Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 04:26 AM EDT

PDB ID	:	5TMC
Title	:	Re-refinement of Thermus thermopiles DNA-directed RNA polymerase structure
Authors	:	Wang, J.
Deposited on	:	2016-10-12
Resolution	:	2.71 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

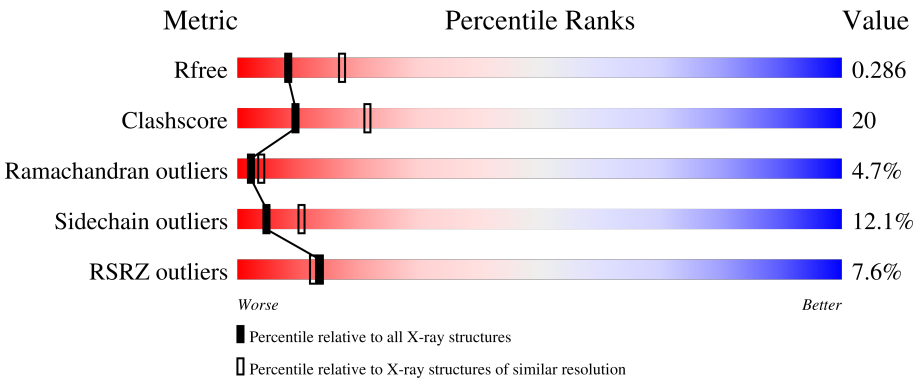
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.71 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	315	3%; 34%, 31%, 8%, 27%
1	B	315	10%; 46%, 27%, ·, 24%
2	C	1119	6%; 52%, 41%, 7%
3	D	1524	8%; 52%, 40%, 7%, ·
4	E	99	7%; 69%, 23%, ·, ·, ·

Continued on next page...

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Mol	Chain	Length	Quality of chain
5	F	423	10% 56% 23% • 17%
6	Z	48	96% •

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 28419 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	1816	1159	315	339	3	0	0	0
1	B	238	1863	1188	322	350	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1119	8829	5581	1577	1647	24	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1504	11864	7518	2091	2219	36	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	95	769	488	133	144	4	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	GLU	VAL	conflict	UNP Q72ID6
E	92	ILE	LEU	conflict	UNP Q72ID6
E	95	GLY	VAL	conflict	UNP Q72ID6

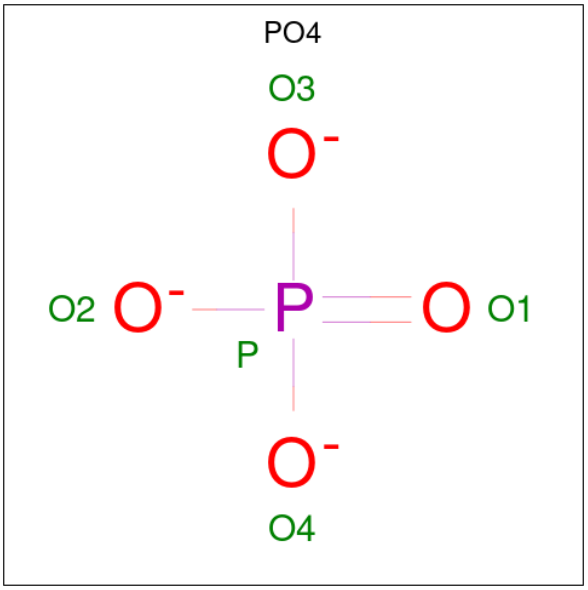
- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	351	2844	1794	515	531	4	0	0	0

- Molecule 6 is a protein called unknown protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	Z	48	240	144	48	48	0	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
7	A	1	5	4	1	0	0

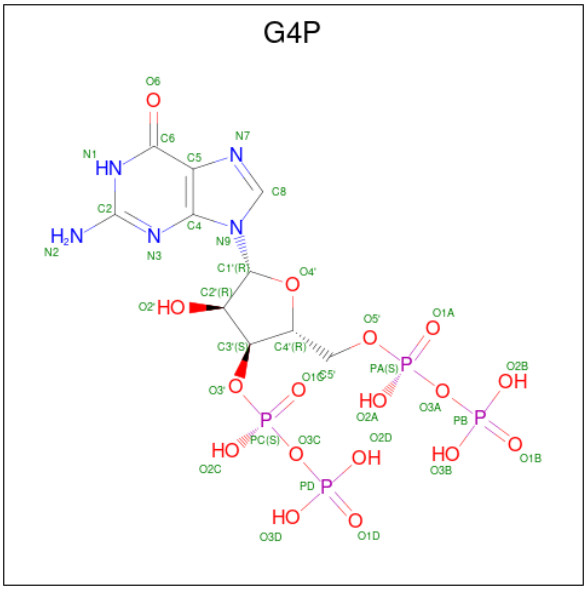
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
8	C	1	1	1	0	0
8	D	3	3	3	0	0

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

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

- Molecule 10 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
10	D	1	36	10	5	17	4	0	0

- Molecule 11 is water.

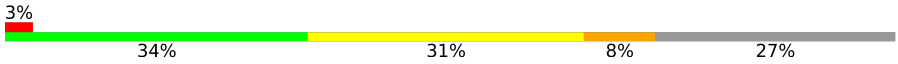
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	15	15	15	0	0
11	B	2	2	2	0	0
11	C	54	54	54	0	0
11	D	62	62	62	0	0
11	E	9	9	9	0	0
11	F	5	5	5	0	0

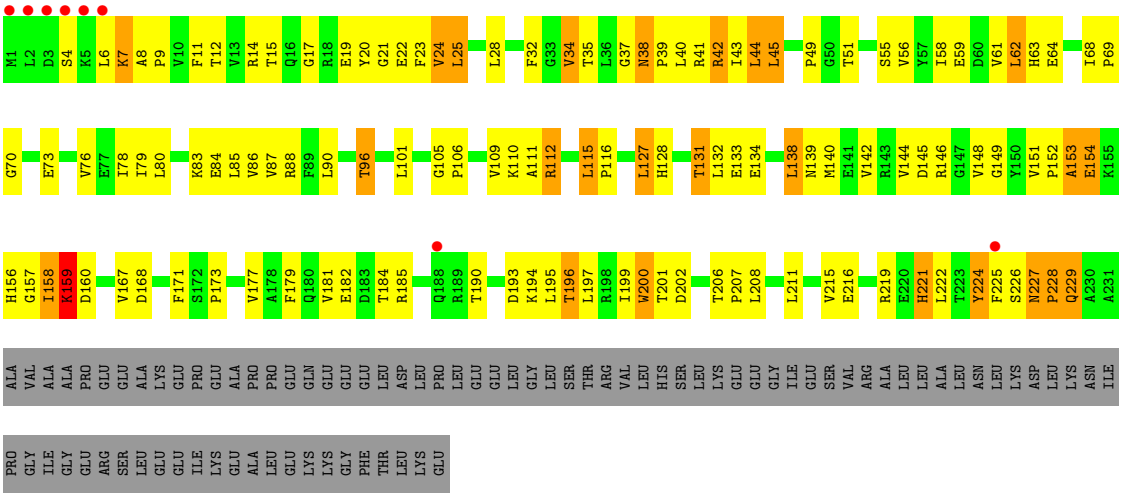
3 Residue-property plots (i)

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha

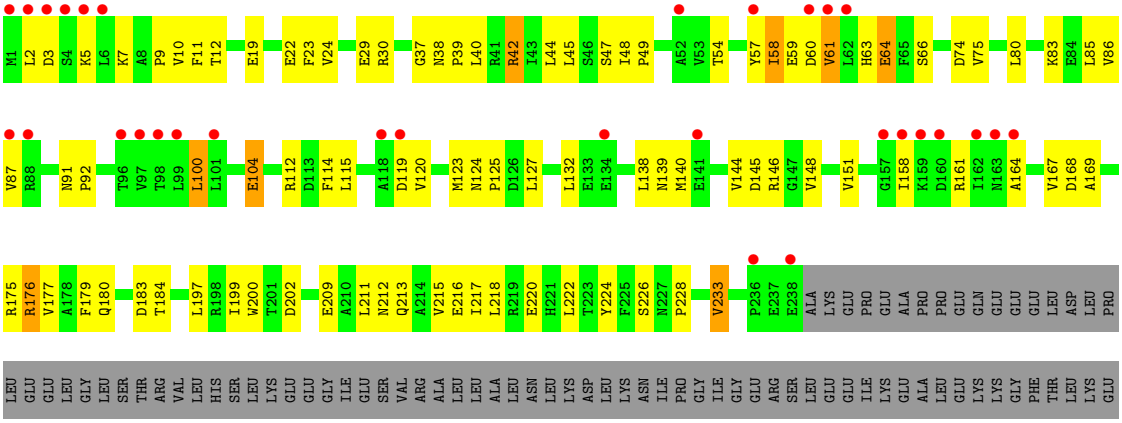
Chain A:





• Molecule 1: DNA-directed RNA polymerase subunit alpha

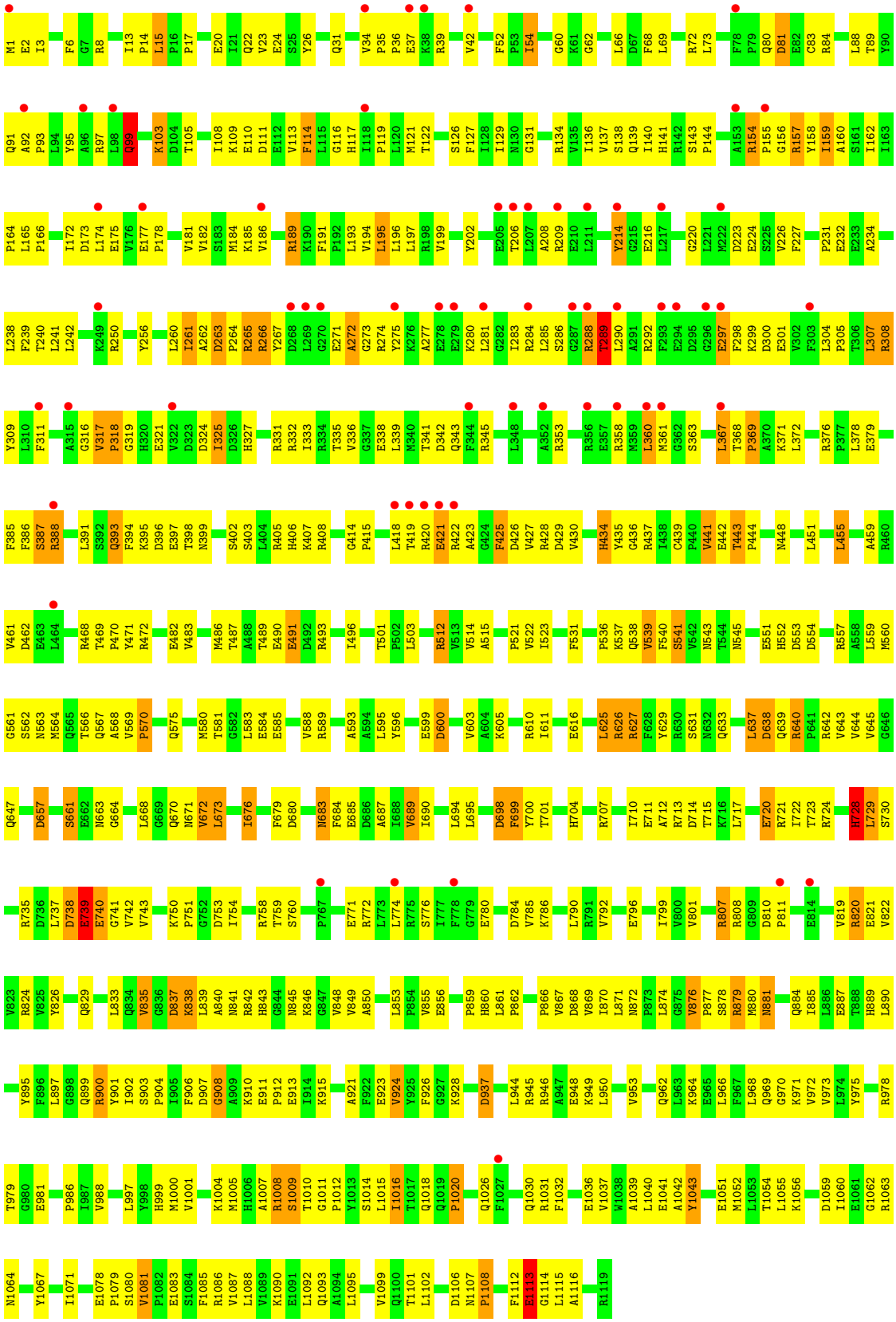
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

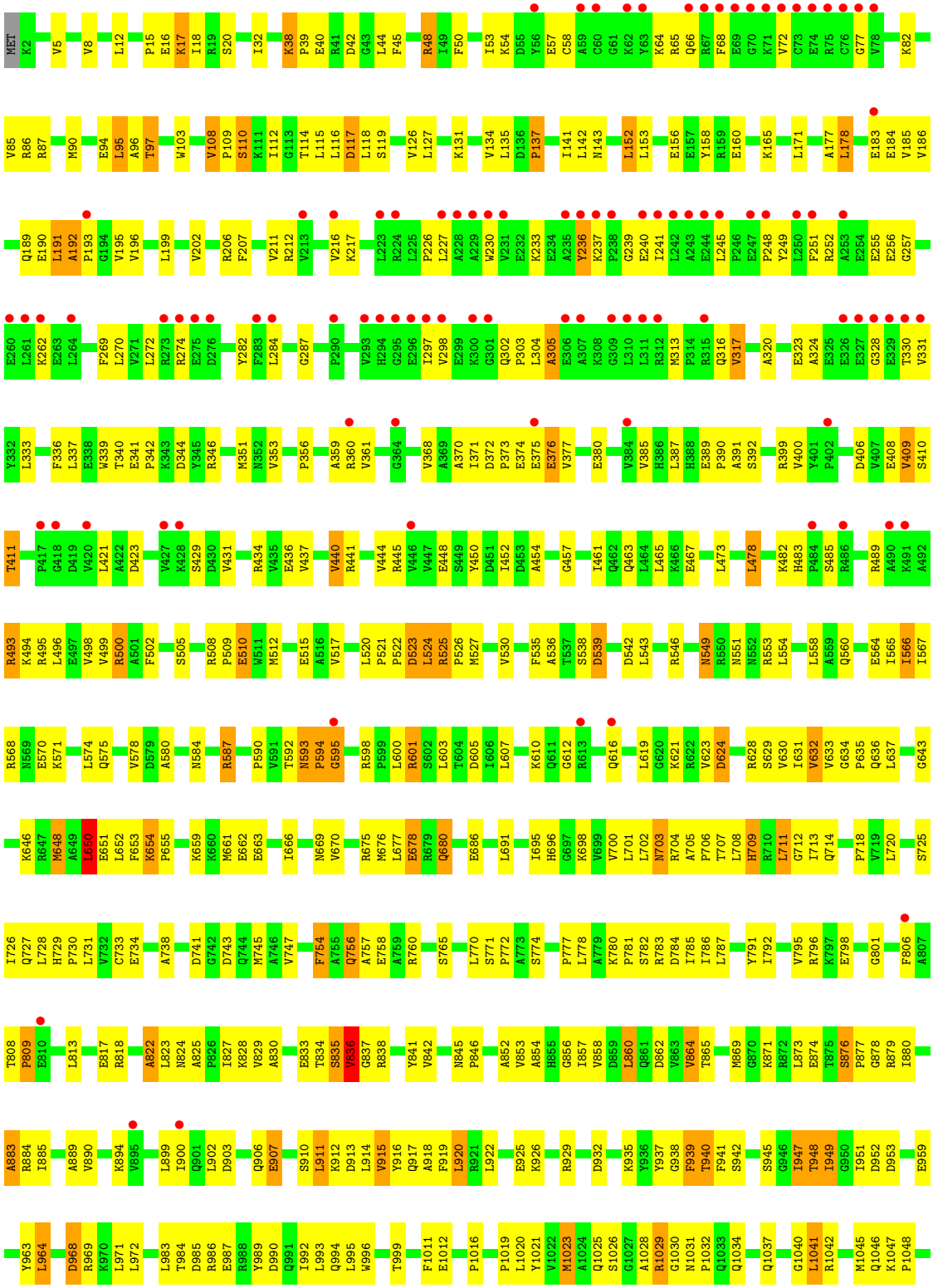
Chain C:

6%
52%
41%
7%


M1 E2 I3 F6 G7 R8 I13 P14 L15 P16 P17 E20 I21 Q22 V23 E24 S25 Y26 Q31 V34 P35 P36 E37 K38 R39 V42 F52 P53 I54 G60 K61 G62 L66 D67 F68 L69 R72 L73 F78 P79 Q80 D81 E82 C83 R84 L88 T89 Y90
Q91 A92 P93 L94 Y95 A96 R97 L98 Q99 K103 D104 T105 I108 K109 E110 D111 E112 V113 F114 L115 G116 H117 I118 P119 L120 M121 T122 S126 F127 I128 I129 N130 G131 R134 V135 I136 V137 S138 Q139 I140 H141 R142 S143 P144 A153 R154 P155 G156 R157 Y158 I159 A160 S161 I162 I163
P164 L165 P166 I172 D173 L174 E175 V176 E177 P178 V181 V182 S183 M184 K185 V186 R189 K190 F191 P192 L193 V194 L195 L196 L197 R198 V199 Y202 E205 T206 L207 A208 R209 E210 L211 Y214 G215 E216 L217 G220 L221 M222 D223 E224 S225 V226 F227 P231 E232 E233 A234
L238 F239 T240 L241 L242 K249 R250 Y256 L260 I261 A262 D263 P264 R265 R266 Y267 D268 L269 G270 E271 A272 G273 R274 Y275 K276 A277 E278 E279 K280 L281 G282 I283 R284 L285 S286 G287 R288 T289 L290 A291 R292 F293 E294 D295 G296 E297 F298 K299 D300 E301 V302 F303 L304 P305 T306 L307 R308
Y309 L310 F311 A315 G316 V317 P318 G319 H320 E321 V322 D323 D324 I325 D326 H327 R331 R332 I333 R334 T335 V336 G337 E338 L339 M340 T341 D342 Q343 F344 R345 L348 A352 R353 R356 E357 R358 M359 L360 M361 G362 S363 L367 T368 P369 A370 K371 L372 R376 P377 L378 E379
F385 F386 S387 R388 L391 S392 Q393 F394 K395 D396 E397 T398 N399 S402 S403 L404 R405 H406 K407 R408 G414 P415 L418 T419 R420 E421 R422 A423 G424 F425 D426 V427 R428 D429 V430 H434 Y435 G436 R437 I438 C439 P440 V441 E442 T443 P444 N448 L451 L455 A459 R460
V461 D462 E463 L464 R468 T469 P470 Y471 R472 E482 V483 M486 T487 A488 T489 E490 E491 D492 R493 I496 T501 P502 L503 R512 V513 V514 A515 P521 V522 I523 F531 P536 K537 Q538 V539 F540 S541 V542 N543 T544 N545 E551 H552 D553 D554 R557 A558 L559 M560
G561 S562 N563 M564 Q565 T566 Q567 A568 V569 P570 Q575 M580 T581 G582 L583 E584 E585 V588 R589 A593 A594 L595 Y596 E599 D600 V603 A604 K605 R610 I611 E616 L625 R626 R627 F628 Y629 R630 S631 N632 Q633 L637 D638 Q639 R640 F641 R642 V643 V644 V645 G646
Q647 D657 S661 E662 N663 G664 L668 G669 Q670 N671 V672 L673 I676 F679 D680 N683 F684 E685 D686 A687 I688 V689 I690 L694 L695 D698 F699 Y700 T701 H704 R707 I710 E711 A712 R713 D714 T715 K716 L717 E720 R721 I722 T723 R724 H728 L729 S730
R735 D736 L737 D738 E739 E740 G741 V742 V743 K750 P751 G752 D753 I754 R758 T759 S760 P767 E771 R772 L773 L774 R775 S776 I777 F778 G779 E780 D784 V785 K786 L790 R791 V792 E796 I799 V800 V801 R807 R808 G809 D810 P811 E814 V819 R820 E821 V822
V823 R824 V825 Y826 Q829 L833 Q834 V835 G836 D837 K838 L839 A840 N841 R842 H843 G844 N845 K846 G847 V848 V849 A850 L853 P854 V855 E856 P859 H860 L861 P862 P866 V867 D868 V869 I870 L871 N872 P873 L874 G875 V876 P877 S878 R879 M880 N881 Q884 I885 L886 E887 T888 H889 L890
Y895 F896 L897 G898 Q899 R900 Y901 I902 S903 P904 I905 F906 D907 G908 A909 K910 E911 P912 E913 I914 K915 A921 F922 E923 V924 Y925 F926 G927 K928 D937 L944 R945 R946 A947 E948 K949 L950 V953 Q962 L963 K964 E965 L966 F967 L968 Q969 G970 K971 V972 V973 L974 Y975 R978
T979 G980 E981 P986 I987 V988 L997 Y998 H999 M1000 V1001 K1004 M1005 H1006 A1007 R1008 S1009 T1010 G1011 P1012 Y1013 S1014 L1015 I1016 T1017 Q1018 Q1019 P1020 Q1026 F1027 Q1030 R1031 F1032 E1036 V1037 W1038 A1039 L1040 E1041 A1042 Y1043 E1051 M1052 L1053 T1054 L1055 K1056 D1059 I1060 E1061 G1062 R1063
N1064 Y1067 I1071 E1078 P1079 S1080 V1081 P1082 E1083 S1084 F1085 R1086 V1087 L1088 Y1089 K1090 E1091 L1092 Q1093 A1094 L1095 V1099 Q1100 T1101 L1102 D1106 N1107 P1108 F1112 E1113 G1114 L1115 A1116 R1119

• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



T1052 F1053 E1054 V1055 P1056 V1057 R1058 T1066 V1067 L1068 E1069 Y1070 F1071 I1072 S1073 S1074 H1075 G1076 A1077 L1086 R1087 T1088 A1089 D1090 S1091 G1092 Y1093 L1094 T1095 R1096 K1097 L1098 V1101 T1102 H1103 E1104 V1107 C1112 T1115 N1116 S1119 Q1124 P1125 D1126 E1127 V1128 S1131 L1132 R1133 L1134 R1135

K1136 D1139 I1140 E1141 A1142 Y1145 A1150 R1151 E1152 V1155 V1158 E1161 E1162 G1163 R1164 Y1165 L1166 S1167 M1168 D1169 D1170 V1171 H1172 L1173 L1174 I1175 V1186 P1187 V1188 R1189 S1190 P1191 L1192 T1193 C1194 V1200 C1201 Q1202 K1203 C1204 Y1205 D1208 L1209 S1210 R1213 P1214 V1215 S1216 I1217 G1218

E1219 A1220 V1221 G1222 A1225 I1229 G1230 E1231 P1232 G1233 T1234 M1238 R1239 T1240 F1241 H1242 T1243 G1244 G1245 V1246 A1247 G1248 A1249 A1250 T1253 Q1254 G1255 L1256 P1257 R1258 E1261 L1262 F1263 E1264 A1265 R1266 R1267 P1268 K1269 A1270 K1271 E1276 I1277 V1281 T1286 E1287 E1288 V1292 E1295 S1296

E1297 S1300 K1301 L1305 P1306 K1307 L1312 V1313 K1314 D1315 G1316 D1317 Y1318 V1319 E1320 Q1323 P1324 L1325 T1326 R1327 D1331 P1332 H1333 Q1334 P1341 E1342 A1343 V1344 E1345 R1346 Y1347 L1348 V1349 E1350 E1351 I1352 Q1353 K1354 V1355 Y1356 R1357 A1358 Q1359 K1362 L1363 H1364 D1365 K1366 H1367 I1368 E1369 I1370 V1371

V1372 M1375 M1376 K1377 Y1378 V1379 E1380 V1381 T1382 D1383 P1384 G1385 D1386 S1387 R1388 L1389 L1390 E1391 V1394 L1395 E1396 K1397 W1398 D1399 V1400 N1404 L1407 I1408 A1409 E1410 G1411 K1412 T1413 P1414 V1415 L1420 L1421 M1422 G1423 V1424 T1425 S1430 T1431 K1432 S1433 W1434 L1435 S1436 A1437 A1438 S1439 F1440 Q1441 N1442

T1443 T1444 A1453 D1457 E1458 L1459 I1460 G1461 L1462 K1463 E1464 I1467 L1468 G1469 R1470 L1471 I1472 P1473 A1474 S1478 D1479 F1480 V1481 R1482 F1483 T1484 Q1485 V1486 V1487 D1488 Q1489 L1492 I1495 E1496 R1499 V1503 E1504 A1505 LYS GLU ARG PRO ALA ALA ARG ARG GLY VAL LYS ARG GLU GLN

PRO GLY LYS GLN ALA

- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 7% 69% 23%

MET A2 L9 F10 G11 R18 L19 K25 R26 A27 Q28 Q29 L30 L31 R32 H33 N37 T38 V39 E43 E52 A60 E61 T62 W63 L68 R72 V80 P81 E82 D83 R84 L85 Q86 K87 E88 M89 E90 R91 E96 ARG GLU GLU

- Molecule 5: RNA polymerase sigma factor SigA

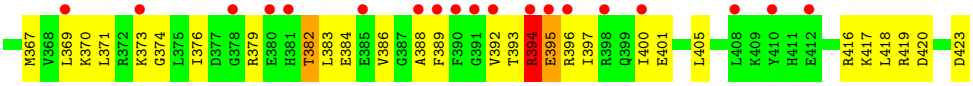
Chain F: 10% 56% 23% 17%

MET LYS LYS SER LYS ARG LYS ASN ALA GLN ALA GLN GLU ALA GLN GLU THR GLU VAL LEU VAL GLN GLU GLU ALA GLU GLU LEU PRO GLU PHE PRO GLU GLY GLU PRO ASP PRO ASP LEU GLU ASP PRO ASP LEU ALA LEU GLU ASP ASP LEU LEU ASP LEU PRO GLU GLU GLU GLY GLU GLY

LEU ASP LEU GLU GLU GLU GLU GLU ASP LEU PRO ILE P73 K74 I75 S76 D79 P80 V81 R82 Q83 I88 V91 P92 L93 L94 T95 E98 E101 R104 S117 T120 G121 L122 D123 P124 D125 R128 R132 I135 L136 G137 R140 V141 I144 P145 G146

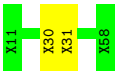
L147 K148 E149 T150 L151 D152 P153 E157 Q161 R172 I176 A177 R178 E179 R184 R193 L194 V195 K200 K201 Y202 R205 G206 L207 S208 F209 L210 D211 L212 I213 Q214 R222 E228 Y229 K230 K234 F235 S236 T237 T240 W241 W242 R249 A255 R256

P261 V262 H263 M264 V265 E266 T267 R276 E290 I291 A292 E293 A294 W299 D300 R303 V304 T307 I310 P314 V315 E318 T319 P320 I321 K325 F328 Y329 I333 P334 D335 E336 P341 A344 L350 L354 E355 K356 A357 L358 S359 K360 L361 S362 E363



- Molecule 6: unknown protein

Chain Z: 96%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	236.35Å 236.35Å 249.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.51 – 2.71 48.50 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.51-2.71) 97.1 (48.50-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.265 , 0.286 0.265 , 0.286	Depositor DCC
R_{free} test set	7447 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å^2)	51.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 89.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.086 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.875 for H, K, L 0.125 for -H-K, K, -L	Depositor
Outliers	1 of 206105 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	28419	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4, G4P, ZN

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	0.47	0/1848	0.64	0/2512
1	B	0.39	0/1896	0.57	0/2579
2	C	0.46	0/8997	0.65	0/12164
3	D	0.45	0/12073	0.65	2/16324 (0.0%)
4	E	0.44	0/783	0.63	0/1054
5	F	0.35	0/2890	0.55	0/3888
All	All	0.44	0/28487	0.63	2/38521 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	95	LEU	CA-CB-CG	5.47	127.89	115.30
3	D	650	LEU	CA-CB-CG	5.43	127.79	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1126	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1816	0	1871	90	0
1	B	1863	0	1914	59	0
2	C	8829	0	8933	408	0
3	D	11864	0	12094	544	0
4	E	769	0	775	20	0
5	F	2844	0	2926	68	0
6	Z	240	0	50	1	0
7	A	5	0	0	0	0
8	C	1	0	0	0	0
8	D	3	0	0	0	0
9	D	2	0	0	0	0
10	D	36	0	11	1	0
11	A	15	0	0	0	0
11	B	2	0	0	2	0
11	C	54	0	0	4	0
11	D	62	0	0	7	0
11	E	9	0	0	1	0
11	F	5	0	0	0	0
All	All	28419	0	28574	1111	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 20.

All (1111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1265:ALA:HA	3:D:1266:ARG:CB	1.60	1.29
3:D:1265:ALA:HA	3:D:1266:ARG:HB2	1.23	1.13
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.32	1.07
2:C:93:PRO:HA	2:C:117:HIS:HB2	1.36	1.06
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.41	1.01
3:D:703:ASN:HA	3:D:712:GLY:O	1.59	1.01
3:D:836:VAL:H	3:D:837:GLY:HA3	1.26	0.97
3:D:1213:ARG:HG2	3:D:1213:ARG:HH11	1.26	0.96
3:D:728:LEU:HD13	3:D:745:MET:HE1	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:964:LEU:HD21	3:D:1058:ARG:HG2	1.45	0.95
3:D:1265:ALA:HA	3:D:1266:ARG:HB3	1.49	0.95
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.32	0.94
2:C:838:LYS:HG3	2:C:997:LEU:HB2	1.48	0.93
2:C:881:ASN:H	2:C:881:ASN:ND2	1.67	0.93
2:C:676:ILE:O	3:D:948:THR:HG22	1.69	0.91
2:C:881:ASN:HD22	2:C:881:ASN:N	1.62	0.91
3:D:1496:GLU:HA	3:D:1499:ARG:HB2	1.50	0.91
3:D:1265:ALA:CA	3:D:1266:ARG:HB2	2.01	0.90
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.53	0.90
2:C:724:ARG:HE	2:C:738:ASP:HA	1.35	0.89
2:C:263:ASP:H	2:C:264:PRO:CD	1.86	0.88
2:C:575:GLN:NE2	2:C:671:ASN:H	1.71	0.88
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.55	0.88
2:C:199:VAL:HG21	2:C:238:LEU:HD11	1.56	0.88
3:D:1265:ALA:CA	3:D:1266:ARG:CB	2.51	0.88
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.55	0.87
2:C:889:HIS:HE1	3:D:951:ILE:H	1.21	0.87
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.40	0.87
3:D:493:ARG:HH12	3:D:1390:LEU:H	1.23	0.86
3:D:675:ARG:HA	3:D:678:GLU:OE1	1.76	0.86
2:C:469:THR:HG22	2:C:538:GLN:HE21	1.37	0.85
2:C:1059:ASP:OD1	2:C:1062:GLY:N	2.10	0.85
1:B:2:LEU:N	1:B:3:ASP:HA	1.91	0.85
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.58	0.85
3:D:1258:ARG:CZ	3:D:1262:LEU:HD21	2.07	0.85
3:D:1377:LYS:HD2	3:D:1378:TYR:CE2	2.12	0.84
3:D:584:ASN:OD1	3:D:590:PRO:HD2	1.78	0.84
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	1.60	0.83
1:A:128:HIS:HE1	1:A:131:THR:HG23	1.43	0.82
1:B:167:VAL:HG12	1:B:168:ASP:H	1.44	0.82
2:C:881:ASN:H	2:C:881:ASN:HD22	0.84	0.82
2:C:34:VAL:N	2:C:35:PRO:HD2	1.93	0.82
5:F:370:LYS:HA	5:F:374:GLY:HA3	1.62	0.81
3:D:984:THR:HG22	3:D:987:GLU:HG3	1.61	0.81
3:D:730:PRO:O	11:D:1701:HOH:O	1.97	0.81
3:D:1094:LEU:O	3:D:1098:LEU:HD13	1.80	0.81
2:C:263:ASP:H	2:C:264:PRO:HD3	1.44	0.81
2:C:157:ARG:HG3	2:C:158:TYR:H	1.44	0.81
3:D:580:ALA:O	3:D:584:ASN:HB2	1.80	0.80
3:D:907:GLU:OE2	3:D:910:SER:HB3	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:93:PRO:HA	2:C:117:HIS:CB	2.10	0.80
2:C:581:THR:HA	2:C:903:SER:O	1.81	0.80
3:D:1042:ARG:HH11	3:D:1042:ARG:HB3	1.45	0.80
3:D:96:ALA:CB	3:D:554:LEU:HD23	2.09	0.80
2:C:13:ILE:HD12	2:C:14:PRO:HD2	1.63	0.80
3:D:1011:PHE:HB3	3:D:1021:TYR:CD2	2.16	0.80
2:C:1081:VAL:HG13	2:C:1086:ARG:HE	1.46	0.79
3:D:117:ASP:HB2	3:D:495:ARG:HH12	1.47	0.79
3:D:964:LEU:O	3:D:968:ASP:HB2	1.82	0.79
2:C:971:LYS:HA	2:C:988:VAL:HA	1.65	0.79
3:D:1434:TRP:NE1	3:D:1457:ASP:HB2	1.98	0.78
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.63	0.78
3:D:836:VAL:N	3:D:837:GLY:HA3	1.96	0.78
2:C:737:LEU:O	2:C:739:GLU:N	2.16	0.78
3:D:1091:SER:C	3:D:1093:TYR:H	1.87	0.78
3:D:152:LEU:HD23	3:D:152:LEU:H	1.49	0.78
2:C:695:LEU:HD21	2:C:833:LEU:HB3	1.65	0.78
2:C:1083:GLU:OE1	3:D:87:ARG:NH1	2.18	0.77
1:B:86:VAL:HG13	1:B:123:MET:HB2	1.66	0.77
3:D:1312:LEU:HD13	3:D:1327:ARG:HG2	1.67	0.76
3:D:1201:CYS:SG	3:D:1204:CYS:HB2	2.25	0.76
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.18	0.76
2:C:878:SER:N	11:C:1301:HOH:O	2.07	0.76
2:C:436:GLY:HA2	2:C:538:GLN:O	1.86	0.76
1:A:23:PHE:HE2	1:A:208:LEU:HD13	1.51	0.75
3:D:1041:LEU:HD12	3:D:1058:ARG:HA	1.66	0.75
3:D:1031:ASN:H	3:D:1034:GLN:HE21	1.34	0.75
4:E:26:ARG:HH21	4:E:30:LEU:HD13	1.52	0.75
3:D:8:VAL:HG12	3:D:1434:TRP:CZ2	2.18	0.75
3:D:632:VAL:O	3:D:727:GLN:HA	1.87	0.75
2:C:859:PRO:O	2:C:867:VAL:HG22	1.87	0.74
3:D:1496:GLU:HA	3:D:1499:ARG:CB	2.16	0.74
2:C:490:GLU:HG2	2:C:493:ARG:HH21	1.51	0.74
3:D:97:THR:HG21	3:D:571:LYS:HD3	1.69	0.74
1:B:58:ILE:HD12	1:B:61:VAL:HB	1.70	0.74
3:D:351:MET:HG2	3:D:370:ALA:HA	1.69	0.74
3:D:885:ILE:HG21	3:D:937:TYR:HD1	1.53	0.74
2:C:261:ILE:O	2:C:264:PRO:HD3	1.88	0.73
3:D:907:GLU:O	3:D:911:LEU:HD12	1.89	0.73
2:C:325:ILE:HD12	2:C:325:ILE:H	1.54	0.73
1:A:96:THR:HB	1:A:145:ASP:OD2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:776:SER:HA	2:C:780:GLU:HB2	1.69	0.72
3:D:698:LYS:HA	3:D:756:GLN:HE22	1.53	0.72
3:D:947:ILE:HG13	3:D:948:THR:N	2.04	0.72
3:D:1378:TYR:HD1	3:D:1422:MET:SD	2.11	0.72
5:F:152:ASP:N	5:F:153:PRO:HD3	2.05	0.72
5:F:208:SER:O	5:F:212:LEU:HG	1.88	0.72
3:D:1368:ILE:HD12	3:D:1368:ILE:H	1.55	0.71
2:C:738:ASP:O	2:C:740:GLU:N	2.22	0.71
3:D:646:LYS:HA	3:D:720:LEU:HD22	1.72	0.71
3:D:1459:LEU:HA	3:D:1464:GLU:HG3	1.72	0.71
3:D:661:MET:HA	3:D:666:ILE:HD12	1.71	0.70
3:D:1380:GLU:HB2	3:D:1420:LEU:HD11	1.73	0.70
1:B:38:ASN:ND2	2:C:979:THR:HA	2.06	0.70
2:C:181:VAL:HA	2:C:220:GLY:HA2	1.74	0.70
2:C:214:TYR:CE1	2:C:311:PHE:HB3	2.26	0.70
5:F:135:ILE:HD11	5:F:178:ARG:HA	1.72	0.70
3:D:1208:ASP:O	3:D:1209:LEU:HB2	1.90	0.70
2:C:15:LEU:HD12	2:C:15:LEU:H	1.57	0.70
2:C:425:PHE:O	2:C:429:ASP:HB2	1.92	0.69
2:C:724:ARG:NE	2:C:738:ASP:HA	2.07	0.69
3:D:158:TYR:HE1	3:D:454:ALA:HB3	1.57	0.69
2:C:277:ALA:HA	2:C:280:LYS:HB2	1.74	0.69
3:D:984:THR:HG22	3:D:987:GLU:CG	2.22	0.69
2:C:672:VAL:HG22	2:C:868:ASP:CB	2.23	0.69
2:C:536:PRO:O	2:C:539:VAL:HG23	1.92	0.69
2:C:848:VAL:CG1	3:D:632:VAL:HG23	2.23	0.69
3:D:791:TYR:CE2	3:D:945:SER:HB2	2.28	0.69
3:D:1213:ARG:HH11	3:D:1213:ARG:CG	2.05	0.69
2:C:430:VAL:HG13	3:D:1075:HIS:HD2	1.58	0.68
2:C:850:ALA:HA	3:D:632:VAL:CG2	2.23	0.68
2:C:850:ALA:HA	3:D:632:VAL:HG22	1.75	0.68
2:C:1093:GLN:HB3	3:D:90:MET:HE2	1.76	0.68
3:D:631:ILE:HG21	3:D:745:MET:HG3	1.75	0.68
3:D:1139:ASP:O	3:D:1142:ALA:HB3	1.94	0.68
2:C:838:LYS:CG	2:C:997:LEU:HB2	2.21	0.67
2:C:263:ASP:N	2:C:264:PRO:HD3	2.10	0.67
2:C:193:LEU:HD21	2:C:307:LEU:HD21	1.76	0.67
2:C:840:ALA:HA	2:C:845:ASN:O	1.95	0.67
2:C:305:PRO:HA	2:C:308:ARG:HG2	1.76	0.67
3:D:317:VAL:HG23	3:D:337:LEU:HA	1.76	0.67
3:D:482:LYS:H	3:D:489:ARG:HG3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:592:THR:HG23	3:D:600:LEU:HD21	1.76	0.67
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.09	0.67
5:F:222:ARG:HG2	5:F:242:TRP:CZ3	2.30	0.67
2:C:704:HIS:HB3	11:C:1308:HOH:O	1.95	0.66
2:C:843:HIS:HE1	2:C:887:GLU:OE1	1.78	0.66
3:D:1351:GLU:HA	3:D:1354:LYS:HD3	1.76	0.66
3:D:836:VAL:H	3:D:837:GLY:CA	2.05	0.66
1:B:45:LEU:HD11	11:B:401:HOH:O	1.95	0.66
3:D:1261:GLU:O	3:D:1265:ALA:HB2	1.96	0.66
3:D:630:VAL:HG13	3:D:725:SER:HB3	1.76	0.66
3:D:964:LEU:CD2	3:D:1058:ARG:HG2	2.23	0.66
5:F:370:LYS:HA	5:F:374:GLY:CA	2.25	0.66
3:D:1225:ALA:O	3:D:1229:ILE:HG13	1.96	0.65
3:D:1397:LYS:HB2	3:D:1398:TRP:CZ3	2.32	0.65
3:D:1442:ASN:HD21	3:D:1444:THR:HB	1.60	0.65
2:C:1102:LEU:HB3	2:C:1106:ASP:HA	1.78	0.65
3:D:108:VAL:HG12	3:D:109:PRO:HA	1.79	0.65
2:C:140:ILE:HD12	2:C:331:ARG:NH2	2.12	0.65
2:C:846:LYS:HE2	3:D:741:ASP:O	1.97	0.65
3:D:885:ILE:CG2	3:D:937:TYR:HD1	2.10	0.65
3:D:1258:ARG:NH2	3:D:1262:LEU:HD21	2.10	0.65
3:D:702:LEU:O	3:D:713:ILE:HA	1.96	0.65
2:C:949:LYS:HD2	3:D:796:ARG:NH2	2.11	0.65
2:C:91:GLN:HB3	2:C:119:PRO:HA	1.79	0.64
2:C:399:ASN:ND2	2:C:568:ALA:HB3	2.12	0.64
2:C:673:LEU:HD11	2:C:895:TYR:CZ	2.31	0.64
1:A:38:ASN:O	1:A:41:ARG:N	2.30	0.64
2:C:317:VAL:N	2:C:318:PRO:HD3	2.13	0.64
2:C:1086:ARG:HD3	2:C:1112:PHE:CD2	2.33	0.64
2:C:588:VAL:HG13	2:C:593:ALA:HB3	1.79	0.64
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.78	0.64
2:C:707:ARG:HG3	2:C:826:TYR:CE2	2.33	0.64
5:F:379:ARG:HD3	5:F:382:THR:HB	1.78	0.64
1:A:200:TRP:HE3	1:A:200:TRP:H	1.45	0.64
2:C:1081:VAL:CG1	2:C:1086:ARG:HE	2.09	0.64
2:C:116:GLY:HA3	2:C:378:LEU:HD23	1.78	0.64
2:C:911:GLU:N	2:C:912:PRO:HD2	2.11	0.64
2:C:1090:LYS:HA	2:C:1093:GLN:HB2	1.80	0.64
3:D:659:LYS:HE3	3:D:663:GLU:HG3	1.77	0.64
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.79	0.64
3:D:1232:PRO:HG2	3:D:1356:TYR:HE2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:574:LEU:O	3:D:578:VAL:HG23	1.98	0.63
2:C:640:ARG:HH11	2:C:642:ARG:HH22	1.46	0.63
3:D:183:GLU:O	3:D:202:VAL:HG13	1.98	0.63
2:C:1052:MET:HG3	3:D:623:VAL:HG21	1.79	0.63
3:D:791:TYR:CD2	3:D:945:SER:HB2	2.34	0.63
2:C:1009:SER:HB3	3:D:651:GLU:OE2	1.98	0.63
3:D:941:PHE:O	3:D:945:SER:HB3	1.98	0.63
1:A:111:ALA:HB2	1:A:127:LEU:HD23	1.79	0.63
3:D:885:ILE:CG2	3:D:937:TYR:CD1	2.82	0.63
5:F:367:MET:HA	5:F:370:LYS:HB2	1.80	0.63
1:A:24:VAL:HG13	1:A:196:THR:HG23	1.80	0.63
2:C:575:GLN:NE2	2:C:670:GLN:HG2	2.14	0.63
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.81	0.62
1:A:73:GLU:HB3	1:A:78:ILE:HG12	1.81	0.62
3:D:535:PHE:O	5:F:314:PRO:HB2	1.99	0.62
3:D:969:ARG:O	3:D:972:LEU:HB2	1.99	0.62
2:C:202:TYR:HE2	2:C:300:ASP:HB3	1.63	0.62
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.11	0.62
2:C:1012:PRO:HD3	2:C:1026:GLN:HG2	1.81	0.62
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.80	0.62
3:D:45:PHE:O	3:D:86:ARG:NH2	2.32	0.62
2:C:363:SER:H	2:C:367:LEU:HD21	1.64	0.62
3:D:1127:GLU:HB3	3:D:1131:SER:HB3	1.82	0.62
1:A:110:LYS:HB2	1:A:112:ARG:HG2	1.81	0.62
2:C:430:VAL:HG13	3:D:1075:HIS:CD2	2.34	0.62
2:C:1018:GLN:HG3	2:C:1060:ILE:HD11	1.80	0.62
3:D:845:ASN:HB2	3:D:846:PRO:CD	2.29	0.62
1:A:206:THR:HG22	1:A:208:LEU:H	1.65	0.61
3:D:728:LEU:HD13	3:D:745:MET:CE	2.27	0.61
2:C:575:GLN:HE21	2:C:671:ASN:H	1.48	0.61
3:D:1074:SER:HA	3:D:1077:ALA:HB3	1.81	0.61
3:D:1341:PRO:HD2	3:D:1342:GLU:OE2	2.00	0.61
2:C:441:VAL:O	2:C:441:VAL:CG2	2.48	0.61
2:C:1087:VAL:HG22	3:D:524:LEU:HD22	1.81	0.61
3:D:1397:LYS:C	3:D:1398:TRP:HE3	2.03	0.61
2:C:194:VAL:HA	2:C:197:LEU:HD12	1.81	0.61
3:D:1152:GLU:HG3	3:D:1161:GLU:HA	1.83	0.61
2:C:843:HIS:CE1	2:C:887:GLU:OE1	2.53	0.61
2:C:1030:GLN:OE1	3:D:628:ARG:HB2	2.00	0.61
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.81	0.61
2:C:720:GLU:HB3	2:C:760:SER:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:838:ARG:HH11	3:D:874:GLU:HB3	1.66	0.61
2:C:759:THR:HB	2:C:785:VAL:HB	1.82	0.61
3:D:703:ASN:ND2	3:D:707:THR:OG1	2.33	0.61
3:D:520:LEU:O	3:D:525:ARG:NH1	2.34	0.60
3:D:616:GLN:HA	3:D:619:LEU:HD12	1.81	0.60
3:D:711:LEU:HD13	3:D:778:LEU:HD23	1.82	0.60
2:C:469:THR:HG22	2:C:538:GLN:NE2	2.12	0.60
2:C:971:LYS:HB2	2:C:986:PRO:HB2	1.83	0.60
2:C:711:GLU:O	2:C:758:ARG:NH1	2.32	0.60
2:C:553:ASP:OD1	2:C:843:HIS:CD2	2.54	0.60
3:D:781:PRO:HG2	3:D:911:LEU:HD22	1.84	0.60
2:C:1039:ALA:HB2	3:D:707:THR:HG21	1.84	0.60
1:B:124:ASN:HD22	1:B:127:LEU:HD13	1.67	0.60
2:C:469:THR:CG2	2:C:538:GLN:HE21	2.10	0.60
2:C:807:ARG:HA	2:C:821:GLU:HB2	1.84	0.60
4:E:25:LYS:HA	4:E:28:GLN:OE1	2.01	0.60
3:D:1433:SER:HA	3:D:1457:ASP:OD2	2.01	0.60
2:C:807:ARG:CZ	2:C:807:ARG:HB3	2.31	0.60
3:D:729:HIS:HE1	3:D:932:ASP:OD1	1.85	0.60
3:D:795:VAL:HG12	3:D:876:SER:HB3	1.84	0.60
3:D:885:ILE:HG23	3:D:937:TYR:CE1	2.36	0.60
2:C:772:ARG:HG2	5:F:373:LYS:HD3	1.84	0.59
2:C:885:ILE:HG22	2:C:889:HIS:CE1	2.36	0.59
3:D:64:LYS:HB3	5:F:376:ILE:HB	1.84	0.59
3:D:1145:TYR:CE2	3:D:1168:MET:HB2	2.36	0.59
2:C:91:GLN:CB	2:C:119:PRO:HA	2.33	0.59
2:C:177:GLU:HG2	2:C:178:PRO:HD2	1.84	0.59
2:C:551:GLU:HG2	2:C:552:HIS:CD2	2.37	0.59
5:F:101:GLU:HG3	5:F:104:ARG:HH12	1.66	0.59
2:C:877:PRO:HG3	3:D:1023:MET:CE	2.32	0.59
3:D:808:THR:N	3:D:809:PRO:HD2	2.17	0.59
3:D:1140:ILE:HD13	3:D:1175:ILE:HG12	1.83	0.59
10:D:1605:G4P:O3C	10:D:1605:G4P:H4'	2.02	0.59
1:B:209:GLU:O	1:B:213:GLN:HG2	2.01	0.59
3:D:1127:GLU:HB3	3:D:1131:SER:CB	2.32	0.59
1:B:226:SER:O	1:B:228:PRO:HD3	2.02	0.59
2:C:3:ILE:HG22	2:C:900:ARG:HB2	1.84	0.59
3:D:17:LYS:O	3:D:20:SER:HB3	2.03	0.59
3:D:709:HIS:ND1	3:D:1231:GLU:HG3	2.18	0.59
1:A:42:ARG:HH21	2:C:978:ARG:HG3	1.67	0.59
2:C:1009:SER:HB2	3:D:651:GLU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1352:ILE:HG21	3:D:1368:ILE:HG21	1.85	0.59
1:B:66:SER:O	1:B:75:VAL:HG23	2.03	0.59
3:D:770:LEU:HA	3:D:777:PRO:HA	1.85	0.59
3:D:890:VAL:O	3:D:926:LYS:HD3	2.02	0.59
3:D:628:ARG:HG2	3:D:629:SER:N	2.18	0.58
1:A:58:ILE:HB	1:A:61:VAL:HG22	1.85	0.58
3:D:558:LEU:HD23	3:D:567:ILE:HD12	1.85	0.58
3:D:838:ARG:HD3	3:D:874:GLU:CD	2.22	0.58
5:F:79:ASP:N	5:F:80:PRO:HD2	2.18	0.58
3:D:527:MET:O	3:D:527:MET:HG3	2.03	0.58
5:F:319:THR:O	5:F:329:TYR:N	2.32	0.58
2:C:640:ARG:NH1	2:C:642:ARG:HH22	2.01	0.58
2:C:1032:PHE:HZ	2:C:1040:LEU:HD11	1.67	0.58
3:D:1091:SER:C	3:D:1093:TYR:N	2.55	0.58
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.03	0.58
2:C:971:LYS:CB	2:C:986:PRO:HB2	2.34	0.58
3:D:65:ARG:HG3	3:D:66:GLN:H	1.67	0.58
3:D:1440:PHE:HE2	3:D:1463:LYS:HZ3	1.52	0.58
3:D:1378:TYR:CE1	3:D:1430:SER:HB2	2.39	0.58
2:C:435:TYR:HA	3:D:1071:PHE:HE2	1.69	0.58
3:D:1400:VAL:HG12	3:D:1404:ASN:HD21	1.69	0.58
2:C:395:LYS:HE2	2:C:403:SER:OG	2.04	0.58
2:C:877:PRO:HG3	3:D:1023:MET:HE3	1.85	0.58
2:C:281:LEU:HB3	2:C:305:PRO:HB2	1.86	0.57
3:D:374:GLU:HB3	3:D:376:GLU:HG3	1.86	0.57
5:F:367:MET:O	5:F:371:LEU:HG	2.04	0.57
1:B:151:VAL:HB	1:B:169:ALA:HB3	1.84	0.57
3:D:1362:LYS:HD3	11:D:1752:HOH:O	2.04	0.57
3:D:1481:VAL:CG1	4:E:18:ARG:HA	2.34	0.57
5:F:350:LEU:O	5:F:354:LEU:HG	2.03	0.57
2:C:140:ILE:HD12	2:C:331:ARG:HH22	1.67	0.57
2:C:441:VAL:O	2:C:441:VAL:HG23	2.03	0.57
3:D:112:ILE:HG22	3:D:512:MET:HE3	1.86	0.57
3:D:860:LEU:HA	3:D:877:PRO:HD2	1.85	0.57
3:D:634:GLY:O	3:D:637:LEU:HB2	2.03	0.57
3:D:852:ALA:HB1	3:D:857:ILE:HG12	1.85	0.57
3:D:1205:TYR:CZ	3:D:1221:VAL:HG22	2.39	0.57
1:A:38:ASN:O	1:A:39:PRO:C	2.41	0.57
3:D:568:ARG:O	3:D:571:LYS:N	2.37	0.57
3:D:992:ILE:O	3:D:995:LEU:HB3	2.03	0.57
3:D:1115:THR:O	3:D:1151:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1295:GLU:HG2	3:D:1300:SER:HA	1.86	0.57
1:A:41:ARG:HG3	1:A:45:LEU:HD12	1.86	0.57
3:D:770:LEU:HD11	3:D:919:PHE:CE1	2.39	0.57
3:D:262:LYS:HD3	3:D:269:PHE:HD2	1.70	0.57
3:D:549:ASN:O	3:D:553:ARG:HB2	2.04	0.57
1:A:181:VAL:HG12	1:A:181:VAL:O	2.05	0.56
3:D:320:ALA:HB3	3:D:336:PHE:HD1	1.70	0.56
2:C:271:GLU:H	2:C:274:ARG:HD3	1.70	0.56
2:C:274:ARG:HD2	2:C:285:LEU:HB3	1.87	0.56
2:C:728:HIS:NE2	2:C:730:SER:O	2.38	0.56
2:C:889:HIS:CD2	2:C:970:GLY:HA3	2.41	0.56
3:D:421:LEU:HD22	3:D:429:SER:HB2	1.85	0.56
1:B:167:VAL:HG12	1:B:168:ASP:N	2.17	0.56
2:C:712:ALA:HB3	2:C:821:GLU:H	1.70	0.56
2:C:713:ARG:HG2	2:C:819:VAL:HG22	1.86	0.56
2:C:890:LEU:HG	2:C:901:TYR:CD1	2.40	0.56
3:D:1155:VAL:HG11	3:D:1174:LEU:HD23	1.88	0.56
2:C:501:THR:O	2:C:503:LEU:HD13	2.06	0.56
5:F:417:LYS:HB2	5:F:418:LEU:HD12	1.87	0.56
2:C:6:PHE:HB2	2:C:902:ILE:O	2.06	0.56
2:C:712:ALA:O	2:C:820:ARG:N	2.38	0.56
2:C:1008:ARG:HH21	2:C:1020:PRO:HB3	1.68	0.56
3:D:935:LYS:HG2	3:D:939:PHE:CE1	2.41	0.56
2:C:17:PRO:O	2:C:20:GLU:HB2	2.05	0.56
2:C:234:ALA:O	2:C:238:LEU:HG	2.05	0.56
2:C:469:THR:HG22	2:C:470:PRO:HD2	1.88	0.56
2:C:695:LEU:HD21	2:C:833:LEU:CB	2.36	0.56
3:D:408:GLU:O	3:D:409:VAL:HG22	2.06	0.56
3:D:1190:SER:OG	3:D:1191:PRO:HD2	2.06	0.56
1:B:86:VAL:HG22	1:B:123:MET:HG3	1.88	0.56
2:C:99:GLN:HB2	2:C:109:LYS:HA	1.88	0.56
3:D:400:VAL:HG12	3:D:445:ARG:HG2	1.86	0.56
3:D:729:HIS:CD2	3:D:730:PRO:HD2	2.41	0.56
3:D:824:ASN:ND2	3:D:862:ASP:OD2	2.39	0.56
3:D:127:LEU:HD11	3:D:461:ILE:HG13	1.87	0.56
3:D:1030:GLY:HA2	3:D:1034:GLN:NE2	2.21	0.56
3:D:1379:VAL:HG13	3:D:1395:LEU:HB2	1.87	0.56
2:C:426:ASP:O	2:C:428:ARG:N	2.38	0.55
3:D:879:ARG:HB3	3:D:902:LEU:CD1	2.36	0.55
3:D:916:TYR:CE2	3:D:920:LEU:HD21	2.40	0.55
2:C:368:THR:HB	2:C:369:PRO:HD3	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:835:VAL:HA	2:C:849:VAL:O	2.05	0.55
2:C:1015:LEU:HA	5:F:335:ASP:HB2	1.89	0.55
3:D:711:LEU:HD13	3:D:778:LEU:CD2	2.35	0.55
2:C:881:ASN:O	2:C:884:GLN:HG2	2.06	0.55
3:D:272:LEU:HG	3:D:282:TYR:HE1	1.71	0.55
2:C:496:ILE:HG12	2:C:531:PHE:HB2	1.88	0.55
5:F:207:LEU:HB3	5:F:212:LEU:HD21	1.88	0.55
2:C:672:VAL:HG22	2:C:868:ASP:HB2	1.89	0.55
2:C:99:GLN:H	2:C:110:GLU:HB2	1.71	0.55
1:A:32:PHE:HA	1:A:35:THR:HB	1.88	0.55
2:C:557:ARG:HD3	2:C:879:ARG:HG3	1.89	0.55
2:C:1032:PHE:CE1	2:C:1052:MET:HG2	2.42	0.55
3:D:522:PRO:HA	3:D:525:ARG:NH1	2.21	0.55
3:D:798:GLU:HG3	3:D:824:ASN:HB2	1.89	0.55
4:E:39:VAL:O	4:E:72:ARG:HD2	2.07	0.55
2:C:553:ASP:OD1	2:C:843:HIS:HD2	1.89	0.55
2:C:1081:VAL:HG13	2:C:1086:ARG:NE	2.20	0.55
3:D:634:GLY:HA3	3:D:637:LEU:HD12	1.88	0.55
3:D:770:LEU:HB2	3:D:1210:SER:HA	1.87	0.55
3:D:1229:ILE:O	3:D:1229:ILE:HG22	2.06	0.55
3:D:1353:GLN:O	3:D:1357:ARG:HG2	2.06	0.55
3:D:1127:GLU:HB3	3:D:1131:SER:OG	2.07	0.54
2:C:595:LEU:HD12	2:C:639:GLN:NE2	2.22	0.54
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.30	0.54
1:A:181:VAL:N	2:C:937:ASP:OD2	2.32	0.54
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.42	0.54
2:C:34:VAL:N	2:C:35:PRO:CD	2.68	0.54
3:D:216:VAL:HG22	3:D:340:THR:HG22	1.87	0.54
3:D:1314:LYS:HB3	3:D:1317:ASP:OD2	2.07	0.54
2:C:83:CYS:HB3	2:C:88:LEU:O	2.07	0.54
2:C:164:PRO:HB2	2:C:166:PRO:HD3	1.89	0.54
2:C:512:ARG:HD3	2:C:523:ILE:HD12	1.90	0.54
3:D:570:GLU:OE2	5:F:214:GLN:NE2	2.36	0.54
3:D:835:SER:N	3:D:838:ARG:HE	2.06	0.54
3:D:1369:GLU:O	3:D:1372:VAL:HG12	2.08	0.54
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.88	0.54
2:C:108:ILE:HD12	2:C:368:THR:HG21	1.90	0.54
3:D:1145:TYR:HE2	3:D:1168:MET:HB2	1.71	0.54
2:C:181:VAL:HG12	2:C:182:VAL:H	1.73	0.54
3:D:436:GLU:HB2	3:D:445:ARG:HB2	1.88	0.54
3:D:835:SER:H	3:D:838:ARG:HE	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1459:LEU:HD12	3:D:1470:ARG:HH11	1.73	0.54
2:C:637:LEU:O	2:C:638:ASP:HB3	2.08	0.54
3:D:353:VAL:HG12	3:D:368:VAL:HG22	1.90	0.54
1:A:38:ASN:O	1:A:40:LEU:N	2.41	0.53
1:A:24:VAL:HG11	1:A:194:LYS:HE2	1.90	0.53
4:E:33:HIS:HB2	4:E:37:ASN:HD21	1.72	0.53
5:F:200:LYS:HA	5:F:209:PHE:CE1	2.44	0.53
3:D:1332:PRO:HB2	3:D:1421:LEU:CD2	2.38	0.53
5:F:300:ASP:HB3	5:F:303:ARG:HB2	1.89	0.53
1:A:23:PHE:CE2	1:A:208:LEU:HD13	2.39	0.53
2:C:861:LEU:CD2	2:C:972:VAL:HG21	2.38	0.53
2:C:897:LEU:HB3	2:C:899:GLN:OE1	2.08	0.53
1:B:85:LEU:HA	1:B:124:ASN:HD21	1.72	0.53
2:C:89:THR:HG23	2:C:129:ILE:HA	1.90	0.53
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.89	0.53
2:C:393:GLN:OE1	2:C:406:HIS:HE1	1.92	0.53
2:C:1114:GLY:O	2:C:1116:ALA:N	2.41	0.53
3:D:1066:THR:HB	3:D:1069:GLU:H	1.74	0.53
2:C:1020:PRO:HG3	3:D:624:ASP:OD1	2.09	0.53
3:D:38:LYS:HG3	3:D:39:PRO:HD2	1.90	0.53
3:D:698:LYS:HA	3:D:756:GLN:NE2	2.22	0.53
3:D:1012:GLU:HA	3:D:1012:GLU:OE1	2.08	0.53
3:D:1264:GLU:HA	3:D:1423:GLY:HA3	1.91	0.53
5:F:117:SER:HB2	5:F:122:LEU:O	2.09	0.53
2:C:84:ARG:HA	2:C:131:GLY:HA2	1.90	0.53
2:C:455:LEU:HG	2:C:459:ALA:HB3	1.89	0.53
2:C:862:PRO:HA	2:C:975:TYR:HE1	1.74	0.53
3:D:15:PRO:HA	3:D:18:ILE:HD12	1.90	0.53
3:D:1046:GLN:N	11:D:1702:HOH:O	2.29	0.53
2:C:468:ARG:HE	2:C:487:THR:HG23	1.73	0.53
3:D:792:ILE:O	3:D:878:GLY:HA3	2.08	0.53
3:D:165:LYS:HD3	3:D:199:LEU:HD11	1.90	0.53
3:D:925:GLU:HG3	4:E:2:ALA:HB3	1.91	0.53
3:D:1397:LYS:HB2	3:D:1398:TRP:HZ3	1.73	0.53
3:D:1481:VAL:O	3:D:1482:ARG:C	2.47	0.53
5:F:152:ASP:N	5:F:153:PRO:CD	2.72	0.53
5:F:416:ARG:HG2	5:F:419:ARG:HD2	1.91	0.53
1:A:70:GLY:HA2	1:A:133:GLU:HG2	1.90	0.52
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.91	0.52
3:D:1370:ILE:HG22	3:D:1371:VAL:N	2.22	0.52
5:F:172:ARG:O	5:F:176:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:885:ILE:HG23	3:D:937:TYR:CD1	2.43	0.52
3:D:1042:ARG:HB3	3:D:1042:ARG:NH1	2.19	0.52
3:D:1462:LEU:HD23	3:D:1473:PRO:HG2	1.91	0.52
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.92	0.52
2:C:292:ARG:HB2	2:C:299:LYS:H	1.75	0.52
2:C:444:PRO:HG2	2:C:448:ASN:O	2.09	0.52
3:D:108:VAL:HA	3:D:109:PRO:C	2.30	0.52
3:D:270:LEU:O	3:D:282:TYR:HB2	2.09	0.52
2:C:1092:LEU:CD1	2:C:1099:VAL:HG21	2.34	0.52
3:D:72:VAL:HG13	3:D:77:GLY:HA2	1.90	0.52
5:F:137:GLY:HA2	5:F:140:ARG:HB3	1.91	0.52
2:C:333:ILE:HD11	2:C:461:VAL:HG11	1.90	0.52
3:D:94:GLU:O	3:D:551:ASN:ND2	2.43	0.52
3:D:871:LYS:HD3	3:D:873:LEU:HD21	1.91	0.52
2:C:1063:ARG:HG3	5:F:341:PRO:HG3	1.92	0.52
3:D:1372:VAL:O	3:D:1375:MET:HB3	2.10	0.52
3:D:1379:VAL:HG11	3:D:1395:LEU:HD13	1.90	0.52
5:F:263:HIS:O	5:F:267:THR:HG23	2.10	0.52
3:D:730:PRO:HA	3:D:733:CYS:SG	2.50	0.52
3:D:704:ARG:CD	3:D:738:ALA:HB2	2.40	0.52
3:D:1213:ARG:HG2	3:D:1213:ARG:NH1	2.05	0.52
5:F:157:GLU:O	5:F:161:GLN:N	2.43	0.52
2:C:551:GLU:HB3	2:C:906:PHE:CD2	2.45	0.52
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.91	0.51
1:A:225:PHE:HD2	1:B:11:PHE:CE1	2.28	0.51
2:C:521:PRO:HG2	3:D:1055:VAL:HG21	1.93	0.51
3:D:948:THR:O	3:D:949:ILE:CG1	2.58	0.51
3:D:1381:VAL:HG13	3:D:1389:LEU:O	2.10	0.51
1:B:177:VAL:HB	11:B:401:HOH:O	2.11	0.51
2:C:72:ARG:HG3	2:C:95:TYR:HB2	1.92	0.51
2:C:157:ARG:HG3	2:C:158:TYR:N	2.21	0.51
2:C:1008:ARG:HD3	2:C:1010:THR:HA	1.92	0.51
3:D:1489:GLN:HA	3:D:1492:LEU:HD12	1.92	0.51
2:C:545:ASN:HB3	2:C:583:LEU:HD12	1.91	0.51
3:D:57:GLU:HG2	3:D:58:CYS:H	1.76	0.51
3:D:96:ALA:HB3	3:D:554:LEU:CD2	2.22	0.51
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.93	0.51
2:C:496:ILE:O	2:C:515:ALA:HB1	2.11	0.51
3:D:361:VAL:HG21	3:D:385:VAL:HG23	1.93	0.51
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.93	0.51
2:C:81:ASP:HB3	2:C:626:ARG:HH22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:387:SER:HB3	2:C:388:ARG:HD3	1.92	0.51
2:C:1052:MET:HG3	3:D:623:VAL:CG2	2.41	0.51
3:D:440:VAL:HG23	3:D:441:ARG:H	1.75	0.51
5:F:95:THR:HB	5:F:98:GLU:H	1.75	0.51
2:C:603:VAL:HG23	2:C:647:GLN:O	2.10	0.51
2:C:1067:TYR:CE2	2:C:1071:ILE:HG13	2.45	0.51
2:C:162:ILE:HB	2:C:172:ILE:HB	1.91	0.51
2:C:443:THR:HG22	2:C:559:LEU:HD11	1.93	0.51
2:C:810:ASP:N	2:C:811:PRO:CD	2.74	0.51
2:C:1031:ARG:HA	3:D:621:LYS:O	2.10	0.51
3:D:593:ASN:CB	3:D:594:PRO:HD3	2.40	0.51
3:D:654:LYS:HB3	3:D:655:PRO:CD	2.35	0.51
3:D:1281:VAL:HB	3:D:1316:GLY:H	1.75	0.51
1:A:56:VAL:HG22	1:A:142:VAL:HG22	1.93	0.51
1:A:156:HIS:HD2	1:A:158:ILE:HB	1.76	0.51
3:D:95:LEU:HD21	3:D:517:VAL:HG23	1.91	0.51
3:D:651:GLU:O	3:D:654:LYS:HB2	2.11	0.51
3:D:778:LEU:HG	3:D:778:LEU:O	2.11	0.51
3:D:1264:GLU:CD	3:D:1425:THR:HG1	2.13	0.51
2:C:585:GLU:HA	2:C:664:GLY:O	2.11	0.50
2:C:672:VAL:HG22	2:C:868:ASP:HB3	1.93	0.50
3:D:731:LEU:HA	11:D:1701:HOH:O	2.11	0.50
3:D:1292:VAL:HG11	3:D:1325:LEU:HD22	1.93	0.50
2:C:657:ASP:OD1	2:C:661:SER:OG	2.29	0.50
2:C:742:VAL:HG12	2:C:743:VAL:N	2.25	0.50
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.15	0.50
1:A:139:ASN:C	1:A:139:ASN:OD1	2.50	0.50
1:A:228:PRO:O	1:A:229:GLN:HB2	2.10	0.50
1:B:63:HIS:CE1	3:D:809:PRO:HB3	2.47	0.50
2:C:141:HIS:CE1	2:C:332:ARG:NH1	2.80	0.50
2:C:625:LEU:O	2:C:626:ARG:C	2.50	0.50
3:D:127:LEU:CD1	3:D:461:ILE:HG13	2.41	0.50
3:D:917:GLN:C	3:D:919:PHE:H	2.14	0.50
3:D:1397:LYS:HB2	3:D:1398:TRP:CE3	2.45	0.50
5:F:120:THR:HB	5:F:122:LEU:HG	1.92	0.50
2:C:842:ARG:NH1	11:C:1302:HOH:O	2.29	0.50
3:D:137:PRO:HA	3:D:452:ILE:HG23	1.92	0.50
3:D:860:LEU:HB3	3:D:878:GLY:N	2.25	0.50
2:C:728:HIS:CG	2:C:729:LEU:H	2.29	0.50
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.47	0.50
2:C:1036:GLU:HG3	3:D:703:ASN:ND2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:192:ALA:HB1	3:D:193:PRO:CD	2.33	0.50
3:D:704:ARG:HD3	3:D:738:ALA:HB2	1.92	0.50
2:C:1036:GLU:O	2:C:1039:ALA:HB3	2.11	0.50
2:C:1083:GLU:O	2:C:1087:VAL:HB	2.12	0.50
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.77	0.50
3:D:206:ARG:HB2	3:D:392:SER:O	2.11	0.50
2:C:285:LEU:HD23	2:C:285:LEU:H	1.76	0.50
2:C:589:ARG:HA	2:C:596:TYR:HE1	1.75	0.50
2:C:536:PRO:HB3	2:C:906:PHE:HB2	1.92	0.50
2:C:754:ILE:N	2:C:754:ILE:HD12	2.27	0.50
3:D:539:ASP:OD2	3:D:598:ARG:NH2	2.43	0.50
3:D:939:PHE:O	3:D:940:THR:C	2.50	0.50
3:D:1372:VAL:O	3:D:1375:MET:CB	2.60	0.50
2:C:266:ARG:HH11	2:C:273:GLY:H	1.60	0.49
2:C:881:ASN:ND2	2:C:881:ASN:N	2.36	0.49
3:D:939:PHE:O	3:D:942:SER:N	2.45	0.49
3:D:1481:VAL:O	3:D:1483:PHE:N	2.45	0.49
5:F:79:ASP:HB3	5:F:83:GLN:HB2	1.93	0.49
2:C:448:ASN:HA	2:C:451:LEU:HD12	1.94	0.49
2:C:753:ASP:O	2:C:792:VAL:HG23	2.12	0.49
2:C:904:PRO:HD2	2:C:908:GLY:CA	2.42	0.49
3:D:1101:VAL:HG11	3:D:1424:VAL:HG12	1.94	0.49
5:F:386:VAL:HG12	5:F:388:ALA:H	1.78	0.49
3:D:543:LEU:HD23	3:D:546:ARG:HD3	1.95	0.49
2:C:15:LEU:HD21	2:C:583:LEU:HD22	1.94	0.49
2:C:196:LEU:HD23	2:C:238:LEU:HD22	1.93	0.49
2:C:580:MET:SD	2:C:584:GLU:HG3	2.53	0.49
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.44	0.49
1:A:185:ARG:HB2	1:A:190:THR:HG22	1.94	0.49
2:C:267:TYR:HB2	2:C:272:ALA:HB3	1.94	0.49
2:C:545:ASN:HB3	2:C:583:LEU:CD1	2.42	0.49
3:D:828:LYS:HB3	3:D:833:GLU:HG2	1.94	0.49
3:D:853:VAL:HG12	3:D:858:VAL:HG13	1.93	0.49
3:D:1463:LYS:O	3:D:1467:ILE:HG22	2.13	0.49
3:D:1213:ARG:HB2	3:D:1214:PRO:CD	2.42	0.49
2:C:486:MET:HE3	2:C:491:GLU:HA	1.92	0.49
3:D:1167:SER:HB3	3:D:1170:ASP:OD2	2.12	0.49
3:D:1320:GLU:O	3:D:1323:GLN:HB2	2.12	0.49
5:F:393:THR:HG22	5:F:397:ILE:HD11	1.93	0.49
2:C:713:ARG:HH11	2:C:713:ARG:HB2	1.78	0.49
2:C:1101:THR:HB	3:D:5:VAL:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.93	0.49
3:D:1378:TYR:HE2	3:D:1394:VAL:HG22	1.75	0.49
3:D:117:ASP:CB	3:D:495:ARG:HH12	2.23	0.49
3:D:915:VAL:HG12	3:D:916:TYR:N	2.27	0.49
2:C:657:ASP:CG	2:C:663:ASN:H	2.16	0.48
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.48	0.48
3:D:1434:TRP:HE1	3:D:1457:ASP:HB2	1.76	0.48
1:B:11:PHE:HZ	1:B:211:LEU:HD21	1.78	0.48
1:B:100:LEU:HB2	1:B:115:LEU:HD13	1.94	0.48
2:C:881:ASN:OD1	2:C:884:GLN:NE2	2.46	0.48
1:B:59:GLU:HB2	1:B:139:ASN:H	1.79	0.48
3:D:605:ASP:HA	3:D:610:LYS:HB2	1.94	0.48
2:C:595:LEU:HB2	2:C:639:GLN:HE21	1.79	0.48
4:E:87:LYS:HE2	4:E:91:ARG:HH22	1.78	0.48
5:F:152:ASP:H	5:F:153:PRO:HD3	1.79	0.48
2:C:724:ARG:HG3	2:C:738:ASP:O	2.13	0.48
3:D:1045:MET:O	3:D:1053:PHE:HD1	1.96	0.48
3:D:1263:PHE:HD2	3:D:1375:MET:HE2	1.78	0.48
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.14	0.48
2:C:92:ALA:O	2:C:117:HIS:HB2	2.12	0.48
2:C:759:THR:HA	2:C:786:LYS:O	2.13	0.48
2:C:1085:PHE:O	2:C:1088:LEU:HB3	2.13	0.48
3:D:444:VAL:O	3:D:444:VAL:HG23	2.14	0.48
3:D:629:SER:OG	3:D:630:VAL:N	2.46	0.48
3:D:695:ILE:O	3:D:696:HIS:C	2.51	0.48
1:A:11:PHE:HB2	1:B:224:TYR:O	2.13	0.48
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.44	0.48
2:C:629:TYR:HD2	11:C:1330:HOH:O	1.96	0.48
2:C:850:ALA:HA	3:D:632:VAL:HG21	1.96	0.48
2:C:904:PRO:HD2	2:C:908:GLY:H	1.79	0.48
2:C:1051:GLU:O	2:C:1056:LYS:HD3	2.14	0.48
2:C:1093:GLN:HB3	3:D:90:MET:CE	2.43	0.48
3:D:233:LYS:HB2	3:D:236:TYR:HD1	1.79	0.48
3:D:356:PRO:HB3	3:D:441:ARG:HG3	1.96	0.48
3:D:785:ILE:HG23	3:D:935:LYS:HA	1.96	0.48
3:D:1028:ALA:O	3:D:1029:ARG:HB2	2.12	0.48
2:C:874:LEU:CD2	3:D:1023:MET:SD	3.02	0.48
3:D:852:ALA:HB1	3:D:857:ILE:CG1	2.44	0.48
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.49	0.48
1:A:39:PRO:O	1:A:43:ILE:HG13	2.14	0.48
2:C:267:TYR:CD2	2:C:271:GLU:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.54	0.48
3:D:754:PHE:O	3:D:757:ALA:HB3	2.13	0.48
3:D:798:GLU:O	3:D:825:ALA:HA	2.13	0.48
3:D:853:VAL:HA	3:D:858:VAL:O	2.14	0.48
3:D:860:LEU:HB3	3:D:878:GLY:CA	2.44	0.48
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.49	0.48
3:D:1404:ASN:OD1	3:D:1408:ILE:HB	2.14	0.48
1:B:23:PHE:HE1	1:B:199:ILE:HD12	1.79	0.48
2:C:343:GLN:OE1	2:C:343:GLN:HA	2.13	0.48
3:D:131:LYS:HD3	3:D:152:LEU:HD12	1.95	0.48
3:D:947:ILE:CG1	3:D:948:THR:N	2.73	0.48
3:D:1140:ILE:O	3:D:1141:GLU:C	2.52	0.48
2:C:272:ALA:O	2:C:275:TYR:HB3	2.13	0.47
2:C:672:VAL:CG2	2:C:868:ASP:HB3	2.44	0.47
2:C:1005:MET:HG2	3:D:629:SER:HB2	1.96	0.47
3:D:233:LYS:HB2	3:D:236:TYR:CD1	2.49	0.47
3:D:883:ALA:HA	3:D:900:ILE:HD13	1.96	0.47
1:A:38:ASN:HB3	1:A:39:PRO:CD	2.44	0.47
2:C:3:ILE:HA	2:C:900:ARG:O	2.13	0.47
2:C:154:ARG:HH21	2:C:156:GLY:HA3	1.79	0.47
2:C:946:ARG:O	2:C:950:LEU:HG	2.14	0.47
3:D:42:ASP:HB2	11:D:1731:HOH:O	2.14	0.47
3:D:48:ARG:HB3	3:D:48:ARG:CZ	2.44	0.47
3:D:406:ASP:HB2	3:D:423:ASP:HA	1.95	0.47
3:D:1021:TYR:CE1	3:D:1025:GLN:HG3	2.49	0.47
3:D:1231:GLU:N	3:D:1232:PRO:CD	2.77	0.47
4:E:37:ASN:H	4:E:37:ASN:ND2	2.13	0.47
5:F:384:GLU:HA	5:F:397:ILE:HD12	1.96	0.47
1:A:55:SER:HB2	1:A:158:ILE:HG21	1.95	0.47
1:B:59:GLU:HB3	1:B:138:LEU:HG	1.96	0.47
2:C:1112:PHE:O	2:C:1113:GLU:C	2.52	0.47
3:D:834:THR:HG23	3:D:838:ARG:HB2	1.96	0.47
3:D:1042:ARG:NH1	3:D:1045:MET:CE	2.77	0.47
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.44	0.47
1:A:151:VAL:HA	1:A:152:PRO:HD3	1.80	0.47
1:B:161:ARG:H	1:B:164:ALA:HB3	1.79	0.47
1:B:175:ARG:HE	1:B:202:ASP:HA	1.79	0.47
2:C:700:TYR:CB	2:C:833:LEU:HD13	2.44	0.47
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.96	0.47
3:D:889:ALA:O	3:D:929:ARG:NH1	2.47	0.47
2:C:944:LEU:HD22	2:C:962:GLN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1007:ALA:HB2	3:D:648:MET:HG2	1.97	0.47
3:D:1158:VAL:HG11	3:D:1173:LEU:HD21	1.96	0.47
2:C:144:PRO:CB	2:C:266:ARG:HB3	2.45	0.47
2:C:191:PHE:HZ	2:C:196:LEU:HD11	1.80	0.47
2:C:575:GLN:HE22	2:C:671:ASN:H	1.56	0.47
2:C:1001:VAL:O	2:C:1004:LYS:HB3	2.14	0.47
3:D:339:TRP:CZ3	3:D:341:GLU:HB2	2.50	0.47
3:D:835:SER:H	3:D:838:ARG:NE	2.12	0.47
1:A:62:LEU:HB2	1:A:63:HIS:HD2	1.80	0.47
2:C:889:HIS:CE1	3:D:951:ILE:H	2.13	0.47
3:D:324:ALA:HA	3:D:331:VAL:HG13	1.97	0.47
3:D:917:GLN:O	3:D:919:PHE:N	2.48	0.47
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.49	0.47
5:F:256:ARG:NH2	5:F:310:ILE:O	2.48	0.47
1:A:221:HIS:HA	1:A:224:TYR:CE1	2.50	0.47
1:B:2:LEU:H	1:B:3:ASP:HA	1.76	0.47
2:C:563:ASN:O	2:C:566:THR:HB	2.15	0.47
2:C:679:PHE:CE2	2:C:853:LEU:HD11	2.49	0.47
2:C:707:ARG:HD2	2:C:824:ARG:HH11	1.79	0.47
3:D:601:ARG:HB2	5:F:318:GLU:HG2	1.97	0.47
1:A:177:VAL:HG22	1:A:199:ILE:HG12	1.97	0.47
2:C:689:VAL:HG22	2:C:870:ILE:HB	1.97	0.47
2:C:897:LEU:HG	2:C:921:ALA:HB2	1.96	0.47
2:C:904:PRO:HD2	2:C:908:GLY:N	2.29	0.47
3:D:1098:LEU:O	3:D:1102:THR:HG23	2.15	0.47
2:C:676:ILE:O	3:D:948:THR:CG2	2.53	0.47
3:D:158:TYR:C	3:D:160:GLU:H	2.18	0.47
3:D:478:LEU:HD12	3:D:478:LEU:HA	1.80	0.47
3:D:705:ALA:HA	3:D:706:PRO:HA	1.59	0.47
3:D:1058:ARG:N	3:D:1069:GLU:OE2	2.48	0.47
5:F:234:LYS:HD2	5:F:236:SER:HB3	1.96	0.47
2:C:265:ARG:HG2	2:C:288:ARG:HD2	1.97	0.46
2:C:644:VAL:HG12	2:C:645:VAL:H	1.80	0.46
3:D:538:SER:OG	3:D:539:ASP:N	2.47	0.46
3:D:567:ILE:O	3:D:571:LYS:HG3	2.15	0.46
1:A:224:TYR:CD1	1:B:9:PRO:HG2	2.49	0.46
3:D:1232:PRO:HG2	3:D:1356:TYR:CE2	2.47	0.46
5:F:392:VAL:HG11	5:F:396:ARG:HH11	1.80	0.46
1:B:47:SER:O	1:B:148:VAL:HG11	2.16	0.46
3:D:134:VAL:HA	3:D:454:ALA:HA	1.97	0.46
3:D:505:SER:HB3	3:D:1453:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:643:GLY:N	3:D:727:GLN:O	2.46	0.46
3:D:651:GLU:HA	3:D:651:GLU:OE1	2.15	0.46
3:D:654:LYS:CB	3:D:655:PRO:HD3	2.40	0.46
2:C:683:ASN:HB2	2:C:687:ALA:O	2.16	0.46
2:C:1008:ARG:NH1	2:C:1011:GLY:N	2.63	0.46
3:D:212:ARG:HD3	3:D:342:PRO:HB3	1.97	0.46
3:D:885:ILE:HG12	3:D:937:TYR:CE1	2.51	0.46
5:F:329:TYR:HE1	5:F:333:ILE:HD11	1.81	0.46
2:C:34:VAL:H	2:C:35:PRO:HD2	1.78	0.46
2:C:1014:SER:O	2:C:1018:GLN:HA	2.15	0.46
3:D:1378:TYR:CE2	3:D:1394:VAL:HG22	2.50	0.46
3:D:813:LEU:O	3:D:817:GLU:HG2	2.15	0.46
3:D:1222:GLY:O	3:D:1225:ALA:HB3	2.16	0.46
3:D:1366:LYS:O	3:D:1369:GLU:HB2	2.16	0.46
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.51	0.46
2:C:841:ASN:ND2	2:C:845:ASN:HB2	2.31	0.46
3:D:1411:GLY:O	3:D:1412:LYS:HB2	2.16	0.46
5:F:261:PRO:O	5:F:265:VAL:HG23	2.15	0.46
5:F:401:GLU:O	5:F:405:LEU:HB2	2.15	0.46
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.98	0.46
1:B:80:LEU:HD23	1:B:83:LYS:HD2	1.98	0.46
1:B:211:LEU:O	1:B:215:VAL:HG13	2.16	0.46
2:C:139:GLN:HG2	2:C:339:LEU:HD21	1.98	0.46
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.97	0.46
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.97	0.46
2:C:710:ILE:HD11	2:C:758:ARG:CZ	2.46	0.46
2:C:771:GLU:HA	2:C:774:LEU:HB3	1.96	0.46
3:D:239:GLY:HA2	3:D:313:MET:HB3	1.98	0.46
3:D:575:GLN:NE2	11:D:1705:HOH:O	2.48	0.46
3:D:701:LEU:O	3:D:747:VAL:HG23	2.15	0.46
3:D:1436:SER:O	3:D:1438:ALA:N	2.49	0.46
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.51	0.46
5:F:394:ARG:HB3	5:F:395:GLU:H	1.61	0.46
1:A:24:VAL:HA	1:A:195:LEU:O	2.16	0.46
2:C:189:ARG:HD2	2:C:241:LEU:HD22	1.97	0.46
2:C:317:VAL:H	2:C:318:PRO:HD3	1.78	0.46
2:C:923:GLU:O	2:C:924:VAL:C	2.54	0.46
3:D:115:LEU:HD11	3:D:499:VAL:HG22	1.97	0.46
3:D:1479:ASP:OD1	3:D:1479:ASP:N	2.49	0.46
1:A:41:ARG:HD2	1:A:177:VAL:HG12	1.98	0.46
2:C:23:VAL:HG12	2:C:121:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.97	0.46
3:D:1112:CYS:HB3	3:D:1201:CYS:HB3	1.58	0.46
3:D:1350:GLU:O	3:D:1352:ILE:N	2.49	0.46
5:F:123:ASP:OD2	5:F:123:ASP:N	2.48	0.46
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.98	0.45
1:B:212:ASN:O	1:B:215:VAL:HG22	2.16	0.45
2:C:62:GLY:HA2	2:C:103:LYS:HG2	1.98	0.45
2:C:126:SER:HB2	2:C:134:ARG:O	2.16	0.45
2:C:266:ARG:NH1	2:C:271:GLU:O	2.49	0.45
2:C:376:ARG:HH12	5:F:276:ARG:HG2	1.80	0.45
2:C:860:HIS:NE2	2:C:975:TYR:HB2	2.32	0.45
2:C:972:VAL:HG23	2:C:973:VAL:N	2.31	0.45
3:D:95:LEU:HA	3:D:551:ASN:HD21	1.81	0.45
3:D:237:LYS:HB2	3:D:240:GLU:HG3	1.98	0.45
3:D:297:ILE:HG23	3:D:298:VAL:HG23	1.98	0.45
1:A:20:TYR:CD1	1:A:21:GLY:N	2.85	0.45
1:B:58:ILE:HG21	1:B:61:VAL:HG12	1.99	0.45
2:C:385:PHE:HD2	2:C:386:PHE:CD1	2.34	0.45
3:D:8:VAL:CG1	3:D:1434:TRP:CZ2	2.96	0.45
3:D:539:ASP:HB3	3:D:600:LEU:HD22	1.97	0.45
3:D:1459:LEU:CA	3:D:1464:GLU:HG3	2.44	0.45
3:D:536:ALA:HA	5:F:315:VAL:O	2.16	0.45
3:D:675:ARG:HH12	5:F:423:ASP:HB2	1.80	0.45
3:D:1194:CYS:SG	3:D:1200:VAL:HA	2.56	0.45
3:D:1350:GLU:O	3:D:1353:GLN:N	2.49	0.45
5:F:104:ARG:HG3	5:F:229:TYR:CZ	2.51	0.45
1:A:79:ILE:CG2	1:A:167:VAL:HG11	2.47	0.45
2:C:54:ILE:HG23	2:C:66:LEU:HB3	1.99	0.45
2:C:144:PRO:HB3	2:C:266:ARG:HB3	1.99	0.45
2:C:428:ARG:HH21	2:C:451:LEU:HD11	1.81	0.45
2:C:751:PRO:HA	2:C:792:VAL:CG1	2.46	0.45
3:D:131:LYS:HB3	3:D:152:LEU:HB2	1.99	0.45
3:D:729:HIS:CD2	3:D:730:PRO:CD	2.99	0.45
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.99	0.45
1:A:173:PRO:O	1:A:201:THR:HB	2.16	0.45
2:C:23:VAL:HG23	2:C:24:GLU:N	2.30	0.45
2:C:560:MET:O	2:C:564:MET:HG3	2.17	0.45
3:D:880:ILE:O	3:D:884:ARG:N	2.49	0.45
3:D:1217:ILE:HD12	3:D:1217:ILE:H	1.82	0.45
3:D:1394:VAL:HB	3:D:1397:LYS:HE2	1.97	0.45
1:B:57:TYR:HD1	1:B:161:ARG:HG3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:72:ARG:O	2:C:95:TYR:N	2.40	0.45
2:C:305:PRO:HA	2:C:308:ARG:HD3	1.99	0.45
2:C:627:ARG:HA	2:C:627:ARG:HD3	1.85	0.45
3:D:95:LEU:HB2	3:D:515:GLU:O	2.17	0.45
3:D:270:LEU:HB3	3:D:284:LEU:HD11	1.99	0.45
3:D:368:VAL:HG23	3:D:377:VAL:HG11	1.98	0.45
3:D:643:GLY:O	3:D:726:ILE:HG23	2.17	0.45
3:D:1478:SER:O	3:D:1480:PHE:N	2.50	0.45
1:A:22:GLU:C	1:A:23:PHE:CD1	2.90	0.45
1:A:42:ARG:O	1:A:43:ILE:C	2.54	0.45
1:A:206:THR:HG22	1:A:208:LEU:N	2.30	0.45
2:C:694:LEU:O	2:C:699:PHE:HB2	2.17	0.45
2:C:1009:SER:O	3:D:624:ASP:O	2.34	0.45
3:D:134:VAL:HG12	3:D:135:LEU:N	2.32	0.45
3:D:659:LYS:HG3	3:D:663:GLU:OE2	2.16	0.45
3:D:662:GLU:OE1	3:D:670:VAL:HG23	2.16	0.45
3:D:959:GLU:HB3	3:D:963:TYR:CE2	2.51	0.45
1:A:55:SER:HB2	1:A:158:ILE:CG2	2.47	0.45
1:B:100:LEU:O	1:B:114:PHE:HA	2.17	0.45
2:C:846:LYS:CE	3:D:741:ASP:O	2.63	0.45
2:C:872:ASN:OD1	2:C:874:LEU:HG	2.17	0.45
3:D:542:ASP:O	3:D:546:ARG:HG2	2.17	0.45
2:C:551:GLU:HB3	2:C:906:PHE:CE2	2.52	0.45
3:D:95:LEU:HD21	3:D:517:VAL:CG2	2.46	0.45
3:D:783:ARG:HB3	3:D:784:ASP:H	1.42	0.45
3:D:854:ALA:C	3:D:856:GLY:H	2.20	0.45
3:D:864:VAL:HG13	3:D:865:THR:N	2.32	0.45
3:D:1208:ASP:O	3:D:1209:LEU:CB	2.60	0.45
3:D:1481:VAL:HG13	4:E:18:ARG:HG3	1.99	0.45
3:D:1484:THR:HG21	4:E:18:ARG:HG2	1.98	0.45
1:A:28:LEU:O	1:A:193:ASP:N	2.50	0.45
1:B:19:GLU:O	1:B:200:TRP:HA	2.17	0.45
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.99	0.45
2:C:668:LEU:HD23	2:C:668:LEU:HA	1.73	0.45
2:C:848:VAL:HG12	3:D:632:VAL:HG23	1.99	0.45
3:D:116:LEU:HD21	3:D:465:LEU:HD23	1.99	0.45
3:D:411:THR:O	5:F:178:ARG:HD2	2.17	0.45
3:D:539:ASP:N	3:D:539:ASP:OD1	2.50	0.45
3:D:1023:MET:HA	3:D:1028:ALA:HB3	1.97	0.45
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.97	0.44
1:B:38:ASN:HB2	1:B:39:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:154:ARG:HE	2:C:156:GLY:HA3	1.82	0.44
2:C:265:ARG:H	2:C:265:ARG:HG3	1.64	0.44
2:C:713:ARG:HB2	2:C:713:ARG:NH1	2.32	0.44
3:D:566:ILE:O	3:D:566:ILE:HG13	2.16	0.44
3:D:675:ARG:NH2	5:F:420:ASP:O	2.50	0.44
3:D:1305:LEU:HA	3:D:1306:PRO:HD2	1.79	0.44
2:C:435:TYR:HA	3:D:1071:PHE:CE2	2.49	0.44
2:C:860:HIS:HA	2:C:866:PRO:HA	1.98	0.44
2:C:915:LYS:O	2:C:968:LEU:HD22	2.17	0.44
3:D:171:LEU:HD21	3:D:192:ALA:HB1	2.00	0.44
3:D:1372:VAL:HA	3:D:1375:MET:HE1	1.98	0.44
4:E:11:GLY:HA3	11:E:103:HOH:O	2.18	0.44
1:A:70:GLY:CA	1:A:133:GLU:HG2	2.47	0.44
2:C:266:ARG:HD2	2:C:273:GLY:HA3	1.99	0.44
2:C:833:LEU:HA	2:C:837:ASP:OD2	2.17	0.44
3:D:661:MET:HE1	3:D:677:LEU:HD21	1.99	0.44
3:D:1378:TYR:O	3:D:1420:LEU:HB2	2.17	0.44
1:A:40:LEU:HD23	1:A:43:ILE:HD12	2.00	0.44
2:C:283:ILE:HG22	2:C:284:ARG:HG2	1.98	0.44
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.97	0.44
2:C:971:LYS:HA	2:C:988:VAL:CA	2.43	0.44
3:D:191:LEU:HD12	3:D:195:VAL:HB	1.99	0.44
3:D:523:ASP:O	3:D:526:PRO:HD3	2.17	0.44
3:D:643:GLY:O	3:D:726:ILE:HA	2.18	0.44
2:C:468:ARG:HE	2:C:487:THR:CG2	2.29	0.44
3:D:1213:ARG:HB2	3:D:1214:PRO:HD2	1.99	0.44
3:D:1440:PHE:HE2	3:D:1463:LYS:NZ	2.15	0.44
1:A:206:THR:O	1:A:207:PRO:C	2.55	0.44
1:A:225:PHE:CD2	1:B:11:PHE:HE1	2.35	0.44
1:B:23:PHE:CE1	1:B:199:ILE:HD12	2.52	0.44
1:B:167:VAL:CG1	1:B:168:ASP:H	2.23	0.44
3:D:186:VAL:O	3:D:189:GLN:HB2	2.16	0.44
3:D:659:LYS:O	3:D:662:GLU:N	2.50	0.44
3:D:1472:ILE:HG23	3:D:1474:ALA:H	1.83	0.44
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.99	0.44
1:A:226:SER:O	1:A:227:ASN:HB3	2.18	0.44
2:C:599:GLU:HG3	2:C:600:ASP:H	1.82	0.44
3:D:787:LEU:HD13	3:D:1023:MET:HG2	2.00	0.44
2:C:13:ILE:HD12	2:C:14:PRO:CD	2.42	0.44
2:C:292:ARG:HD3	2:C:299:LYS:HB3	1.99	0.44
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:834:THR:HA	3:D:838:ARG:HE	1.83	0.44
2:C:605:LYS:O	2:C:611:ILE:HG23	2.18	0.44
2:C:721:ARG:O	2:C:758:ARG:HG3	2.18	0.44
3:D:16:GLU:O	3:D:20:SER:N	2.51	0.44
3:D:152:LEU:HD23	3:D:152:LEU:N	2.25	0.44
3:D:496:LEU:HD11	3:D:500:ARG:HH12	1.83	0.44
3:D:947:ILE:O	3:D:948:THR:HG23	2.17	0.44
2:C:69:LEU:HD13	2:C:97:ARG:HB3	2.00	0.43
2:C:393:GLN:HG3	2:C:406:HIS:HE2	1.82	0.43
3:D:493:ARG:NH1	3:D:1389:LEU:HB3	2.33	0.43
3:D:631:ILE:HG12	3:D:743:ASP:O	2.17	0.43
3:D:786:ILE:HG21	3:D:1026:SER:O	2.18	0.43
3:D:1104:GLU:HA	3:D:1461:GLY:HA2	1.99	0.43
5:F:91:VAL:HA	5:F:92:PRO:HD3	1.80	0.43
5:F:132:ARG:HH21	5:F:184:ARG:NE	2.16	0.43
2:C:159:ILE:HG23	2:C:175:GLU:HB2	1.99	0.43
2:C:540:PHE:CE1	2:C:906:PHE:HE1	2.36	0.43
2:C:728:HIS:CG	2:C:729:LEU:N	2.85	0.43
3:D:885:ILE:HG21	3:D:937:TYR:CD1	2.40	0.43
3:D:1443:THR:O	3:D:1444:THR:C	2.57	0.43
3:D:1481:VAL:HG13	4:E:18:ARG:HA	1.99	0.43
5:F:79:ASP:N	5:F:80:PRO:CD	2.82	0.43
5:F:379:ARG:HD2	5:F:383:LEU:HB2	2.00	0.43
1:A:216:GLU:CD	1:A:219:ARG:HH21	2.22	0.43
1:B:44:LEU:HA	1:B:48:ILE:HD13	2.00	0.43
2:C:561:GLY:O	2:C:562:SER:C	2.55	0.43
3:D:841:TYR:HB2	3:D:864:VAL:HG22	2.00	0.43
1:A:83:LYS:HE3	1:A:168:ASP:O	2.18	0.43
1:A:87:VAL:HG21	1:A:144:VAL:HG11	2.01	0.43
2:C:713:ARG:HA	2:C:819:VAL:HA	2.00	0.43
3:D:156:GLU:CD	3:D:156:GLU:H	2.22	0.43
3:D:493:ARG:NH1	3:D:1390:LEU:H	2.01	0.43
2:C:434:HIS:O	2:C:435:TYR:C	2.56	0.43
2:C:683:ASN:CG	2:C:872:ASN:HB2	2.38	0.43
2:C:876:VAL:O	2:C:877:PRO:C	2.55	0.43
4:E:9:LEU:O	4:E:19:LEU:HD13	2.19	0.43
1:B:112:ARG:NH1	1:B:112:ARG:HB3	2.33	0.43
2:C:537:LYS:O	2:C:539:VAL:N	2.51	0.43
2:C:690:ILE:HD13	2:C:690:ILE:HA	1.72	0.43
3:D:114:THR:HG21	3:D:498:VAL:HG21	2.00	0.43
3:D:986:ARG:HG3	3:D:990:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1190:SER:OG	3:D:1191:PRO:CD	2.66	0.43
3:D:1400:VAL:HG12	3:D:1404:ASN:ND2	2.32	0.43
5:F:201:LYS:HA	5:F:201:LYS:HD2	1.86	0.43
1:A:51:THR:HG22	1:A:146:ARG:HA	2.01	0.43
1:A:73:GLU:CB	1:A:78:ILE:HG12	2.48	0.43
2:C:52:PHE:HD2	2:C:68:PHE:HB2	1.84	0.43
2:C:141:HIS:HE1	2:C:332:ARG:HH12	1.65	0.43
2:C:274:ARG:HA	2:C:277:ALA:HB3	2.01	0.43
2:C:724:ARG:HE	2:C:738:ASP:CA	2.19	0.43
3:D:757:ALA:O	3:D:758:GLU:C	2.56	0.43
3:D:836:VAL:N	3:D:837:GLY:CA	2.73	0.43
3:D:1219:GLU:O	3:D:1221:VAL:N	2.49	0.43
1:A:149:GLY:O	1:A:171:PHE:HB2	2.19	0.43
2:C:195:LEU:HB3	2:C:238:LEU:CD2	2.49	0.43
2:C:589:ARG:NH2	2:C:596:TYR:CD2	2.87	0.43
2:C:751:PRO:HB2	3:D:680:GLN:HG3	2.00	0.43
3:D:508:ARG:C	3:D:510:GLU:H	2.21	0.43
3:D:948:THR:O	3:D:949:ILE:HG13	2.19	0.43
5:F:222:ARG:HG2	5:F:242:TRP:CE3	2.54	0.43
2:C:266:ARG:H	2:C:266:ARG:NE	2.16	0.43
2:C:683:ASN:HA	2:C:687:ALA:HB3	2.00	0.43
2:C:997:LEU:HD23	2:C:997:LEU:HA	1.77	0.43
3:D:126:VAL:HG21	3:D:461:ILE:HD11	2.01	0.43
3:D:372:ASP:O	3:D:374:GLU:N	2.52	0.43
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.18	0.43
1:A:68:ILE:HA	1:A:69:PRO:HD2	1.83	0.43
2:C:238:LEU:C	2:C:240:THR:H	2.21	0.43
2:C:437:ARG:NH2	2:C:487:THR:O	2.52	0.43
2:C:1095:LEU:HD13	3:D:103:TRP:CH2	2.53	0.43
3:D:117:ASP:HB2	3:D:495:ARG:NH1	2.26	0.43
3:D:272:LEU:HG	3:D:282:TYR:CE1	2.52	0.43
3:D:953:ASP:HB3	3:D:1019:PRO:HG2	2.01	0.43
3:D:969:ARG:HA	3:D:972:LEU:HD23	2.00	0.43
3:D:1042:ARG:HD3	3:D:1057:VAL:HG11	2.01	0.43
5:F:320:PRO:HA	5:F:328:PHE:HA	2.00	0.43
5:F:397:ILE:HA	5:F:400:ILE:HB	1.99	0.43
1:A:49:PRO:HB3	1:A:148:VAL:HG22	2.00	0.42
1:A:177:VAL:HG12	1:A:177:VAL:O	2.19	0.42
1:B:58:ILE:HD13	1:B:59:GLU:N	2.33	0.42
1:B:176:ARG:HB3	1:B:200:TRP:CE3	2.54	0.42
2:C:698:ASP:OD1	2:C:701:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1008:ARG:HH11	2:C:1011:GLY:N	2.17	0.42
3:D:116:LEU:HB3	3:D:118:LEU:HD12	2.01	0.42
3:D:806:PHE:H	3:D:829:VAL:HG12	1.84	0.42
1:A:58:ILE:HB	1:A:61:VAL:CG2	2.48	0.42
2:C:231:PRO:HA	2:C:234:ALA:HB3	2.01	0.42
2:C:317:VAL:N	2:C:318:PRO:CD	2.82	0.42
2:C:341:THR:HG22	2:C:345:ARG:HE	1.84	0.42
2:C:414:GLY:HA3	2:C:415:PRO:HD3	1.86	0.42
2:C:1107:ASN:O	2:C:1108:PRO:C	2.58	0.42
3:D:272:LEU:HB3	3:D:274:ARG:NH1	2.34	0.42
3:D:594:PRO:HB2	3:D:595:GLY:H	1.63	0.42
5:F:292:ALA:C	5:F:294:ALA:H	2.22	0.42
1:A:80:LEU:HD23	1:A:83:LYS:HG3	2.01	0.42
1:A:84:GLU:O	1:A:85:LEU:C	2.58	0.42
2:C:121:MET:HG3	2:C:127:PHE:CE1	2.54	0.42
2:C:360:LEU:HG	2:C:361:MET:H	1.83	0.42
2:C:569:VAL:HA	2:C:570:PRO:HD2	1.87	0.42
2:C:724:ARG:HB2	2:C:741:GLY:H	1.84	0.42
3:D:207:PHE:HB2	3:D:391:ALA:HB3	2.01	0.42
3:D:1087:ARG:HB3	3:D:1091:SER:HB2	2.01	0.42
3:D:1150:ALA:C	3:D:1151:ARG:HG2	2.39	0.42
3:D:1341:PRO:O	3:D:1344:VAL:HG12	2.19	0.42
4:E:31:LEU:HD12	4:E:60:ALA:HB2	2.00	0.42
1:A:40:LEU:O	1:A:44:LEU:HB2	2.19	0.42
1:B:216:GLU:OE2	1:B:220:GLU:HB2	2.19	0.42
2:C:575:GLN:HE21	2:C:670:GLN:HA	1.85	0.42
3:D:650:LEU:HB2	3:D:691:LEU:HD22	2.02	0.42
3:D:996:TRP:HA	3:D:999:THR:HB	2.02	0.42
3:D:1486:VAL:HG11	4:E:26:ARG:HB2	2.01	0.42
1:B:104:GLU:HA	1:B:132:LEU:HD22	2.01	0.42
2:C:182:VAL:HG13	2:C:220:GLY:HA3	2.01	0.42
2:C:263:ASP:N	2:C:264:PRO:CD	2.62	0.42
2:C:964:LYS:O	2:C:968:LEU:HG	2.19	0.42
2:C:1037:VAL:O	2:C:1041:GLU:HG3	2.19	0.42
3:D:256:GLU:OE1	3:D:302:GLN:HB3	2.19	0.42
3:D:835:SER:HB2	3:D:838:ARG:HG3	2.02	0.42
3:D:938:GLY:O	3:D:939:PHE:O	2.37	0.42
3:D:1119:SER:HA	3:D:1186:VAL:O	2.20	0.42
3:D:1314:LYS:HB3	3:D:1314:LYS:HE2	1.88	0.42
4:E:25:LYS:O	4:E:28:GLN:HB2	2.19	0.42
2:C:136:ILE:HB	2:C:336:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:948:THR:HB	3:D:949:ILE:H	1.49	0.42
3:D:1375:MET:HE3	3:D:1375:MET:HB2	1.78	0.42
3:D:1378:TYR:HD2	3:D:1394:VAL:HA	1.85	0.42
1:A:41:ARG:NH1	1:A:45:LEU:HD11	2.35	0.42
1:A:152:PRO:O	1:A:153:ALA:C	2.57	0.42
1:A:154:GLU:H	1:A:154:GLU:CD	2.22	0.42
1:B:29:GLU:O	1:B:30:ARG:C	2.58	0.42
2:C:472:ARG:HA	2:C:483:VAL:HA	2.02	0.42
2:C:1054:THR:HB	2:C:1059:ASP:HB2	2.02	0.42
3:D:141:ILE:C	3:D:143:ASN:H	2.23	0.42
3:D:374:GLU:HG3	3:D:375:GLU:N	2.34	0.42
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.72	0.42
1:B:144:VAL:HG12	1:B:145:ASP:H	1.84	0.42
2:C:139:GLN:O	2:C:333:ILE:HA	2.20	0.42
2:C:173:ASP:HB2	2:C:185:LYS:HB3	2.01	0.42
2:C:589:ARG:HA	2:C:596:TYR:CE1	2.53	0.42
3:D:567:ILE:HG22	3:D:571:LYS:NZ	2.35	0.42
1:A:34:VAL:HA	1:A:179:PHE:HE1	1.84	0.42
1:A:225:PHE:CD2	1:B:11:PHE:CE1	3.06	0.42
1:B:37:GLY:HA3	1:B:179:PHE:CE1	2.55	0.42
2:C:15:LEU:HD12	2:C:15:LEU:N	2.30	0.42
2:C:297:GLU:HB3	2:C:298:PHE:H	1.68	0.42
2:C:540:PHE:HE1	2:C:906:PHE:HE1	1.68	0.42
5:F:125:ASP:HA	5:F:128:ARG:NH2	2.35	0.42
2:C:260:LEU:HD12	2:C:288:ARG:HG2	2.02	0.42
3:D:226:PRO:HA	3:D:330:THR:HG22	2.02	0.42
3:D:714:GLN:HE21	3:D:765:SER:CB	2.32	0.42
3:D:913:ASP:O	3:D:914:LEU:C	2.58	0.42
3:D:1372:VAL:HA	3:D:1375:MET:CE	2.50	0.42
5:F:369:LEU:O	5:F:374:GLY:N	2.50	0.42
1:A:132:LEU:HD11	1:A:138:LEU:HB3	2.02	0.41
2:C:309:TYR:HE1	2:C:319:GLY:HA3	1.85	0.41
2:C:700:TYR:HB3	2:C:833:LEU:HD13	2.01	0.41
2:C:910:LYS:C	2:C:912:PRO:HD2	2.40	0.41
2:C:1009:SER:N	3:D:651:GLU:HG3	2.35	0.41
3:D:700:VAL:HG13	3:D:718:PRO:HG3	2.01	0.41
3:D:835:SER:O	3:D:836:VAL:HG23	2.20	0.41
3:D:911:LEU:O	3:D:912:LYS:C	2.59	0.41
3:D:1161:GLU:OE2	3:D:1164:ARG:HG3	2.18	0.41
3:D:1242:HIS:CE1	3:D:1245:GLY:HA3	2.55	0.41
1:A:37:GLY:HA3	1:A:195:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ASN:O	1:B:42:ARG:HG2	2.21	0.41
2:C:408:ARG:NH2	2:C:455:LEU:HD23	2.35	0.41
2:C:1107:ASN:HA	2:C:1108:PRO:HD2	1.91	0.41
3:D:463:GLN:NE2	3:D:467:GLU:HG3	2.34	0.41
3:D:493:ARG:HH21	3:D:494:LYS:HZ3	1.66	0.41
3:D:662:GLU:OE2	3:D:669:ASN:HA	2.20	0.41
3:D:760:ARG:NH2	4:E:62:THR:OG1	2.53	0.41
3:D:916:TYR:O	3:D:919:PHE:HB3	2.20	0.41
3:D:1042:ARG:NH1	3:D:1045:MET:HE1	2.35	0.41
3:D:1046:GLN:HA	3:D:1052:THR:HA	2.01	0.41
3:D:1459:LEU:HD11	3:D:1468:LEU:HD13	2.02	0.41
4:E:30:LEU:HD21	4:E:63:TRP:HB3	2.02	0.41
1:B:12:THR:HB	1:B:24:VAL:HB	2.01	0.41
2:C:121:MET:HG3	2:C:127:PHE:CZ	2.55	0.41
2:C:707:ARG:HD2	2:C:824:ARG:NH1	2.35	0.41
2:C:850:ALA:CA	3:D:632:VAL:HG22	2.48	0.41
2:C:1032:PHE:CD1	2:C:1052:MET:HG2	2.54	0.41
2:C:1040:LEU:HA	2:C:1043:TYR:HB2	2.01	0.41
3:D:539:ASP:HB3	3:D:600:LEU:HB3	2.02	0.41
3:D:1377:LYS:HD2	3:D:1378:TYR:HE2	1.78	0.41
5:F:88:ILE:HD13	5:F:88:ILE:HA	1.70	0.41
5:F:291:ILE:HG23	5:F:304:VAL:HG21	2.02	0.41
1:A:11:PHE:HA	1:A:25:LEU:HD12	2.01	0.41
2:C:1060:ILE:O	2:C:1064:ASN:ND2	2.53	0.41
3:D:727:GLN:HB2	3:D:727:GLN:HE21	1.54	0.41
3:D:756:GLN:HE21	3:D:756:GLN:HB3	1.68	0.41
3:D:1225:ALA:HA	3:D:1367:HIS:ND1	2.34	0.41
3:D:1254:GLN:O	3:D:1257:PRO:HG2	2.19	0.41
1:B:64:GLU:HB2	1:B:75:VAL:HG11	2.02	0.41
2:C:284:ARG:HA	2:C:284:ARG:HH11	1.85	0.41
2:C:338:GLU:HG2	2:C:342:ASP:OD2	2.21	0.41
2:C:439:CYS:HB2	2:C:541:SER:H	1.85	0.41
2:C:842:ARG:NH2	2:C:887:GLU:OE2	2.52	0.41
2:C:1059:ASP:OD1	2:C:1062:GLY:CA	2.68	0.41
3:D:108:VAL:HA	3:D:110:SER:N	2.35	0.41
3:D:653:PHE:N	3:D:653:PHE:CD1	2.89	0.41
3:D:1431:THR:HG21	11:D:1713:HOH:O	2.20	0.41
2:C:264:PRO:HB2	2:C:289:THR:HG21	2.02	0.41
2:C:839:LEU:HA	2:C:839:LEU:HD23	1.62	0.41
2:C:926:PHE:C	2:C:928:LYS:H	2.23	0.41
3:D:53:ILE:HG22	3:D:54:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:226:PRO:HG3	3:D:249:TYR:HB2	2.02	0.41
3:D:257:GLY:H	3:D:272:LEU:HD22	1.85	0.41
3:D:304:LEU:O	3:D:305:ALA:HB3	2.21	0.41
3:D:387:LEU:H	3:D:387:LEU:HD12	1.86	0.41
3:D:473:LEU:HD11	3:D:495:ARG:HH21	1.85	0.41
3:D:772:PRO:O	3:D:1209:LEU:HD23	2.21	0.41
3:D:984:THR:HG23	3:D:987:GLU:H	1.86	0.41
3:D:1031:ASN:HB2	3:D:1032:PRO:HD2	2.00	0.41
3:D:1383:ASP:HA	3:D:1384:PRO:HD3	1.90	0.41
4:E:81:PRO:HB2	4:E:84:ARG:HB2	2.02	0.41
5:F:208:SER:HB3	5:F:211:ASP:HB2	2.01	0.41
1:A:101:LEU:HB3	1:A:140:MET:HG2	2.02	0.41
2:C:405:ARG:HB2	2:C:543:ASN:HD21	1.85	0.41
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.56	0.41
2:C:949:LYS:HD2	3:D:796:ARG:HH21	1.81	0.41
3:D:211:VAL:HG12	3:D:387:LEU:HA	2.02	0.41
3:D:1364:HIS:ND1	3:D:1366:LYS:HG2	2.35	0.41
2:C:418:LEU:O	2:C:420:ARG:N	2.48	0.41
2:C:776:SER:CA	2:C:780:GLU:HB2	2.44	0.41
3:D:356:PRO:HB2	3:D:359:ALA:HB2	2.02	0.41
3:D:539:ASP:CG	3:D:598:ARG:HH21	2.23	0.41
3:D:786:ILE:O	3:D:787:LEU:C	2.58	0.41
2:C:95:TYR:CG	2:C:114:PHE:HB3	2.56	0.41
2:C:1056:LYS:HB3	3:D:624:ASP:H	1.86	0.41
3:D:731:LEU:HA	3:D:731:LEU:HD23	1.91	0.41
3:D:1135:ARG:O	3:D:1136:LYS:C	2.58	0.41
3:D:1397:LYS:C	3:D:1398:TRP:CE3	2.90	0.41
3:D:1459:LEU:HD22	3:D:1464:GLU:HB2	2.03	0.41
3:D:1495:ILE:O	3:D:1499:ARG:HB2	2.21	0.41
1:A:115:LEU:HA	1:A:116:PRO:HD2	1.84	0.41
2:C:137:VAL:O	2:C:391:LEU:HG	2.21	0.41
2:C:286:SER:OG	2:C:301:GLU:HB2	2.21	0.41
2:C:421:GLU:O	2:C:423:ALA:N	2.49	0.41
2:C:1095:LEU:HD12	3:D:607:LEU:HD12	2.03	0.41
3:D:177:ALA:O	3:D:178:LEU:HB2	2.20	0.41
3:D:1264:GLU:CB	3:D:1266:ARG:HH21	2.33	0.41
2:C:154:ARG:NE	2:C:157:ARG:H	2.18	0.40
3:D:368:VAL:HB	3:D:377:VAL:HG21	2.02	0.40
3:D:912:LYS:HB3	3:D:912:LYS:HE2	1.73	0.40
3:D:1267:ARG:HD2	3:D:1271:LYS:NZ	2.36	0.40
1:A:23:PHE:CD2	1:A:211:LEU:HD23	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:HIS:CE1	2:C:801:VAL:HG12	2.56	0.40
1:A:158:ILE:H	1:A:159:LYS:NZ	2.18	0.40
1:B:74:ASP:OD2	1:B:75:VAL:N	2.54	0.40
2:C:1059:ASP:OD2	2:C:1080:SER:N	2.54	0.40
3:D:217:LYS:HD2	3:D:339:TRP:CZ2	2.55	0.40
3:D:935:LYS:HB3	3:D:935:LYS:HE2	1.76	0.40
3:D:1271:LYS:HD2	3:D:1334:GLN:OE1	2.21	0.40
3:D:1413:THR:HA	3:D:1414:PRO:HD3	1.79	0.40
5:F:88:ILE:HG23	5:F:193:ARG:HG2	2.03	0.40
6:Z:30:UNK:HA	6:Z:31:UNK:HA	1.61	0.40
1:B:91:ASN:HA	1:B:92:PRO:HD3	1.85	0.40
2:C:224:GLU:HB3	2:C:227:PHE:HB2	2.04	0.40
3:D:410:SER:OG	3:D:411:THR:N	2.55	0.40
3:D:450:TYR:HB2	3:D:452:ILE:HD11	2.03	0.40
3:D:774:SER:HB3	3:D:1362:LYS:O	2.21	0.40
3:D:1103:HIS:CE1	3:D:1463:LYS:HB2	2.56	0.40
3:D:1141:GLU:HA	3:D:1171:VAL:HG11	2.02	0.40
3:D:1350:GLU:O	3:D:1351:GLU:C	2.60	0.40
1:A:7:LYS:HE2	1:A:7:LYS:HB3	1.98	0.40
1:A:101:LEU:HD21	1:A:109:VAL:CG1	2.52	0.40
1:A:115:LEU:HD13	1:A:116:PRO:HD2	2.04	0.40
1:A:179:PHE:CG	1:A:179:PHE:O	2.75	0.40
1:B:213:GLN:O	1:B:217:ILE:HG13	2.21	0.40
2:C:271:GLU:O	2:C:273:GLY:N	2.54	0.40
2:C:948:GLU:HB3	2:C:953:VAL:HG23	2.02	0.40
3:D:206:ARG:H	3:D:390:PRO:HB3	1.86	0.40
3:D:879:ARG:HB3	3:D:902:LEU:HD12	2.03	0.40
3:D:906:GLN:HA	3:D:910:SER:OG	2.22	0.40
3:D:1364:HIS:O	3:D:1365:ASP:C	2.60	0.40
2:C:807:ARG:HA	2:C:821:GLU:CB	2.51	0.40
3:D:341:GLU:HA	3:D:342:PRO:HD3	1.88	0.40
3:D:1011:PHE:O	3:D:1016:PRO:HA	2.21	0.40
3:D:1037:GLN:HG2	3:D:1042:ARG:HA	2.03	0.40
3:D:1066:THR:HB	3:D:1069:GLU:HB2	2.04	0.40
3:D:1255:GLY:O	3:D:1258:ARG:N	2.51	0.40
3:D:1365:ASP:HA	3:D:1368:ILE:HD13	2.03	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	A	229/315 (73%)	175 (76%)	40 (18%)	14 (6%)	1 2
1	B	236/315 (75%)	186 (79%)	45 (19%)	5 (2%)	7 16
2	C	1117/1119 (100%)	877 (78%)	187 (17%)	53 (5%)	2 4
3	D	1502/1524 (99%)	1160 (77%)	260 (17%)	82 (6%)	2 3
4	E	93/99 (94%)	76 (82%)	14 (15%)	3 (3%)	4 8
5	F	349/423 (82%)	286 (82%)	54 (16%)	9 (3%)	5 12
All	All	3526/3795 (93%)	2760 (78%)	600 (17%)	166 (5%)	2 4

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
2	C	42	VAL
2	C	263	ASP
2	C	272	ALA
2	C	738	ASP
2	C	739	GLU
2	C	1115	LEU
3	D	137	PRO
3	D	587	ARG
3	D	593	ASN
3	D	594	PRO
3	D	809	PRO
3	D	939	PHE
3	D	940	THR
3	D	1128	VAL
3	D	1386	ASP
3	D	1391	GLU
3	D	1437	ALA
3	D	1441	GLN
3	D	1482	ARG

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Mol	Chain	Res	Type
4	E	82	GLU
1	A	14	ARG
1	A	105	GLY
1	A	153	ALA
1	A	158	ILE
1	A	159	LYS
1	B	233	VAL
2	C	60	GLY
2	C	80	GLN
2	C	105	THR
2	C	223	ASP
2	C	262	ALA
2	C	316	GLY
2	C	369	PRO
2	C	419	THR
2	C	1016	ILE
3	D	110	SER
3	D	178	LEU
3	D	192	ALA
3	D	196	VAL
3	D	409	VAL
3	D	525	ARG
3	D	549	ASN
3	D	595	GLY
3	D	822	ALA
3	D	823	LEU
3	D	830	ALA
3	D	918	ALA
3	D	949	ILE
3	D	1209	LEU
3	D	1220	ALA
3	D	1266	ARG
3	D	1297	GLU
3	D	1341	PRO
3	D	1412	LYS
3	D	1444	THR
5	F	141	VAL
5	F	153	PRO
1	A	38	ASN
1	B	125	PRO
1	B	158	ILE
2	C	208	ALA

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Mol	Chain	Res	Type
2	C	288	ARG
2	C	422	ARG
2	C	541	SER
2	C	626	ARG
2	C	728	HIS
2	C	876	VAL
2	C	908	GLY
2	C	1042	ALA
2	C	1108	PRO
2	C	1113	GLU
3	D	82	LYS
3	D	119	SER
3	D	230	TRP
3	D	287	GLY
3	D	483	HIS
3	D	603	LEU
3	D	652	LEU
3	D	835	SER
3	D	1166	LEU
3	D	1245	GLY
3	D	1269	LYS
3	D	1348	LEU
3	D	1389	LEU
3	D	1390	LEU
3	D	1442	ASN
5	F	255	ALA
1	A	59	GLU
1	A	160	ASP
2	C	31	GLN
2	C	261	ILE
2	C	482	GLU
2	C	638	ASP
2	C	735	ARG
2	C	880	MET
2	C	1079	PRO
3	D	117	ASP
3	D	248	PRO
3	D	255	GLU
3	D	316	GLN
3	D	373	PRO
3	D	437	VAL
3	D	509	PRO

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Mol	Chain	Res	Type
3	D	601	ARG
3	D	654	LYS
3	D	801	GLY
3	D	836	VAL
3	D	1040	GLY
3	D	1238	MET
3	D	1248	GLY
3	D	1349	VAL
5	F	394	ARG
1	A	227	ASN
2	C	36	PRO
2	C	37	GLU
2	C	99	GLN
2	C	111	ASP
2	C	195	LEU
2	C	820	ARG
2	C	835	VAL
2	C	907	ASP
2	C	945	ARG
3	D	245	LEU
3	D	303	PRO
3	D	440	VAL
3	D	485	SER
3	D	869	MET
3	D	883	ALA
3	D	1365	ASP
3	D	1408	ILE
4	E	86	GLN
5	F	389	PHE
5	F	395	GLU
1	A	4	SER
1	A	228	PRO
1	B	49	PRO
2	C	289	THR
2	C	570	PRO
2	C	784	ASP
2	C	796	GLU
2	C	808	ARG
3	D	227	LEU
3	D	305	ALA
3	D	1023	MET
3	D	1072	ILE

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Mol	Chain	Res	Type
3	D	1125	PRO
3	D	1410	GLU
4	E	39	VAL
5	F	80	PRO
5	F	152	ASP
1	A	17	GLY
2	C	427	VAL
3	D	328	GLY
3	D	457	GLY
3	D	530	VAL
3	D	1067	VAL
1	A	157	GLY
2	C	318	PRO
2	C	924	VAL
2	C	1020	PRO
2	C	226	VAL
1	B	120	VAL
2	C	155	PRO
3	D	612	GLY
5	F	314	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	202/273 (74%)	171 (85%)	31 (15%)	2 6
1	B	206/273 (76%)	183 (89%)	23 (11%)	6 13
2	C	941/941 (100%)	816 (87%)	125 (13%)	4 8
3	D	1264/1279 (99%)	1111 (88%)	153 (12%)	5 10
4	E	83/87 (95%)	75 (90%)	8 (10%)	8 19
5	F	306/370 (83%)	283 (92%)	23 (8%)	13 30
All	All	3002/3223 (93%)	2639 (88%)	363 (12%)	5 10

All (363) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	7	LYS
1	A	12	THR
1	A	15	THR
1	A	19	GLU
1	A	24	VAL
1	A	25	LEU
1	A	34	VAL
1	A	42	ARG
1	A	44	LEU
1	A	45	LEU
1	A	62	LEU
1	A	86	VAL
1	A	88	ARG
1	A	90	LEU
1	A	96	THR
1	A	112	ARG
1	A	115	LEU
1	A	127	LEU
1	A	131	THR
1	A	138	LEU
1	A	154	GLU
1	A	159	LYS
1	A	182	GLU
1	A	184	THR
1	A	196	THR
1	A	197	LEU
1	A	200	TRP
1	A	202	ASP
1	A	221	HIS
1	A	224	TYR
1	B	5	LYS
1	B	7	LYS
1	B	10	VAL
1	B	22	GLU
1	B	40	LEU
1	B	42	ARG
1	B	54	THR
1	B	58	ILE
1	B	60	ASP
1	B	61	VAL
1	B	64	GLU
1	B	87	VAL

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Mol	Chain	Res	Type
1	B	100	LEU
1	B	104	GLU
1	B	119	ASP
1	B	140	MET
1	B	146	ARG
1	B	176	ARG
1	B	180	GLN
1	B	183	ASP
1	B	184	THR
1	B	197	LEU
1	B	233	VAL
2	C	1	MET
2	C	2	GLU
2	C	8	ARG
2	C	15	LEU
2	C	26	TYR
2	C	39	ARG
2	C	54	ILE
2	C	73	LEU
2	C	81	ASP
2	C	99	GLN
2	C	103	LYS
2	C	113	VAL
2	C	114	PHE
2	C	122	THR
2	C	138	SER
2	C	143	SER
2	C	154	ARG
2	C	157	ARG
2	C	159	ILE
2	C	165	LEU
2	C	184	MET
2	C	186	VAL
2	C	189	ARG
2	C	206	THR
2	C	209	ARG
2	C	214	TYR
2	C	216	GLU
2	C	232	GLU
2	C	239	PHE
2	C	242	LEU
2	C	250	ARG

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Mol	Chain	Res	Type
2	C	256	TYR
2	C	265	ARG
2	C	266	ARG
2	C	289	THR
2	C	290	LEU
2	C	297	GLU
2	C	307	LEU
2	C	308	ARG
2	C	317	VAL
2	C	321	GLU
2	C	325	ILE
2	C	335	THR
2	C	353	ARG
2	C	358	ARG
2	C	360	LEU
2	C	367	LEU
2	C	371	LYS
2	C	372	LEU
2	C	379	GLU
2	C	387	SER
2	C	388	ARG
2	C	393	GLN
2	C	394	PHE
2	C	398	THR
2	C	402	SER
2	C	421	GLU
2	C	425	PHE
2	C	434	HIS
2	C	441	VAL
2	C	443	THR
2	C	455	LEU
2	C	489	THR
2	C	491	GLU
2	C	512	ARG
2	C	514	VAL
2	C	522	VAL
2	C	539	VAL
2	C	554	ASP
2	C	600	ASP
2	C	610	ARG
2	C	616	GLU
2	C	625	LEU

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Mol	Chain	Res	Type
2	C	627	ARG
2	C	637	LEU
2	C	640	ARG
2	C	657	ASP
2	C	661	SER
2	C	672	VAL
2	C	673	LEU
2	C	676	ILE
2	C	680	ASP
2	C	683	ASN
2	C	685	GLU
2	C	689	VAL
2	C	698	ASP
2	C	699	PHE
2	C	714	ASP
2	C	715	THR
2	C	717	LEU
2	C	720	GLU
2	C	722	ILE
2	C	723	THR
2	C	728	HIS
2	C	729	LEU
2	C	739	GLU
2	C	740	GLU
2	C	750	LYS
2	C	799	ILE
2	C	807	ARG
2	C	822	VAL
2	C	829	GLN
2	C	837	ASP
2	C	838	LYS
2	C	855	VAL
2	C	856	GLU
2	C	869	VAL
2	C	871	LEU
2	C	879	ARG
2	C	881	ASN
2	C	900	ARG
2	C	913	GLU
2	C	937	ASP
2	C	969	GLN
2	C	981	GLU

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Mol	Chain	Res	Type
2	C	999	HIS
2	C	1000	MET
2	C	1008	ARG
2	C	1009	SER
2	C	1016	ILE
2	C	1043	TYR
2	C	1055	LEU
2	C	1078	GLU
2	C	1081	VAL
2	C	1113	GLU
3	D	12	LEU
3	D	17	LYS
3	D	32	ILE
3	D	38	LYS
3	D	40	GLU
3	D	48	ARG
3	D	68	PHE
3	D	85	VAL
3	D	97	THR
3	D	108	VAL
3	D	142	LEU
3	D	152	LEU
3	D	153	LEU
3	D	184	GLU
3	D	185	VAL
3	D	190	GLU
3	D	191	LEU
3	D	236	TYR
3	D	241	ILE
3	D	251	PHE
3	D	252	ARG
3	D	317	VAL
3	D	323	GLU
3	D	333	LEU
3	D	344	ASP
3	D	346	ARG
3	D	360	ARG
3	D	371	ILE
3	D	376	GLU
3	D	380	GLU
3	D	389	GLU
3	D	399	ARG

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Mol	Chain	Res	Type
3	D	411	THR
3	D	431	VAL
3	D	434	ARG
3	D	448	GLU
3	D	478	LEU
3	D	493	ARG
3	D	500	ARG
3	D	502	PHE
3	D	510	GLU
3	D	523	ASP
3	D	524	LEU
3	D	539	ASP
3	D	560	GLN
3	D	564	GLU
3	D	565	ILE
3	D	566	ILE
3	D	587	ARG
3	D	624	ASP
3	D	632	VAL
3	D	636	GLN
3	D	648	MET
3	D	650	LEU
3	D	676	MET
3	D	678	GLU
3	D	680	GLN
3	D	686	GLU
3	D	703	ASN
3	D	708	LEU
3	D	709	HIS
3	D	711	LEU
3	D	734	GLU
3	D	754	PHE
3	D	756	GLN
3	D	771	SER
3	D	780	LYS
3	D	782	SER
3	D	818	ARG
3	D	827	ILE
3	D	836	VAL
3	D	842	VAL
3	D	860	LEU
3	D	864	VAL

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Mol	Chain	Res	Type
3	D	876	SER
3	D	894	LYS
3	D	903	ASP
3	D	907	GLU
3	D	911	LEU
3	D	915	VAL
3	D	920	LEU
3	D	922	LEU
3	D	947	ILE
3	D	948	THR
3	D	952	ASP
3	D	964	LEU
3	D	968	ASP
3	D	971	LEU
3	D	983	LEU
3	D	985	ASP
3	D	994	GLN
3	D	1020	LEU
3	D	1029	ARG
3	D	1041	LEU
3	D	1055	VAL
3	D	1086	LEU
3	D	1096	ARG
3	D	1116	ASN
3	D	1119	SER
3	D	1124	GLN
3	D	1133	ARG
3	D	1155	VAL
3	D	1161	GLU
3	D	1162	GLU
3	D	1170	ASP
3	D	1188	VAL
3	D	1192	LEU
3	D	1202	GLN
3	D	1204	CYS
3	D	1208	ASP
3	D	1213	ARG
3	D	1216	SER
3	D	1234	THR
3	D	1238	MET
3	D	1239	ARG
3	D	1241	PHE

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Mol	Chain	Res	Type
3	D	1253	THR
3	D	1266	ARG
3	D	1276	GLU
3	D	1277	ILE
3	D	1286	THR
3	D	1287	GLU
3	D	1288	GLU
3	D	1297	GLU
3	D	1301	LYS
3	D	1305	LEU
3	D	1307	LYS
3	D	1313	VAL
3	D	1314	LYS
3	D	1319	VAL
3	D	1331	ASP
3	D	1344	VAL
3	D	1346	ARG
3	D	1348	LEU
3	D	1350	GLU
3	D	1359	GLN
3	D	1363	LEU
3	D	1368	ILE
3	D	1388	ARG
3	D	1390	LEU
3	D	1396	GLU
3	D	1398	TRP
3	D	1415	VAL
3	D	1422	MET
3	D	1424	VAL
3	D	1430	SER
3	D	1431	THR
3	D	1467	ILE
3	D	1468	LEU
3	D	1479	ASP
3	D	1482	ARG
3	D	1487	VAL
3	D	1496	GLU
4	E	10	PHE
4	E	19	LEU
4	E	31	LEU
4	E	37	ASN
4	E	39	VAL

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Mol	Chain	Res	Type
4	E	43	GLU
4	E	68	LEU
4	E	80	VAL
5	F	81	VAL
5	F	88	ILE
5	F	123	ASP
5	F	141	VAL
5	F	150	THR
5	F	179	GLU
5	F	205	ARG
5	F	208	SER
5	F	228	GLU
5	F	230	LYS
5	F	237	THR
5	F	249	ARG
5	F	256	ARG
5	F	264	MET
5	F	290	GLU
5	F	304	VAL
5	F	307	THR
5	F	319	THR
5	F	336	GLU
5	F	358	LEU
5	F	361	LEU
5	F	382	THR
5	F	394	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	91	ASN
1	A	95	GLN
1	A	128	HIS
1	A	156	HIS
1	A	212	ASN
1	B	38	ASN
2	C	22	GLN
2	C	179	ASN
2	C	187	ASN
2	C	393	GLN
2	C	406	HIS

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Mol	Chain	Res	Type
2	C	498	GLN
2	C	552	HIS
2	C	575	GLN
2	C	639	GLN
2	C	683	ASN
2	C	829	GLN
2	C	843	HIS
2	C	845	ASN
2	C	881	ASN
2	C	884	GLN
2	C	889	HIS
2	C	920	GLN
3	D	33	ASN
3	D	294	HIS
3	D	302	GLN
3	D	442	ASN
3	D	463	GLN
3	D	507	ASN
3	D	636	GLN
3	D	680	GLN
3	D	703	ASN
3	D	714	GLN
3	D	727	GLN
3	D	729	HIS
3	D	901	GLN
3	D	906	GLN
3	D	1034	GLN
3	D	1075	HIS
3	D	1172	HIS
3	D	1195	GLN
3	D	1242	HIS
3	D	1353	GLN
3	D	1442	ASN
4	E	33	HIS
4	E	37	ASN
5	F	175	HIS
5	F	248	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
7	PO4	A	401	-	4,4,4	1.00	0	6,6,6	0.40	0
10	G4P	D	1605	8	30,38,38	1.46	1 (3%)	42,61,61	1.33	5 (11%)

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
10	G4P	D	1605	8	-	6/23/43/43	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1605	G4P	O6-C6	6.65	1.36	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	1605	G4P	PA-O3A-PB	-3.63	120.36	132.83
10	D	1605	G4P	PC-O3C-PD	-2.92	122.80	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	1605	G4P	C5-C6-N1	2.55	118.45	113.95
10	D	1605	G4P	C2-N1-C6	-2.45	120.58	125.10
10	D	1605	G4P	C8-N7-C5	2.45	107.66	102.99

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	1605	G4P	C5'-O5'-PA-O3A
10	D	1605	G4P	C5'-O5'-PA-O1A
10	D	1605	G4P	C5'-O5'-PA-O2A
10	D	1605	G4P	O4'-C4'-C5'-O5'
10	D	1605	G4P	C4'-C3'-O3'-PC
10	D	1605	G4P	C3'-C4'-C5'-O5'

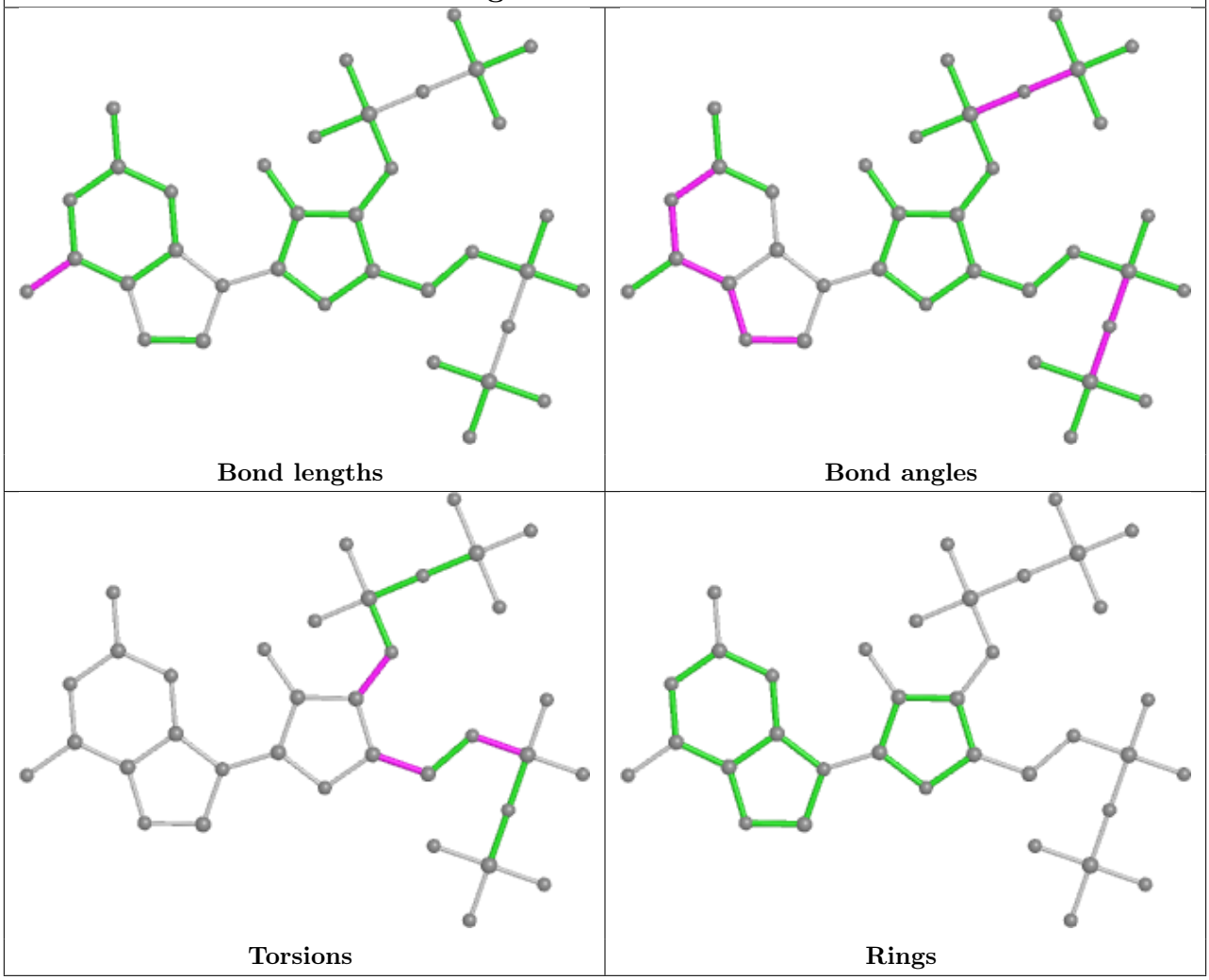
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1605	G4P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand G4P D 1605



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	A	231/315 (73%)	-0.02	8 (3%)	44	44	51, 78, 162, 212	1 (0%)
1	B	238/315 (75%)	0.53	31 (13%)	3	3	70, 149, 236, 260	0
2	C	1119/1119 (100%)	0.07	64 (5%)	23	23	53, 97, 222, 263	2 (0%)
3	D	1504/1524 (98%)	0.22	116 (7%)	13	12	52, 95, 245, 296	4 (0%)
4	E	95/99 (95%)	0.06	7 (7%)	14	13	58, 104, 192, 203	0
5	F	351/423 (82%)	0.60	44 (12%)	3	3	68, 124, 245, 277	2 (0%)
6	Z	0/48	-	-			-	-
All	All	3538/3843 (92%)	0.21	270 (7%)	13	12	51, 102, 232, 296	9 (0%)

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	391	GLY	25.7
3	D	1247	ALA	17.6
1	A	1	MET	14.6
5	F	390	PHE	13.7
1	A	3	ASP	13.7
1	A	5	LYS	13.5
3	D	375	GLU	13.4
5	F	73	PRO	13.0
3	D	328	GLY	12.6
1	A	4	SER	12.2
2	C	269	LEU	11.2
1	B	97	VAL	11.0
5	F	75	ILE	10.4
3	D	1243	THR	10.1
3	D	310	LEU	10.1
3	D	236	TYR	10.0
3	D	248	PRO	9.9
1	B	157	GLY	9.8

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Mol	Chain	Res	Type	RSRZ
3	D	235	ALA	9.7
1	B	158	ILE	9.3
2	C	268	ASP	9.2
3	D	1248	GLY	9.1
1	B	238	GLU	9.1
3	D	1245	GLY	8.7
3	D	251	PHE	8.6
2	C	222	MET	8.6
1	B	1	MET	8.4
5	F	381	HIS	8.4
2	C	293	PHE	8.3
3	D	237	LYS	8.0
1	B	162	ILE	8.0
5	F	74	LYS	7.9
3	D	241	ILE	7.7
5	F	378	GLY	7.4
3	D	229	ALA	7.3
3	D	1249	ALA	7.2
5	F	380	GLU	7.2
3	D	1246	VAL	7.1
5	F	394	ARG	7.1
3	D	227	LEU	7.0
3	D	293	VAL	6.9
3	D	295	GLY	6.9
5	F	148	LYS	6.8
3	D	1408	ILE	6.7
3	D	223	LEU	6.6
3	D	1244	GLY	6.5
1	B	96	THR	6.4
3	D	1505	ALA	6.4
2	C	420	ARG	6.2
2	C	287	GLY	6.2
1	A	2	LEU	6.1
1	B	62	LEU	6.1
2	C	205	GLU	6.1
3	D	296	GLU	6.0
1	B	57	TYR	5.9
3	D	230	TRP	5.9
2	C	275	TYR	5.9
1	A	6	LEU	5.8
3	D	326	GLU	5.7
5	F	369	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
5	F	355	GLU	5.5
1	B	98	THR	5.4
3	D	330	THR	5.4
1	B	141	GLU	5.4
1	B	2	LEU	5.4
3	D	309	GLY	5.4
5	F	359	SER	5.2
5	F	392	VAL	5.2
5	F	147	LEU	5.2
1	B	236	PRO	5.1
2	C	211	LEU	5.1
3	D	78	VAL	5.1
3	D	193	PRO	5.0
5	F	236	SER	5.0
3	D	260	GLU	5.0
3	D	428	LYS	5.0
1	B	61	VAL	4.9
3	D	283	PHE	4.9
3	D	250	LEU	4.9
3	D	329	GLU	4.8
3	D	418	GLY	4.8
1	B	99	LEU	4.6
3	D	486	ARG	4.6
3	D	75	ARG	4.6
3	D	895	VAL	4.5
3	D	300	LYS	4.5
2	C	418	LEU	4.5
1	B	3	ASP	4.5
5	F	76	SER	4.4
3	D	298	VAL	4.4
1	B	60	ASP	4.3
5	F	389	PHE	4.3
2	C	814	GLU	4.3
4	E	85	LEU	4.2
2	C	284	ARG	4.2
3	D	243	ALA	4.2
3	D	59	ALA	4.2
2	C	186	VAL	4.1
3	D	1399	ASP	4.1
3	D	613	ARG	4.1
3	D	76	CYS	4.1
3	D	294	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
3	D	274	ARG	4.0
2	C	278	GLU	4.0
4	E	52	GLU	4.0
3	D	70	GLY	4.0
4	E	87	LYS	4.0
2	C	767	PRO	4.0
5	F	144	ILE	4.0
5	F	400	ILE	4.0
5	F	385	GLU	4.0
2	C	297	GLU	3.9
3	D	312	ARG	3.8
1	B	160	ASP	3.8
3	D	306	GLU	3.8
1	B	4	SER	3.8
3	D	240	GLU	3.8
3	D	327	GLU	3.7
2	C	294	GLU	3.7
3	D	73	CYS	3.7
2	C	296	GLY	3.7
2	C	177	GLU	3.6
2	C	360	LEU	3.6
3	D	1242	HIS	3.6
2	C	279	GLU	3.6
3	D	1250	ALA	3.5
3	D	216	VAL	3.5
5	F	363	GLU	3.5
3	D	420	VAL	3.5
3	D	446	VAL	3.5
4	E	89	MET	3.4
3	D	402	PRO	3.4
3	D	1089	ALA	3.4
3	D	213	VAL	3.4
3	D	616	GLN	3.4
5	F	388	ALA	3.3
2	C	811	PRO	3.3
3	D	238	PRO	3.3
2	C	270	GLY	3.3
3	D	595	GLY	3.3
3	D	69	GLU	3.3
3	D	261	LEU	3.3
3	D	245	LEU	3.2
2	C	281	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	206	THR	3.2
3	D	68	PHE	3.2
2	C	118	ILE	3.2
3	D	417	PRO	3.2
2	C	421	GLU	3.2
3	D	253	ALA	3.2
3	D	231	VAL	3.1
3	D	67	ARG	3.1
3	D	490	ALA	3.1
2	C	217	LEU	3.1
3	D	315	ARG	3.1
1	B	163	ASN	3.1
2	C	42	VAL	3.1
3	D	273	ARG	3.1
2	C	214	TYR	3.0
3	D	224	ARG	3.0
5	F	408	LEU	3.0
4	E	91	ARG	3.0
3	D	290	PRO	3.0
5	F	373	LYS	3.0
1	B	118	ALA	3.0
2	C	348	LEU	3.0
3	D	60	CYS	3.0
3	D	72	VAL	2.9
1	A	188	GLN	2.9
3	D	1503	VAL	2.9
3	D	71	LYS	2.9
5	F	202	TYR	2.9
2	C	153	ALA	2.9
5	F	354	LEU	2.9
3	D	810	GLU	2.9
1	B	5	LYS	2.9
3	D	384	VAL	2.9
3	D	307	ALA	2.8
2	C	207	LEU	2.8
5	F	356	LYS	2.8
3	D	228	ALA	2.8
5	F	237	THR	2.8
3	D	56	TYR	2.8
5	F	410	TYR	2.8
2	C	155	PRO	2.8
3	D	242	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	778	PHE	2.7
2	C	34	VAL	2.7
3	D	484	PRO	2.7
5	F	325	LYS	2.7
3	D	247	GLU	2.7
3	D	297	ILE	2.7
3	D	900	ILE	2.7
2	C	774	LEU	2.7
2	C	249	LYS	2.7
5	F	360	LYS	2.7
2	C	311	PHE	2.7
2	C	1027	PHE	2.7
3	D	1318	TYR	2.7
1	B	164	ALA	2.6
5	F	412	GLU	2.6
3	D	275	GLU	2.6
2	C	92	ALA	2.6
2	C	37	GLU	2.6
5	F	195	VAL	2.6
2	C	356	ARG	2.6
5	F	93	LEU	2.6
2	C	38	LYS	2.6
5	F	395	GLU	2.5
2	C	361	MET	2.5
3	D	264	LEU	2.5
2	C	419	THR	2.5
2	C	464	LEU	2.5
3	D	74	GLU	2.5
5	F	321	ILE	2.5
1	B	6	LEU	2.5
1	B	87	VAL	2.4
3	D	491	LYS	2.4
1	B	119	ASP	2.4
1	B	52	ALA	2.4
3	D	62	LYS	2.4
4	E	84	ARG	2.4
2	C	96	ALA	2.4
5	F	358	LEU	2.4
3	D	262	LYS	2.4
3	D	1409	ALA	2.3
3	D	244	GLU	2.3
2	C	358	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
5	F	240	THR	2.3
2	C	315	ALA	2.3
1	A	225	PHE	2.3
3	D	360	ARG	2.3
2	C	98	LEU	2.3
3	D	331	VAL	2.3
2	C	352	ALA	2.2
5	F	344	ALA	2.2
2	C	388	ARG	2.2
3	D	301	GLY	2.2
3	D	364	GLY	2.2
3	D	276	ASP	2.2
3	D	183	GLU	2.2
1	B	159	LYS	2.2
2	C	209	ARG	2.2
2	C	78	PHE	2.2
3	D	1407	LEU	2.2
5	F	146	GLY	2.2
2	C	174	LEU	2.2
5	F	201	LYS	2.2
3	D	77	GLY	2.2
5	F	396	ARG	2.2
2	C	290	LEU	2.1
3	D	311	LEU	2.1
2	C	288	ARG	2.1
2	C	344	PHE	2.1
2	C	422	ARG	2.1
1	B	88	ARG	2.1
5	F	398	ARG	2.1
1	B	101	LEU	2.1
3	D	284	LEU	2.1
2	C	322	VAL	2.1
3	D	1440	PHE	2.1
2	C	367	LEU	2.1
4	E	86	GLN	2.1
3	D	806	PHE	2.1
2	C	1	MET	2.0
3	D	66	GLN	2.0
3	D	427	VAL	2.0
3	D	63	TYR	2.0
2	C	303	PHE	2.0
1	B	134	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

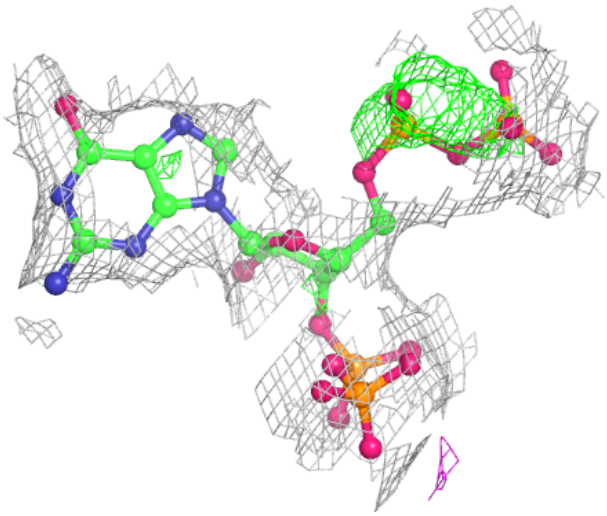
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

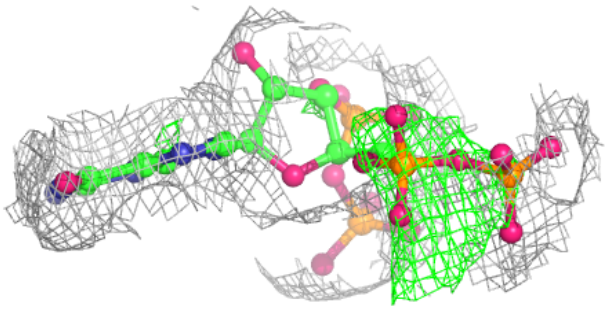
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	ZN	D	1602	1/1	0.60	0.08	225,225,225,225	0
8	MG	C	1201	1/1	0.90	0.22	131,131,131,131	0
10	G4P	D	1605	36/36	0.91	0.21	183,197,222,224	0
8	MG	D	1604	1/1	0.94	0.24	86,86,86,86	0
7	PO4	A	401	5/5	0.95	0.31	143,144,148,149	0
9	ZN	D	1603	1/1	0.96	0.11	168,168,168,168	0
8	MG	D	1606	1/1	0.97	0.17	155,155,155,155	0
8	MG	D	1601	1/1	0.98	0.35	133,133,133,133	0

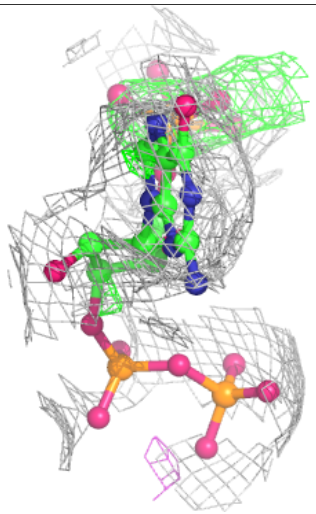
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around G4P D 1605:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.