'	2.20	0.42
1:B:501:HIS:HA	1:B:536:TYR:HD1	1.82	0.42
1:U:1056:GLN:HB2	1:U:1058:MET:SD	2.59	0.42
1:U:1233:ALA:O	1:U:1335:MET:HE2	2.19	0.42
1:U:637:ALA:HB1	1:U:639:TYR:CE1	2.55	0.42
1:S:1050:LEU:HD23	1:S:1050:LEU:N	2.35	0.42
1:B:565:LEU:CD1	1:B:569:LEU:HG	2.50	0.41
1:S:544:LEU:HG	1:S:545:TYR:CD1	2.55	0.41
1:B:1083:ASP:C	1:B:1085:SER:N	2.72	0.41
1:U:1138:ASP:HA	1:U:1141:LYS:HD3	2.02	0.41
1:S:1183:ILE:HA	1:S:1184:PRO:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:609:GLU:HA	1:D:609:GLU:OE1	2.20	0.41
1:B:565:LEU:CB	1:U:1004:LEU:HD12	2.42	0.41
1:D:458:ARG:NH2	2:F:11:DC:H5'	2.35	0.41
1:B:583:LEU:HD22	1:B:591:LEU:HD11	2.02	0.41
1:B:586:MET:SD	1:B:591:LEU:HD13	2.59	0.41
1:S:522:THR:HG23	1:S:618:PHE:HD2	1.85	0.41
1:S:1385:ARG:HB3	1:S:1438:ARG:NH1	2.35	0.41
1:B:1195:VAL:HG22	1:B:1352:LEU:HD13	2.01	0.41
1:S:464:VAL:HG12	1:S:472:ILE:HD13	2.02	0.41
1:D:1183:ILE:HA	1:D:1184:PRO:HD3	1.78	0.41
1:S:601:ARG:NH1	1:S:603:LEU:CD1	2.83	0.41
1:S:1466:LEU:HD21	1:S:1470:ARG:HH21	1.85	0.41
1:S:1204:ILE:HG23	1:S:1204:ILE:O	2.20	0.41
1:D:1257:GLN:H	1:D:1308:VAL:HG12	1.84	0.41
1:D:539:ILE:HG22	1:D:539:ILE:O	2.20	0.41
1:D:595:THR:HG22	1:D:595:THR:O	2.18	0.41
1:S:1002:ALA:CA	1:S:1003:GLU:C	2.85	0.41
2:E:13:DC:N3	2:F:9:DG:N2	2.67	0.41
1:D:1050:LEU:N	1:D:1050:LEU:HD23	2.36	0.41
1:S:1374:ALA:HB1	1:S:1452:ILE:HD11	2.01	0.41
1:U:508:ASP:O	1:U:513:GLY:HA3	2.21	0.41
1:B:1064:TYR:HB3	1:B:1125:GLU:CB	2.50	0.41
1:U:1135:LEU:HD21	1:U:1164:PHE:CE2	2.55	0.41
1:D:1136:LEU:HD23	1:D:1136:LEU:N	2.36	0.41
1:U:432:PHE:HE2	1:U:504:VAL:HG11	1.84	0.41
1:U:606:VAL:HG11	1:U:1014:ILE:HD13	2.02	0.41
1:B:623:GLY:O	1:B:629:ARG:NH1	2.53	0.41
1:U:543:PRO:HD2	1:U:586:MET:CE	2.49	0.41
1:D:1192:ILE:CG2	1:D:1473:LEU:HB3	2.51	0.41
1:S:529:ARG:HG3	1:S:529:ARG:O	2.19	0.41
1:D:562:LEU:HD22	1:D:566:LYS:HE2	2.03	0.41
1:D:1191:LEU:HD23	1:D:1213:ILE:CD1	2.50	0.41
1:U:581:LYS:HE2	1:U:1080:PRO:O	2.21	0.41
1:U:614:ALA:O	1:U:618:PHE:HD1	2.03	0.41
1:D:1104:VAL:HG12	1:D:1105:ASP:H	1.86	0.41
1:U:1233:ALA:HA	1:U:1238:ARG:O	2.20	0.41
1:U:1135:LEU:HD23	1:U:1135:LEU:HA	1.76	0.41
1:S:1289:ILE:O	1:S:1289:ILE:HG22	2.20	0.41
1:D:433:LEU:HD11	1:D:503:ILE:CG2	2.50	0.41
1:B:507:THR:HG21	1:B:516:ILE:CG2	2.51	0.41
1:D:460:LYS:HA	1:D:516:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:445:SER:O	1:U:1298:LEU:HD13	2.21	0.41
1:U:541:GLN:HA	1:U:542:PRO:HD3	1.82	0.41
1:B:570:ASN:N	1:B:571:PRO:CD	2.84	0.41
1:U:1394:ILE:HG12	1:U:1394:ILE:H	1.71	0.41
1:S:601:ARG:HH11	1:S:603:LEU:HG	1.86	0.41
1:D:545:TYR:CE2	1:D:579:ARG:HG3	2.56	0.41
1:S:1040:ASP:CG	1:S:1047:ARG:HH21	2.24	0.41
1:U:506:MET:HB2	1:U:540:ALA:HB3	2.03	0.41
1:B:461:ILE:HG23	1:B:462:LEU:N	2.35	0.41
1:D:1289:ILE:H	1:D:1289:ILE:HG12	1.34	0.41
1:B:1272:ARG:O	1:B:1276:LYS:HG3	2.21	0.41
1:B:1377:ARG:O	1:B:1380:ILE:HB	2.21	0.41
1:B:549:GLN:CG	1:B:573:PRO:HD2	2.50	0.41
1:U:1015:THR:O	1:U:1019:ARG:HG3	2.21	0.41
1:D:462:LEU:HD21	1:D:472:ILE:HG23	2.02	0.41
1:B:431:ILE:HD11	1:B:455:LEU:HB2	2.02	0.41
1:B:1252:ARG:HG2	1:B:1252:ARG:O	2.19	0.41
1:D:1327:LEU:HA	1:D:1327:LEU:HD13	1.78	0.41
1:D:502:LYS:HG2	1:D:538:TYR:CE1	2.55	0.41
2:E:20:DT:N3	2:F:1:5UA:N1	2.69	0.41
1:S:1060:PRO:HD2	1:S:1133:LEU:HD11	2.02	0.41
1:S:1296:THR:HG23	1:S:1301:GLY:C	2.41	0.41
1:D:1168:LEU:HD23	1:D:1168:LEU:HA	1.89	0.41
1:U:1200:LYS:HB2	1:U:1200:LYS:HE3	1.82	0.41
1:D:570:ASN:O	1:D:573:PRO:HD3	2.21	0.41
1:S:455:LEU:O	1:S:455:LEU:CG	2.60	0.41
1:S:419:ALA:O	1:S:447:ARG:NH2	2.49	0.41
1:B:1265:PRO:HB2	1:B:1268:VAL:HG21	2.03	0.41
1:U:503:ILE:N	1:U:536:TYR:O	2.49	0.41
1:U:536:TYR:N	1:U:536:TYR:CD1	2.89	0.41
1:B:509:ALA:HB3	1:B:544:LEU:CD1	2.51	0.41
1:U:1031:VAL:O	1:U:1338:LEU:HD11	2.20	0.41
1:D:1007:SER:C	1:D:1009:ILE:H	2.23	0.41
1:B:1215:GLY:HA2	1:B:1234:TYR:OH	2.20	0.41
1:B:1348:LEU:O	1:B:1348:LEU:HD12	2.21	0.41
1:S:531:LEU:O	1:S:536:TYR:HB2	2.20	0.41
1:B:1101:TYR:HB3	1:B:1131:ILE:HD13	2.02	0.41
1:B:514:ALA:HB1	1:B:1021:SER:HB3	2.02	0.41
1:U:1308:VAL:HG12	1:U:1309:ARG:N	2.35	0.41
1:S:632:PHE:C	1:S:632:PHE:CD2	2.94	0.41
3:V:3:DC:H5"	3:V:3:DC:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:5UA:H3'	2:E:2:DG:P	2.61	0.41
1:B:1004:LEU:CB	1:B:1005:PRO:HD2	2.47	0.41
1:U:1367:THR:HG22	1:U:1455:LEU:HD22	2.02	0.41
1:D:1335:MET:HE3	1:D:1347:ASN:HA	2.02	0.41
1:D:1227:LYS:O	1:D:1231:ARG:HB2	2.21	0.41
1:B:1490:LEU:H	1:B:1490:LEU:HD12	1.85	0.41
1:S:1218:PHE:HA	1:S:1219:PRO:HD3	1.86	0.40
1:B:1265:PRO:HB2	1:B:1268:VAL:CG2	2.51	0.40
1:S:1085:SER:O	1:S:1089:ALA:HB2	2.21	0.40
1:B:455:LEU:HA	1:B:456:PRO:HD2	1.80	0.40
1:D:1035:LEU:HA	1:D:1036:PRO:HD2	1.81	0.40
1:B:625:VAL:HG11	1:B:628:ASN:ND2	2.36	0.40
1:D:1198:LEU:HD23	1:D:1356:LEU:HD22	2.01	0.40
1:D:457:LEU:O	1:D:458:ARG:HG3	2.21	0.40
1:S:1273:MET:HB3	1:S:1273:MET:HE2	2.00	0.40
1:U:1053:LEU:O	1:U:1055:GLU:N	2.54	0.40
1:U:1008:ARG:HG2	1:U:1008:ARG:H	1.39	0.40
1:U:1143:THR:HA	1:U:1365:ARG:NE	2.37	0.40
1:U:1031:VAL:HG23	1:U:1032:ALA:N	2.35	0.40
1:B:1060:PRO:HG3	1:B:1128:MET:HB3	2.04	0.40
1:U:1035:LEU:HA	1:U:1036:PRO:HD3	1.67	0.40
1:D:1333:VAL:CG1	1:D:1334:ASN:N	2.84	0.40
1:S:1440:LYS:HA	1:S:1443:ALA:HB3	2.03	0.40
1:S:477:GLU:O	1:S:478:ILE:C	2.59	0.40
1:B:1309:ARG:CZ	1:B:1312:ALA:HB2	2.49	0.40
3:V:13:DC:C5	3:V:14:DT:C7	3.04	0.40
1:D:549:GLN:HG2	1:D:573:PRO:CG	2.52	0.40
1:U:571:PRO:O	1:U:572:THR:C	2.58	0.40
1:D:557:TYR:N	1:D:557:TYR:HD1	2.18	0.40
1:B:585:GLU:CG	1:B:585:GLU:O	2.69	0.40
1:B:1383:GLY:O	1:B:1425:ILE:HD11	2.21	0.40
1:U:427:GLU:HA	1:U:501:HIS:CG	2.56	0.40
1:U:1030:ILE:HG22	1:U:1343:PRO:HG3	2.04	0.40
1:S:1245:SER:CB	1:S:1263:GLU:O	2.69	0.40
1:S:1264:ILE:HB	1:S:1265:PRO:CD	2.50	0.40
1:B:1160:LEU:CD1	1:B:1160:LEU:N	2.85	0.40
3:W:4:DC:C2'	3:W:5:DG:O5'	2.70	0.40
1:S:1274:ILE:HD11	1:S:1294:ASP:OD2	2.21	0.40
1:U:537:VAL:O	1:U:606:VAL:HG23	2.21	0.40
1:S:1086:ILE:O	1:S:1089:ALA:HB3	2.21	0.40
1:D:443:THR:HG22	1:D:454:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1326:PRO:C	1:B:1328:GLN:N	2.75	0.40
4:W:1020[A]:RXV:H202	4:W:1020[A]:RXV:H132	1.80	0.40
1:S:1322:TYR:HB3	1:S:1328:GLN:HB2	2.03	0.40
1:B:1218:PHE:N	1:B:1218:PHE:CD2	2.89	0.40
1:U:1049:ILE:O	1:U:1053:LEU:HG	2.21	0.40
1:B:1448:LEU:HD23	1:B:1448:LEU:HA	1.89	0.40
1:B:430:GLU:HA	1:B:500:TYR:HB3	2.04	0.40
1:B:1003:GLU:HA	1:B:1004:LEU:CB	2.49	0.40
1:B:637:ALA:O	1:B:638:VAL:HG23	2.21	0.40
1:S:1169:ALA:N	1:S:1191:LEU:HD11	2.37	0.40
1:B:1100:ARG:NH1	1:B:1485:ARG:CZ	2.84	0.40
1:S:630:ARG:NH1	1:S:634:GLU:OE2	2.51	0.40
1:S:511:VAL:HG21	1:S:1028:SER:OG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	716/726 (99%)	596 (83%)	102 (14%)	18 (2%)	7	46
1	D	717/726 (99%)	599 (84%)	97 (14%)	21 (3%)	6	42
1	S	716/726 (99%)	598 (84%)	95 (13%)	23 (3%)	5	40
1	U	715/726 (98%)	607 (85%)	86 (12%)	22 (3%)	5	41
All	All	2864/2904 (99%)	2400 (84%)	380 (13%)	84 (3%)	6	42

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	579	ARG
1	B	644	PHE

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Mol	Chain	Res	Type
1	B	1004	LEU
1	B	1005	PRO
1	B	1007	SER
1	B	1162	ALA
1	D	637	ALA
1	D	1002	ALA
1	D	1008	ARG
1	D	1162	ALA
1	D	1335	MET
1	D	1418	SER
1	S	644	PHE
1	S	1003	GLU
1	S	1006	GLN
1	S	1007	SER
1	S	1008	ARG
1	S	1327	LEU
1	U	570	ASN
1	U	574	LYS
1	U	1002	ALA
1	U	1004	LEU
1	U	1008	ARG
1	U	1114	ASP
1	U	1391	ILE
1	B	463	ASN
1	B	1149	ASN
1	D	581	LYS
1	D	593	GLU
1	D	1007	SER
1	S	482	ILE
1	S	574	LYS
1	S	1033	ARG
1	S	1221	ALA
1	S	1326	PRO
1	S	1481	GLY
1	U	490	GLY
1	U	508	ASP
1	U	577	ILE
1	U	1054	ASN
1	U	1124	THR
1	D	1120	ALA
1	D	1266	PHE
1	S	417	LYS

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Mol	Chain	Res	Type
1	S	1004	LEU
1	S	1138	ASP
1	S	1416	LYS
1	U	552	GLN
1	U	1056	GLN
1	U	1118	ALA
1	U	1176	ALA
1	B	578	ALA
1	B	638	VAL
1	B	1063	SER
1	B	1221	ALA
1	B	1236	THR
1	D	638	VAL
1	S	643	ASP
1	U	643	ASP
1	U	1009	ILE
1	B	574	LYS
1	B	1033	ARG
1	B	1171	GLY
1	D	508	ASP
1	D	574	LYS
1	D	1033	ARG
1	D	1416	LYS
1	S	550	GLY
1	S	1063	SER
1	S	1325	THR
1	U	1221	ALA
1	D	1161	PRO
1	S	1080	PRO
1	U	1005	PRO
1	U	1074	VAL
1	B	1157	PRO
1	U	542	PRO
1	B	1219	PRO
1	D	570	ASN
1	D	573	PRO
1	D	1004	LEU
1	S	573	PRO
1	D	572	THR
1	S	505	ILE

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	B	611/624 (98%)	543 (89%)	68 (11%)	8	35
1	D	610/624 (98%)	541 (89%)	69 (11%)	7	34
1	S	611/624 (98%)	531 (87%)	80 (13%)	5	27
1	U	611/624 (98%)	539 (88%)	72 (12%)	6	31
All	All	2443/2496 (98%)	2154 (88%)	289 (12%)	6	31

All (289) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	438	SER
1	B	443	THR
1	B	447	ARG
1	B	461	ILE
1	B	462	LEU
1	B	464	VAL
1	B	468	ARG
1	B	471	ARG
1	B	489	ILE
1	B	492	ASP
1	B	560	ARG
1	B	575	TRP
1	B	576	SER
1	B	577	ILE
1	B	581	LYS
1	B	593	GLU
1	B	597	ASN
1	B	609	GLU
1	B	620	MET
1	B	635	ASP
1	B	1006	GLN
1	B	1007	SER
1	B	1012	ARG
1	B	1015	THR

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Mol	Chain	Res	Type
1	B	1016	SER
1	B	1045	VAL
1	B	1059	THR
1	B	1067	SER
1	B	1074	VAL
1	B	1107	GLN
1	B	1121	MET
1	B	1122	ARG
1	B	1141	LYS
1	B	1160	LEU
1	B	1177	VAL
1	B	1181	THR
1	B	1206	ILE
1	B	1224	ILE
1	B	1232	ARG
1	B	1236	THR
1	B	1245	SER
1	B	1256	ARG
1	B	1260	VAL
1	B	1262	THR
1	B	1299	ARG
1	B	1300	THR
1	B	1302	VAL
1	B	1306	ILE
1	B	1327	LEU
1	B	1329	THR
1	B	1331	PHE
1	B	1334	ASN
1	B	1338	LEU
1	B	1345	LEU
1	B	1348	LEU
1	B	1350	GLU
1	B	1368	GLN
1	B	1384	LEU
1	B	1388	LEU
1	B	1404	ASP
1	B	1415	PHE
1	B	1423	GLN
1	B	1457	THR
1	B	1462	GLU
1	B	1465	LEU
1	B	1466	LEU

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Mol	Chain	Res	Type
1	B	1474	THR
1	B	1489	GLN
1	D	418	LEU
1	D	423	SER
1	D	430	GLU
1	D	450	ARG
1	D	462	LEU
1	D	472	ILE
1	D	474	ASN
1	D	476	ASN
1	D	495	LEU
1	D	497	LYS
1	D	501	HIS
1	D	516	ILE
1	D	555	TYR
1	D	556	VAL
1	D	557	TYR
1	D	576	SER
1	D	577	ILE
1	D	590	GLN
1	D	591	LEU
1	D	617	THR
1	D	622	MET
1	D	625	VAL
1	D	636	ASN
1	D	638	VAL
1	D	1013	ASN
1	D	1015	THR
1	D	1045	VAL
1	D	1050	LEU
1	D	1055	GLU
1	D	1059	THR
1	D	1067	SER
1	D	1083	ASP
1	D	1085	SER
1	D	1092	ARG
1	D	1122	ARG
1	D	1137	ARG
1	D	1139	ILE
1	D	1151	ASP
1	D	1206	ILE
1	D	1213	ILE

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Mol	Chain	Res	Type
1	D	1224	ILE
1	D	1228	SER
1	D	1238	ARG
1	D	1248	VAL
1	D	1249	ILE
1	D	1268	VAL
1	D	1270	LYS
1	D	1272	ARG
1	D	1280	LEU
1	D	1289	ILE
1	D	1294	ASP
1	D	1307	ASP
1	D	1308	VAL
1	D	1327	LEU
1	D	1329	THR
1	D	1334	ASN
1	D	1344	LYS
1	D	1365	ARG
1	D	1373	LYS
1	D	1392	ASP
1	D	1411	LEU
1	D	1420	LYS
1	D	1429	ARG
1	D	1438	ARG
1	D	1441	ILE
1	D	1455	LEU
1	D	1468	LEU
1	D	1475	GLU
1	D	1485	ARG
1	S	418	LEU
1	S	425	SER
1	S	427	GLU
1	S	445	SER
1	S	449	SER
1	S	450	ARG
1	S	451	THR
1	S	461	ILE
1	S	462	LEU
1	S	464	VAL
1	S	474	ASN
1	S	480	GLN
1	S	495	LEU

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Mol	Chain	Res	Type
1	S	499	ARG
1	S	511	VAL
1	S	518	THR
1	S	529	ARG
1	S	547	LEU
1	S	553	LYS
1	S	554	TYR
1	S	560	ARG
1	S	567	SER
1	S	577	ILE
1	S	597	ASN
1	S	600	HIS
1	S	604	LEU
1	S	608	LEU
1	S	617	THR
1	S	638	VAL
1	S	642	LEU
1	S	643	ASP
1	S	644	PHE
1	S	1008	ARG
1	S	1012	ARG
1	S	1014	ILE
1	S	1015	THR
1	S	1024	ASP
1	S	1050	LEU
1	S	1058	MET
1	S	1073	ASP
1	S	1092	ARG
1	S	1093	MET
1	S	1107	GLN
1	S	1132	THR
1	S	1150	TYR
1	S	1154	GLU
1	S	1156	GLU
1	S	1168	LEU
1	S	1188	LEU
1	S	1220	THR
1	S	1245	SER
1	S	1248	VAL
1	S	1251	GLU
1	S	1261	VAL
1	S	1273	MET

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Mol	Chain	Res	Type
1	S	1299	ARG
1	S	1304	VAL
1	S	1306	ILE
1	S	1323	LYS
1	S	1330	SER
1	S	1334	ASN
1	S	1339	VAL
1	S	1368	GLN
1	S	1385	ARG
1	S	1392	ASP
1	S	1402	ASP
1	S	1403	THR
1	S	1408	MET
1	S	1425	ILE
1	S	1428	MET
1	S	1431	ARG
1	S	1434	THR
1	S	1440	LYS
1	S	1448	LEU
1	S	1449	LEU
1	S	1457	THR
1	S	1468	LEU
1	S	1476	ILE
1	S	1488	ILE
1	S	1490	LEU
1	U	418	LEU
1	U	430	GLU
1	U	450	ARG
1	U	452	GLN
1	U	457	LEU
1	U	458	ARG
1	U	462	LEU
1	U	473	LEU
1	U	495	LEU
1	U	526	ARG
1	U	531	LEU
1	U	532	ILE
1	U	547	LEU
1	U	567	SER
1	U	569	LEU
1	U	583	LEU
1	U	592	TRP

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Mol	Chain	Res	Type
1	U	599	GLU
1	U	613	GLU
1	U	625	VAL
1	U	1008	ARG
1	U	1012	ARG
1	U	1021	SER
1	U	1024	ASP
1	U	1044	PRO
1	U	1050	LEU
1	U	1058	MET
1	U	1059	THR
1	U	1061	ASP
1	U	1062	LYS
1	U	1063	SER
1	U	1069	ARG
1	U	1083	ASP
1	U	1090	MET
1	U	1122	ARG
1	U	1131	ILE
1	U	1132	THR
1	U	1133	LEU
1	U	1138	ASP
1	U	1139	ILE
1	U	1141	LYS
1	U	1147	ILE
1	U	1159	VAL
1	U	1167	LEU
1	U	1203	ASP
1	U	1225	LEU
1	U	1241	ILE
1	U	1248	VAL
1	U	1252	ARG
1	U	1259	ILE
1	U	1262	THR
1	U	1272	ARG
1	U	1292	LEU
1	U	1304	VAL
1	U	1305	VAL
1	U	1306	ILE
1	U	1328	GLN
1	U	1334	ASN
1	U	1356	LEU

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Mol	Chain	Res	Type
1	U	1367	THR
1	U	1396	SER
1	U	1400	GLU
1	U	1404	ASP
1	U	1411	LEU
1	U	1425	ILE
1	U	1432	ARG
1	U	1438	ARG
1	U	1452	ILE
1	U	1466	LEU
1	U	1468	LEU
1	U	1486	THR
1	U	1488	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	474	ASN
1	B	501	HIS
1	B	515	HIS
1	B	549	GLN
1	B	597	ASN
1	B	605	GLN
1	B	636	ASN
1	B	1010	ASN
1	B	1046	HIS
1	B	1081	HIS
1	B	1334	ASN
1	B	1354	HIS
1	B	1368	GLN
1	B	1423	GLN
1	D	476	ASN
1	D	605	GLN
1	D	1013	ASN
1	D	1046	HIS
1	D	1079	HIS
1	D	1081	HIS
1	D	1095	GLN
1	D	1201	ASN
1	D	1359	GLN
1	D	1368	GLN
1	S	474	ASN

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Mol	Chain	Res	Type
1	S	501	HIS
1	S	597	ASN
1	S	600	HIS
1	S	605	GLN
1	S	1056	GLN
1	S	1081	HIS
1	S	1107	GLN
1	S	1109	ASN
1	S	1187	ASN
1	S	1334	ASN
1	S	1368	GLN
1	S	1412	GLN
1	S	1450	ASN
1	U	476	ASN
1	U	587	ASN
1	U	600	HIS
1	U	616	GLN
1	U	1013	ASN
1	U	1081	HIS
1	U	1313	ASN
1	U	1334	ASN
1	U	1358	HIS
1	U	1368	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5UA	E	1	-	16,23,23	2.70	2 (12%)	17,33,33	4.76	3 (17%)
2	5UA	F	1	-	16,23,23	2.68	2 (12%)	17,33,33	4.92	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5UA	E	1	-	-	0/3/21/21	0/3/3/3
2	5UA	F	1	-	-	0/3/21/21	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	5UA	C2-N1	6.53	1.46	1.33
2	F	1	5UA	C2-N1	6.60	1.46	1.33
2	F	1	5UA	C2-N3	7.97	1.46	1.32
2	E	1	5UA	C2-N3	8.09	1.46	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	5UA	N3-C2-N1	-19.45	114.00	128.89
2	E	1	5UA	N3-C2-N1	-18.88	114.44	128.89
2	F	1	5UA	C4-C5-N7	-3.93	105.86	109.48
2	E	1	5UA	C4-C5-N7	-3.91	105.88	109.48
2	F	1	5UA	O4'-C1'-N9	2.11	111.37	107.72
2	E	1	5UA	C2-N1-C6	2.78	123.73	118.77
2	F	1	5UA	C2-N1-C6	3.00	124.12	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	5UA	1	0
2	F	1	5UA	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	RXV	E	1021[A]	-	35,37,37	2.45	4 (11%)	40,51,51	2.52	14 (35%)
4	RXV	E	1021[B]	-	35,37,37	2.31	4 (11%)	40,51,51	1.46	10 (25%)
4	RXV	W	1020[A]	-	35,37,37	2.11	3 (8%)	40,51,51	1.46	6 (15%)
4	RXV	W	1020[B]	-	35,37,37	2.00	6 (17%)	40,51,51	1.56	8 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	RXV	E	1021[A]	-	-	0/14/30/30	0/4/5/5
4	RXV	E	1021[B]	-	-	0/14/30/30	0/4/5/5
4	RXV	W	1020[A]	-	-	0/14/30/30	0/4/5/5
4	RXV	W	1020[B]	-	-	0/14/30/30	0/4/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1021[A]	RXV	C9-C10	-11.92	1.26	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1021[B]	RXV	C9-C10	-10.23	1.29	1.44
4	W	1020[B]	RXV	C9-C10	-9.80	1.29	1.44
4	W	1020[A]	RXV	C9-C10	-9.58	1.30	1.44
4	E	1021[B]	RXV	C8-C9	-7.03	1.31	1.39
4	W	1020[A]	RXV	C8-C9	-5.29	1.33	1.39
4	E	1021[A]	RXV	C9-C12	-4.45	1.35	1.41
4	E	1021[B]	RXV	C33-C32	-2.55	1.37	1.42
4	W	1020[B]	RXV	C12-C32	-2.49	1.38	1.43
4	W	1020[B]	RXV	C33-C32	-2.28	1.37	1.42
4	W	1020[B]	RXV	C32-C6	-2.19	1.39	1.42
4	E	1021[B]	RXV	C12-C32	-2.18	1.39	1.43
4	W	1020[B]	RXV	C29-C25	-2.10	1.36	1.40
4	W	1020[A]	RXV	C32-C6	-2.02	1.39	1.42
4	W	1020[B]	RXV	C8-N7	2.67	1.36	1.31
4	E	1021[A]	RXV	C8-N7	3.09	1.37	1.31
4	E	1021[A]	RXV	C8-C9	4.18	1.44	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1021[A]	RXV	C9-C10-N11	-5.67	167.99	177.82
4	E	1021[A]	RXV	C4-C5-C6	-5.47	114.95	120.88
4	E	1021[A]	RXV	C9-C8-N7	-5.11	116.65	124.30
4	E	1021[A]	RXV	C32-C6-N7	-4.91	117.65	122.88
4	W	1020[B]	RXV	C9-C10-N11	-4.70	169.66	177.82
4	W	1020[A]	RXV	C32-C6-N7	-3.28	119.39	122.88
4	E	1021[B]	RXV	C32-C6-N7	-3.21	119.46	122.88
4	W	1020[B]	RXV	C9-C8-N7	-2.66	120.31	124.30
4	E	1021[B]	RXV	O2-C3-C33	-2.65	117.96	124.62
4	W	1020[A]	RXV	O2-C3-C33	-2.45	118.45	124.62
4	W	1020[B]	RXV	C23-C22-N21	-2.31	108.34	113.39
4	W	1020[A]	RXV	C29-C30-N31	-2.28	118.80	122.72
4	W	1020[B]	RXV	C17-C16-N15	-2.27	107.25	110.96
4	W	1020[B]	RXV	C29-C30-N31	-2.27	118.81	122.72
4	E	1021[A]	RXV	C29-C30-N31	-2.25	118.85	122.72
4	E	1021[A]	RXV	O2-C3-C33	-2.23	119.01	124.62
4	E	1021[B]	RXV	C13-C14-N15	-2.15	104.21	114.49
4	E	1021[B]	RXV	C14-N15-C20	-2.15	105.75	111.27
4	E	1021[B]	RXV	C24-C23-N31	-2.09	120.04	122.95
4	E	1021[A]	RXV	C4-C3-C33	-2.09	117.84	120.84
4	E	1021[A]	RXV	C24-C23-N31	-2.07	120.06	122.95
4	E	1021[B]	RXV	C29-C30-N31	-2.05	119.20	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	1020[A]	RXV	O28-C29-C25	2.02	112.51	109.80
4	E	1021[B]	RXV	C13-C12-C32	2.08	122.99	119.16
4	W	1020[B]	RXV	C5-C6-C32	2.08	121.42	119.07
4	E	1021[B]	RXV	C8-N7-C6	2.24	119.50	116.95
4	E	1021[B]	RXV	C22-C23-N31	2.31	120.46	116.19
4	E	1021[B]	RXV	O28-C29-C25	2.38	113.00	109.80
4	W	1020[B]	RXV	C8-N7-C6	2.40	119.68	116.95
4	E	1021[A]	RXV	C24-C25-S26	2.44	126.40	123.50
4	W	1020[B]	RXV	O28-C29-C25	2.49	113.14	109.80
4	E	1021[A]	RXV	C13-C12-C32	2.52	123.79	119.16
4	E	1021[A]	RXV	O28-C29-C25	2.70	113.43	109.80
4	W	1020[A]	RXV	C22-C23-N31	2.86	121.47	116.19
4	E	1021[A]	RXV	C5-C4-C3	3.29	124.24	120.14
4	W	1020[A]	RXV	C8-N7-C6	4.17	121.70	116.95
4	E	1021[A]	RXV	C5-C6-C32	4.26	123.87	119.07
4	E	1021[A]	RXV	C8-N7-C6	6.55	124.41	116.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1021[A]	RXV	5	0
4	E	1021[B]	RXV	4	0
4	W	1020[A]	RXV	7	0
4	W	1020[B]	RXV	5	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	B	718/726 (98%)	-0.64	2 (0%) 94 91	78, 126, 188, 218	0
1	D	719/726 (99%)	-0.65	0 100 100	63, 111, 184, 221	0
1	S	718/726 (98%)	-0.70	0 100 100	64, 116, 171, 203	0
1	U	717/726 (98%)	-0.69	1 (0%) 95 94	64, 123, 171, 222	0
2	E	19/20 (95%)	-0.46	0 100 100	103, 115, 196, 218	0
2	F	19/20 (95%)	-0.52	0 100 100	97, 112, 188, 193	0
3	V	20/20 (100%)	-0.30	0 100 100	91, 116, 209, 268	0
3	W	18/20 (90%)	-0.42	0 100 100	100, 119, 173, 202	0
All	All	2948/2984 (98%)	-0.66	3 (0%) 95 94	63, 120, 181, 268	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1254	GLY	2.6
1	B	1255	GLY	2.4
1	U	1254	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	5UA	F	1	21/21	0.89	0.42	-	220,235,239,241	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	5UA	E	1	21/21	0.89	0.30	-	193,198,206,208	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	RXV	E	1021[B]	33/33	0.88	0.29	5.32	110,128,143,146	33
4	RXV	E	1021[A]	33/33	0.88	0.29	5.18	111,129,144,148	33
4	RXV	W	1020[A]	33/33	0.94	0.20	1.63	100,108,111,111	33
4	RXV	W	1020[B]	33/33	0.94	0.20	1.50	100,108,110,110	33

6.5 Other polymers [i](#)

There are no such residues in this entry.