Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2021 – 10:06 am BST

PDB ID	:	6ZPN
Title	:	Crystal structure of Chaetomium thermophilum Raptor
Authors	:	Imseng, S.; Boehm, R.; Jakob, R.P.; Hall, M.N.; Hiller, S.; Maier, T.
Deposited on	:	2020-07-08
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

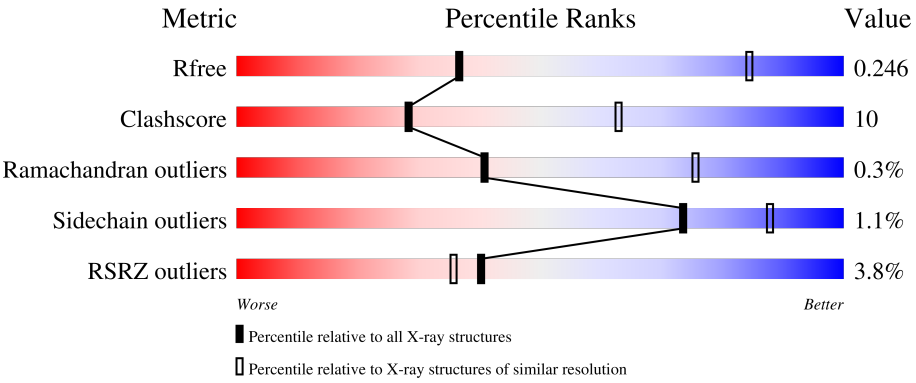
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (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 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	1504	4% 56% 15% 28%
1	B	1504	2% 55% 17% 28%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 34649 atoms, of which 17243 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 WD_REPEATS_REGION domain-containing protein.

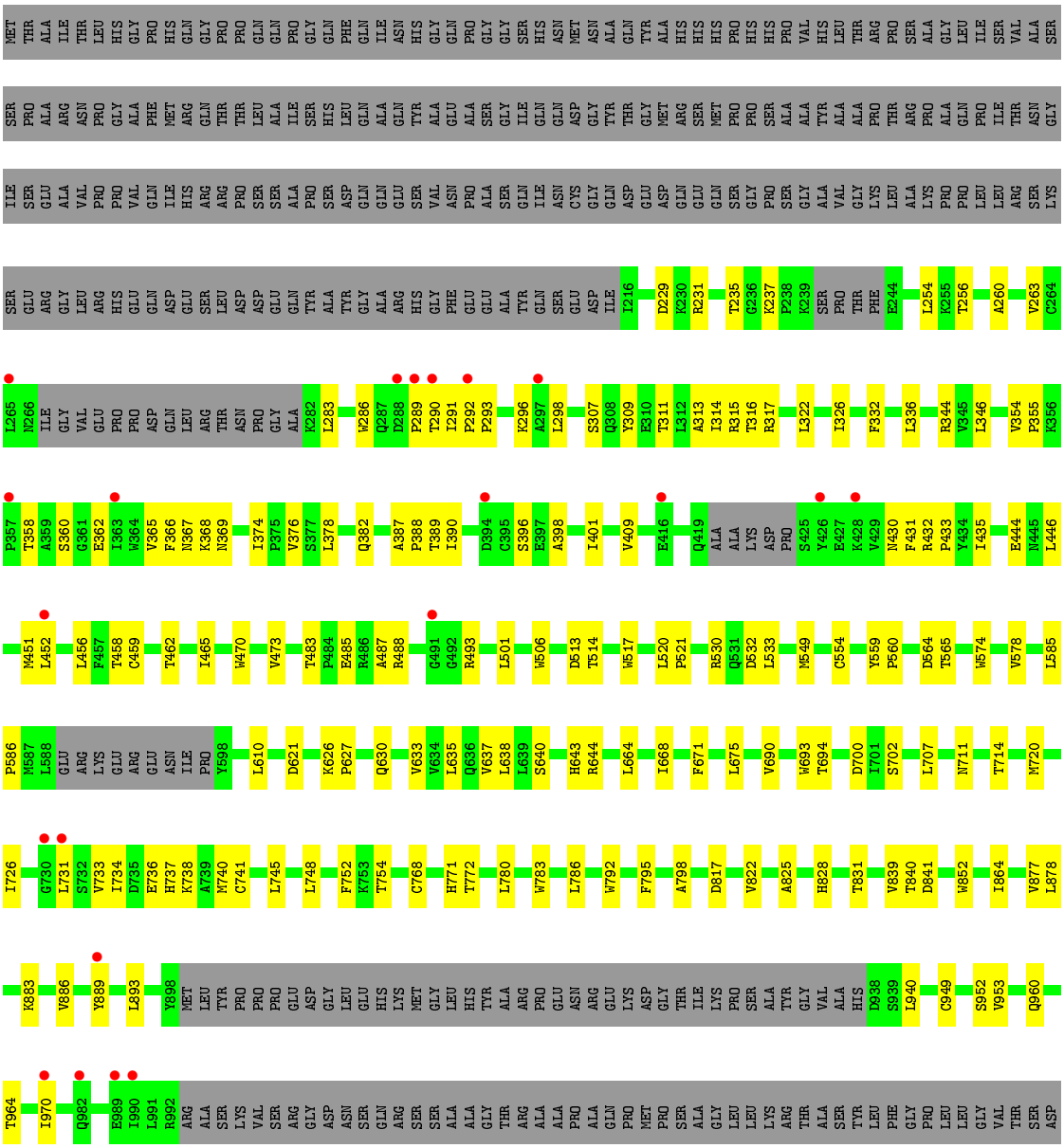
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1079	Total	C	H	N	O	S	0	0	0
			17340	5566	8626	1516	1581	51			
1	B	1079	Total	C	H	N	O	S	0	0	0
			17309	5549	8617	1515	1576	52			

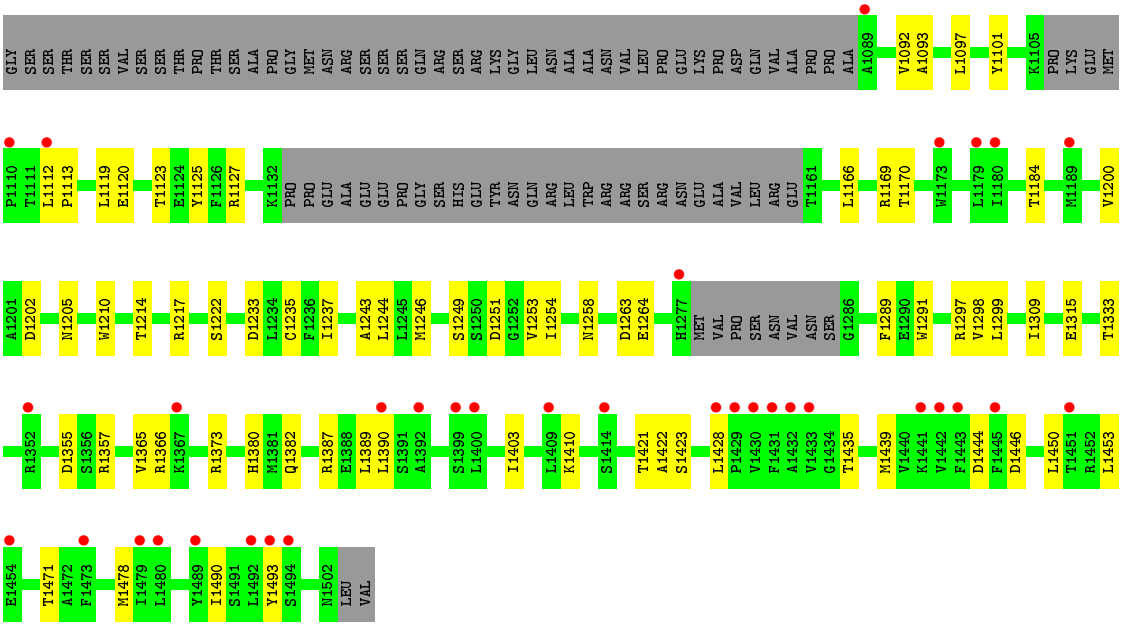
3 Residue-property plots (i)

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: WD_REPEATS_REGION domain-containing protein

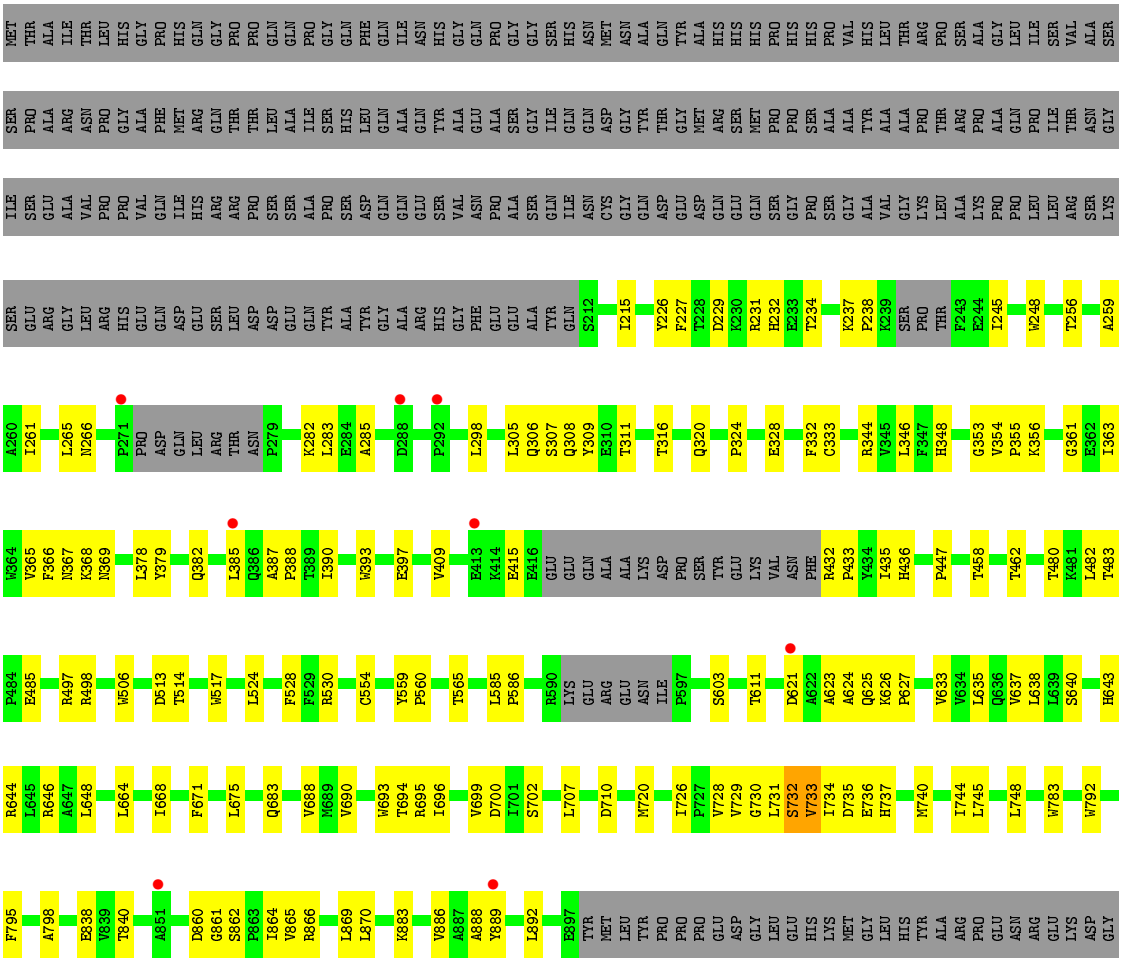
Chain A:

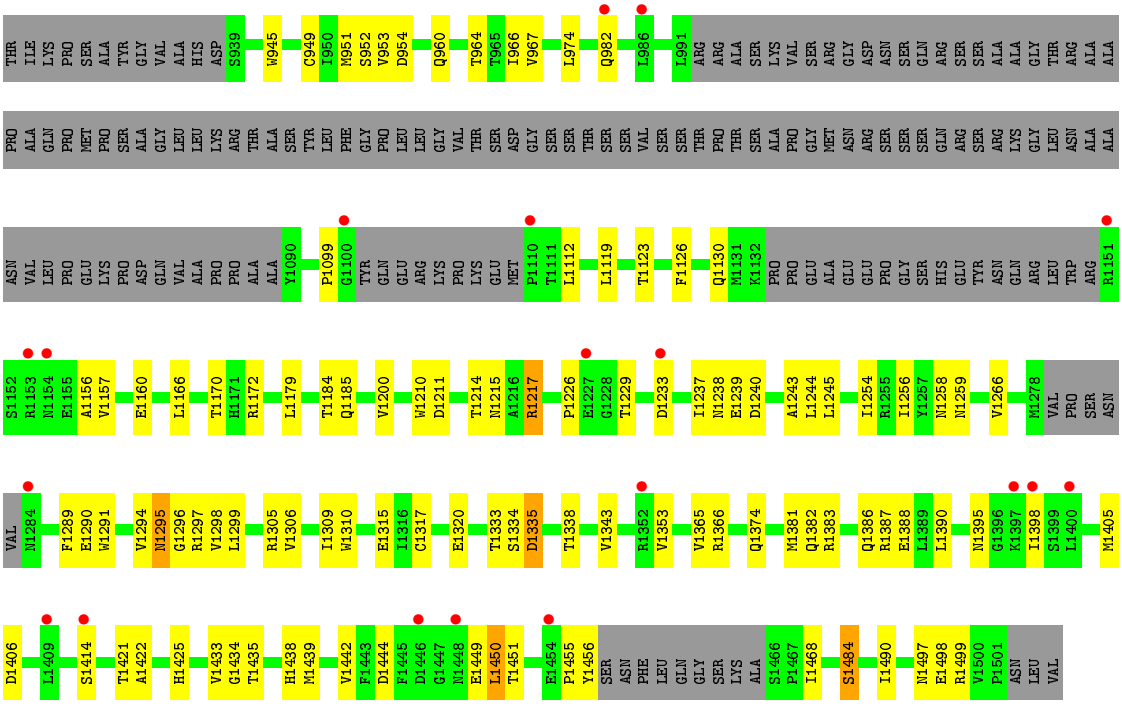




• Molecule 1: WD_REPEATS_REGION domain-containing protein

Chain B:




THR ILE LYS PRO SER ALA TYR GLY VAL ALA HIS ASP S939 W945 C949 I950 M951 S952 V953 D954 Q960 T964 T965 I966 V967 L974 Q982 L986 L991 ARG ARG ALA SER LYS VAL SER ARG GLY ASP ASN SER GLN ARG SER SER ALA ALA GLY THR ARG ALA ALA
PRO ALA GLN PRO MET PRO SER ALA GLY LEU LEU LYS ARG THR ALA SER TYR LEU PHE GLY PRO LEU LEU GLY VAL THR SER ASP GLY SER SER THR SER SER VAL SER SER THR PRO THR SER ALA PRO GLY MET ASN ARG SER SER SER GLN ARG SER SER ARG LYS GLY LEU ASN ALA ALA
ASN VAL LEU PRO GLU LYS PRO ASP GLN VAL ALA PRO PRO ALA ALA Y1090 P1099 G1100 TYR GLN GLU ARG LYS PRO LYS GLU MET P1110 T1111 L1112 L1119 T1123 F1126 Q1130 N1131 K1132 PRO PRO GLU ALA GLU GLU PRO GLY SER HIS GLU TYR ASN GLN ARG LEU TRP ARG R1151
S1152 R1153 N1154 E1155 A1156 V1157 E1160 L1166 T1170 H1171 R1172 L1179 T1184 Q1185 V1200 W1210 D1211 T1214 N1215 A1216 R1217 P1226 E1227 G1228 T1229 D1233 I1237 N1238 E1239 D1240 A1243 L1244 L1245 I1254 R1255 I1256 Y1257 N1258 N1259 V1266 M1278 VAL PRO SER ASN
VAL N1284 F1289 E1290 W1291 V1294 M1295 G1296 R1297 V1298 L1299 R1305 V1306 I1309 W1310 E1315 I1316 C1317 E1320 T1333 S1334 D1335 T1338 V1343 R1352 V1353 V1365 R1366 Q1374 M1381 Q1382 R1383 Q1386 R1387 E1388 L1389 L1390 N1395 G1396 K1397 I1398 S1399 L1400 M1405
D1406 L1409 S1414 T1421 A1422 H1425 V1433 G1434 T1435 H1438 M1439 V1442 F1443 D1444 F1445 D1446 G1447 N1448 E1449 L1450 T1451 E1454 P1455 Y1456 SER ASN PHE LEU GLN GLY SER LYS ALA S1466 P1467 I1468 S1484 I1490 N1497 E1498 R1499 V1500 P1501 ASN LEU VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	183.31Å 183.31Å 271.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.61 – 3.50 47.61 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.61-3.50) 99.6 (47.61-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.228 , 0.245 0.228 , 0.246	Depositor DCC
R_{free} test set	2957 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	133.1	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 152.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	34649	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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

5.1 Standard geometry

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	0.31	0/8931	0.54	0/12125
1	B	0.30	0/8907	0.54	0/12093
All	All	0.30	0/17838	0.54	0/24218

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8714	8626	8618	163	0
1	B	8692	8617	8610	177	0
All	All	17406	17243	17228	340	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 10.

All (340) 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:B:700:ASP:OD1	1:B:702:SER:OG	1.85	0.91
1:A:736:GLU:OE1	1:A:1125:TYR:OH	1.93	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:PRO:O	1:A:290:THR:OG1	1.95	0.83
1:A:878:LEU:CD1	1:A:1112:LEU:HD23	2.12	0.80
1:A:690:VAL:O	1:A:694:THR:HG23	1.81	0.80
1:B:1238:ASN:O	1:B:1240:ASP:N	2.14	0.79
1:A:231:ARG:NH1	1:A:1315:GLU:OE2	2.17	0.78
1:B:1119:LEU:O	1:B:1123:THR:HG23	1.85	0.77
1:B:256:THR:O	1:B:316:THR:HG22	1.85	0.76
1:B:732:SER:O	1:B:734:ILE:N	2.19	0.75
1:A:731:LEU:HD12	1:A:731:LEU:O	1.87	0.74
1:A:298:LEU:HD23	1:A:322:LEU:HD12	1.68	0.74
1:B:1200:VAL:HG11	1:B:1490:ILE:HD11	1.69	0.74
1:A:1200:VAL:HG11	1:A:1490:ILE:HD11	1.69	0.74
1:B:234:THR:HG23	1:B:234:THR:O	1.87	0.74
1:A:451:MET:O	1:A:452:LEU:HD12	1.88	0.74
1:B:1366:ARG:NH2	1:B:1405:MET:O	2.22	0.72
1:A:1244:LEU:HD22	1:A:1258:ASN:HA	1.71	0.72
1:B:695:ARG:NH2	1:B:1126:PHE:O	2.23	0.71
1:A:260:ALA:HB2	1:A:336:LEU:HD11	1.71	0.71
1:B:1343:VAL:HG22	1:B:1353:VAL:HG22	1.70	0.71
1:B:514:THR:HG21	1:B:633:VAL:HG23	1.72	0.70
1:B:379:TYR:OH	1:B:415:GLU:OE1	2.09	0.69
1:A:1444:ASP:HB2	1:A:1450:LEU:HD21	1.75	0.68
1:B:838:GLU:HG2	1:B:840:THR:HG23	1.74	0.68
1:A:574:TRP:O	1:A:578:VAL:HG23	1.95	0.67
1:A:1453:LEU:HD21	1:A:1493:TYR:CZ	2.30	0.67
1:B:1244:LEU:HD22	1:B:1258:ASN:HA	1.75	0.67
1:A:430:ASN:O	1:A:432:ARG:HG3	1.95	0.66
1:A:256:THR:HG23	1:A:532:ASP:OD2	1.95	0.66
1:A:263:VAL:CG2	1:A:322:LEU:HD13	2.26	0.66
1:B:1382:GLN:NE2	1:B:1425:HIS:O	2.28	0.66
1:B:690:VAL:O	1:B:694:THR:HG23	1.95	0.65
1:B:390:ILE:HD13	1:B:435:ILE:HB	1.78	0.65
1:B:720:MET:CE	1:B:745:LEU:HD12	2.27	0.65
1:B:1374:GLN:OE1	1:B:1395:ASN:ND2	2.30	0.64
1:A:256:THR:O	1:A:316:THR:HG22	1.97	0.64
1:B:387:ALA:HB1	1:B:388:PRO:CD	2.27	0.64
1:A:1119:LEU:O	1:A:1123:THR:HG23	1.98	0.64
1:A:298:LEU:CD2	1:A:322:LEU:HD12	2.28	0.63
1:A:786:LEU:HD22	1:A:825:ALA:HB1	1.80	0.63
1:B:1442:VAL:O	1:B:1449:GLU:O	2.16	0.63
1:A:720:MET:CE	1:A:745:LEU:HD12	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LYS:HD2	1:A:1120:GLU:HB3	1.81	0.63
1:A:877:VAL:CG1	1:A:970:ILE:HD11	2.29	0.63
1:A:514:THR:HG21	1:A:633:VAL:HG23	1.82	0.62
1:B:1434:GLY:HA3	1:B:1468:ILE:HD11	1.81	0.62
1:B:245:ILE:HD13	1:B:699:VAL:HG11	1.82	0.62
1:A:452:LEU:HA	1:A:470:TRP:HH2	1.65	0.62
1:B:733:VAL:HG11	1:B:1130:GLN:O	2.00	0.61
1:B:1468:ILE:HA	1:B:1484:SER:HA	1.83	0.61
1:A:517:TRP:CZ3	1:A:668:ILE:HD11	2.36	0.61
1:A:513:ASP:OD2	1:A:530:ARG:NH2	2.33	0.60
1:A:313:ALA:O	1:A:315:ARG:N	2.33	0.60
1:B:298:LEU:O	1:B:298:LEU:HD23	2.01	0.60
1:A:1237:ILE:HG22	1:A:1291:TRP:CD1	2.37	0.60
1:A:387:ALA:HB1	1:A:388:PRO:CD	2.31	0.60
1:B:1365:VAL:HG12	1:B:1366:ARG:HG2	1.85	0.59
1:B:1382:GLN:O	1:B:1382:GLN:HG3	2.01	0.59
1:B:227:PHE:HA	1:B:232:HIS:CE1	2.38	0.59
1:A:291:ILE:HG22	1:A:293:PRO:HD2	1.84	0.58
1:B:517:TRP:CZ3	1:B:668:ILE:HD11	2.39	0.58
1:B:728:VAL:HG12	1:B:730:GLY:H	1.67	0.58
1:B:1211:ASP:O	1:B:1215:ASN:N	2.36	0.58
1:A:387:ALA:HB1	1:A:388:PRO:HD2	1.85	0.58
1:A:235:THR:HG22	1:A:864:ILE:HD12	1.85	0.58
1:A:1365:VAL:HG12	1:A:1366:ARG:HG2	1.85	0.58
1:B:1254:ILE:HD13	1:B:1298:VAL:HG11	1.86	0.57
1:A:1243:ALA:O	1:A:1244:LEU:HD23	2.03	0.57
1:A:726:ILE:HB	1:A:737:HIS:NE2	2.20	0.57
1:A:828:HIS:HA	1:A:831:THR:HG22	1.86	0.57
1:A:771:HIS:CG	1:A:780:LEU:HD21	2.40	0.57
1:B:231:ARG:NH2	1:B:1315:GLU:OE2	2.37	0.57
1:B:745:LEU:HD23	1:B:748:LEU:HD12	1.87	0.57
1:A:1214:THR:HG22	1:A:1214:THR:O	2.04	0.57
1:A:365:VAL:HG12	1:A:366:PHE:N	2.19	0.57
1:A:398:ALA:O	1:A:401:ILE:HG22	2.05	0.57
1:A:1355:ASP:OD1	1:A:1357:ARG:N	2.37	0.56
1:B:733:VAL:O	1:B:733:VAL:HG22	2.05	0.56
1:A:734:ILE:HD11	1:A:736:GLU:OE2	2.04	0.56
1:B:237:LYS:HG3	1:B:237:LYS:O	2.05	0.56
1:B:1366:ARG:HH22	1:B:1406:ASP:HA	1.69	0.56
1:B:1156:ALA:O	1:B:1160:GLU:N	2.40	0.55
1:A:307:SER:O	1:A:311:THR:HG23	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ASN:O	1:A:432:ARG:N	2.39	0.55
1:B:949:CYS:O	1:B:952:SER:OG	2.16	0.55
1:B:960:GLN:O	1:B:964:THR:HG23	2.07	0.55
1:B:356:LYS:NZ	1:B:397:GLU:OE2	2.26	0.55
1:B:783:TRP:HH2	1:B:1123:THR:HG22	1.71	0.55
1:A:452:LEU:HA	1:A:470:TRP:CH2	2.42	0.55
1:A:949:CYS:O	1:A:952:SER:OG	2.20	0.55
1:B:635:LEU:HA	1:B:638:LEU:HD12	1.89	0.55
1:B:866:ARG:NH1	1:B:954:ASP:OD2	2.40	0.55
1:A:635:LEU:HA	1:A:638:LEU:HD12	1.87	0.54
1:B:361:GLY:O	1:B:378:LEU:HD21	2.07	0.54
1:A:953:VAL:HG12	1:A:953:VAL:O	2.08	0.54
1:A:783:TRP:HH2	1:A:1123:THR:HG22	1.71	0.54
1:B:248:TRP:NE1	1:B:700:ASP:OD2	2.31	0.54
1:A:1263:ASP:O	1:A:1264:GLU:HG2	2.08	0.54
1:A:458:THR:O	1:A:462:THR:OG1	2.24	0.54
1:A:396:SER:OG	1:A:446:LEU:HD22	2.07	0.54
1:B:1310:TRP:HA	1:B:1317:CYS:HA	1.90	0.54
1:A:263:VAL:HG22	1:A:322:LEU:HD13	1.89	0.53
1:A:711:ASN:O	1:A:714:THR:HG22	2.09	0.53
1:B:648:LEU:HB3	1:B:688:VAL:HG11	1.89	0.53
1:A:637:VAL:HG13	1:A:643:HIS:HB2	1.91	0.53
1:A:365:VAL:HG12	1:A:366:PHE:H	1.72	0.53
1:A:745:LEU:HD23	1:A:748:LEU:HD12	1.89	0.53
1:B:860:ASP:OD1	1:B:861:GLY:N	2.42	0.53
1:A:559:TYR:HB3	1:A:560:PRO:HD3	1.91	0.52
1:B:307:SER:O	1:B:311:THR:HG23	2.10	0.52
1:B:506:TRP:HH2	1:B:640:SER:HB2	1.73	0.52
1:A:565:THR:HG22	1:A:565:THR:O	2.08	0.52
1:A:817:ASP:OD2	1:A:822:VAL:HG11	2.09	0.52
1:A:390:ILE:HD13	1:A:435:ILE:HB	1.91	0.52
1:B:245:ILE:HD13	1:B:699:VAL:CG1	2.39	0.52
1:A:700:ASP:OD1	1:A:702:SER:OG	2.22	0.52
1:B:309:TYR:CE1	1:B:346:LEU:HD21	2.45	0.52
1:B:458:THR:O	1:B:462:THR:OG1	2.26	0.52
1:B:559:TYR:HB3	1:B:560:PRO:HD3	1.90	0.52
1:B:1237:ILE:HG22	1:B:1291:TRP:CD1	2.45	0.52
1:A:387:ALA:CB	1:A:388:PRO:HD2	2.40	0.52
1:B:731:LEU:HD12	1:B:734:ILE:HD12	1.92	0.51
1:A:483:THR:HG22	1:A:485:GLU:H	1.76	0.51
1:A:368:LYS:O	1:A:369:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:PHE:CE2	1:A:675:LEU:HD11	2.45	0.51
1:B:627:PRO:HB3	1:B:664:LEU:HD11	1.93	0.51
1:B:888:ALA:O	1:B:892:LEU:HD23	2.10	0.51
1:B:365:VAL:HG12	1:B:366:PHE:N	2.25	0.51
1:B:1259:ASN:HB2	1:B:1266:VAL:HA	1.92	0.51
1:B:1306:VAL:HG11	1:B:1320:GLU:HG2	1.93	0.51
1:B:953:VAL:HG12	1:B:953:VAL:O	2.10	0.51
1:A:387:ALA:O	1:A:389:THR:HG23	2.11	0.51
1:A:382:GLN:HE22	1:A:409:VAL:HG23	1.75	0.51
1:A:532:ASP:OD1	1:A:533:LEU:N	2.43	0.51
1:B:234:THR:HG22	1:B:1099:PRO:HG2	1.92	0.51
1:B:734:ILE:HG22	1:B:734:ILE:O	2.11	0.51
1:A:960:GLN:O	1:A:964:THR:HG23	2.10	0.51
1:B:1434:GLY:CA	1:B:1468:ILE:HD11	2.41	0.51
1:A:952:SER:HB2	1:A:964:THR:HG22	1.93	0.51
1:B:624:ALA:C	1:B:625:GLN:HG2	2.31	0.51
1:B:282:LYS:NZ	1:B:447:PRO:O	2.39	0.51
1:A:298:LEU:HD23	1:A:298:LEU:O	2.10	0.50
1:A:564:ASP:OD1	1:A:565:THR:N	2.44	0.50
1:B:671:PHE:CE2	1:B:675:LEU:HD11	2.46	0.50
1:B:696:ILE:O	1:B:699:VAL:O	2.29	0.50
1:A:1097:LEU:HD13	1:A:1101:TYR:HB3	1.94	0.50
1:B:365:VAL:HG12	1:B:366:PHE:H	1.76	0.50
1:B:1214:THR:O	1:B:1214:THR:HG22	2.12	0.50
1:A:1289:PHE:HA	1:A:1299:LEU:O	2.11	0.50
1:B:387:ALA:HB1	1:B:388:PRO:HD3	1.94	0.49
1:A:451:MET:O	1:A:470:TRP:CH2	2.65	0.49
1:B:306:GLN:OE1	1:B:320:GLN:NE2	2.45	0.49
1:A:694:THR:HG21	1:A:740:MET:HB3	1.93	0.49
1:A:1390:LEU:C	1:A:1390:LEU:HD23	2.33	0.49
1:A:1166:LEU:HA	1:A:1169:ARG:HB2	1.95	0.49
1:A:786:LEU:HD12	1:A:1119:LEU:HD12	1.95	0.49
1:B:1449:GLU:O	1:B:1451:THR:N	2.43	0.49
1:A:293:PRO:HB2	1:A:296:LYS:HB3	1.95	0.49
1:B:1289:PHE:HA	1:B:1299:LEU:O	2.13	0.49
1:A:1403:ILE:HD12	1:A:1403:ILE:H	1.78	0.49
1:A:506:TRP:HH2	1:A:640:SER:HB2	1.78	0.48
1:B:694:THR:HG21	1:B:740:MET:HB3	1.95	0.48
1:A:1169:ARG:O	1:A:1450:LEU:HD11	2.13	0.48
1:B:1398:ILE:HD11	1:B:1433:VAL:HG11	1.95	0.48
1:A:852:TRP:CD1	1:A:940:LEU:HD22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:THR:O	1:A:565:THR:CG2	2.60	0.48
1:A:786:LEU:HD12	1:A:1119:LEU:CD1	2.44	0.48
1:A:771:HIS:ND1	1:A:780:LEU:HD21	2.28	0.48
1:B:870:LEU:HD21	1:B:951:MET:SD	2.54	0.48
1:B:1179:LEU:HD13	1:B:1456:TYR:CZ	2.49	0.48
1:B:621:ASP:HB2	1:B:626:LYS:HB3	1.95	0.48
1:A:326:ILE:HG21	1:A:374:ILE:HD12	1.95	0.47
1:B:344:ARG:HA	1:B:388:PRO:O	2.14	0.47
1:B:729:VAL:HG12	1:B:729:VAL:O	2.13	0.47
1:B:974:LEU:HG	1:B:982:GLN:HG3	1.95	0.47
1:A:354:VAL:HB	1:A:355:PRO:HD2	1.97	0.47
1:A:1423:SER:OG	1:A:1471:THR:O	2.32	0.47
1:B:1243:ALA:O	1:B:1244:LEU:HD23	2.15	0.47
1:B:1306:VAL:CG1	1:B:1320:GLU:HG2	2.44	0.47
1:A:256:THR:HG22	1:A:344:ARG:HD2	1.97	0.47
1:A:358:THR:C	1:A:360:SER:H	2.17	0.47
1:B:726:ILE:HD13	1:B:737:HIS:NE2	2.30	0.47
1:B:731:LEU:CD1	1:B:734:ILE:HD12	2.45	0.47
1:B:945:TRP:CH2	1:B:967:VAL:HG13	2.50	0.47
1:B:1237:ILE:HD11	1:B:1244:LEU:HD12	1.97	0.47
1:A:1435:THR:HG22	1:A:1439:MET:O	2.15	0.47
1:B:1335:ASP:HB2	1:B:1383:ARG:HD2	1.97	0.47
1:B:869:LEU:HD23	1:B:869:LEU:O	2.15	0.47
1:B:514:THR:CG2	1:B:633:VAL:HG23	2.45	0.47
1:B:1184:THR:HG22	1:B:1185:GLN:H	1.80	0.46
1:A:795:PHE:HD2	1:A:798:ALA:HB2	1.80	0.46
1:B:1226:PRO:O	1:B:1229:THR:OG1	2.34	0.46
1:B:483:THR:HG22	1:B:485:GLU:H	1.80	0.46
1:A:362:GLU:HA	1:A:376:VAL:O	2.16	0.46
1:A:1428:LEU:HD11	1:A:1478:MET:HG2	1.96	0.46
1:A:517:TRP:CH2	1:A:668:ILE:HD11	2.50	0.46
1:B:378:LEU:O	1:B:382:GLN:HG3	2.16	0.46
1:B:728:VAL:CG1	1:B:730:GLY:H	2.29	0.46
1:A:1387:ARG:O	1:A:1387:ARG:HG2	2.16	0.46
1:B:226:TYR:CZ	1:B:1296:GLY:HA3	2.50	0.46
1:A:640:SER:O	1:A:644:ARG:HB3	2.16	0.46
1:A:1333:THR:HG21	1:A:1380:HIS:HA	1.98	0.46
1:B:367:ASN:OD1	1:B:368:LYS:N	2.49	0.46
1:A:1410:LYS:HE3	1:A:1446:ASP:HA	1.98	0.45
1:B:565:THR:O	1:B:565:THR:CG2	2.65	0.45
1:B:623:ALA:O	1:B:624:ALA:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:LEU:HB2	1:A:521:PRO:HD2	1.99	0.45
1:A:1251:ASP:OD1	1:A:1251:ASP:N	2.49	0.45
1:B:1294:VAL:HG13	1:B:1295:ASN:N	2.32	0.45
1:B:333:CYS:HA	1:B:385:LEU:HD21	1.97	0.45
1:A:1237:ILE:HD11	1:A:1244:LEU:HD12	1.98	0.45
1:B:864:ILE:HG23	1:B:865:VAL:HG23	1.99	0.45
1:B:1438:HIS:NE2	1:B:1455:PRO:O	2.43	0.45
1:A:637:VAL:O	1:A:640:SER:N	2.50	0.45
1:B:261:ILE:HA	1:B:348:HIS:HB3	1.98	0.45
1:B:382:GLN:HE22	1:B:409:VAL:HG23	1.82	0.45
1:B:732:SER:C	1:B:734:ILE:H	2.19	0.45
1:A:256:THR:HG22	1:A:344:ARG:HB3	1.99	0.44
1:A:444:GLU:HB3	1:A:554:CYS:HB3	1.99	0.44
1:B:265:LEU:HA	1:B:353:GLY:HA3	1.98	0.44
1:A:286:TRP:HE1	1:A:488:ARG:HG2	1.82	0.44
1:A:465:ILE:HG21	1:A:501:LEU:HD12	1.98	0.44
1:B:387:ALA:O	1:B:388:PRO:C	2.56	0.44
1:B:1157:VAL:HG12	1:B:1157:VAL:O	2.16	0.44
1:B:1386:GLN:HB3	1:B:1388:GLU:HG3	1.98	0.44
1:B:1335:ASP:OD2	1:B:1338:THR:N	2.45	0.44
1:B:1398:ILE:HD12	1:B:1414:SER:HB3	1.99	0.44
1:B:1497:ASN:O	1:B:1498:GLU:HG3	2.17	0.44
1:A:621:ASP:HB2	1:A:626:LYS:HG3	1.99	0.44
1:B:862:SER:OG	1:B:864:ILE:HG22	2.17	0.44
1:A:1184:THR:OG1	1:A:1202:ASP:OD2	2.34	0.44
1:B:513:ASP:OD2	1:B:530:ARG:NH2	2.50	0.44
1:B:1456:TYR:CD1	1:B:1456:TYR:N	2.86	0.44
1:A:292:PRO:HG2	1:A:293:PRO:HD3	1.99	0.44
1:A:326:ILE:HD12	1:A:376:VAL:HG22	1.99	0.44
1:A:387:ALA:CB	1:A:388:PRO:CD	2.95	0.44
1:B:795:PHE:HD2	1:B:798:ALA:HB2	1.82	0.44
1:A:840:THR:HG22	1:A:841:ASP:N	2.32	0.44
1:B:1435:THR:HG22	1:B:1439:MET:O	2.18	0.44
1:A:693:TRP:CE3	1:A:707:LEU:HD11	2.53	0.44
1:B:215:ILE:HD12	1:B:215:ILE:O	2.18	0.44
1:B:524:LEU:O	1:B:528:PHE:HD1	2.01	0.43
1:B:733:VAL:C	1:B:735:ASP:H	2.21	0.43
1:A:367:ASN:OD1	1:A:368:LYS:N	2.51	0.43
1:A:378:LEU:O	1:A:382:GLN:HG3	2.18	0.43
1:B:517:TRP:CH2	1:B:668:ILE:HD11	2.53	0.43
1:A:1120:GLU:OE1	1:A:1120:GLU:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:PHE:CG	1:B:1256:ILE:CD1	3.01	0.43
1:B:497:ARG:O	1:B:498:ARG:HB3	2.18	0.43
1:A:286:TRP:HH2	1:A:459:CYS:HB3	1.83	0.43
1:A:254:LEU:HD21	1:A:344:ARG:HH12	1.83	0.43
1:B:838:GLU:CG	1:B:840:THR:HG23	2.44	0.43
1:B:480:THR:OG1	1:B:482:LEU:HD12	2.19	0.43
1:B:864:ILE:HG23	1:B:865:VAL:N	2.34	0.43
1:A:1254:ILE:HD13	1:A:1298:VAL:HG11	2.01	0.43
1:A:1421:THR:HG22	1:A:1422:ALA:N	2.34	0.43
1:B:883:LYS:O	1:B:886:VAL:HG13	2.19	0.43
1:B:1444:ASP:HB2	1:B:1450:LEU:HD11	2.00	0.43
1:A:237:LYS:HE2	1:A:1127:ARG:HH12	1.82	0.43
1:A:456:LEU:HB3	1:A:549:MET:CE	2.49	0.43
1:A:1092:VAL:HG23	1:A:1093:ALA:N	2.34	0.43
1:B:1172:ARG:HG3	1:B:1450:LEU:O	2.19	0.43
1:B:1179:LEU:HD13	1:B:1456:TYR:CE1	2.54	0.43
1:A:630:GLN:O	1:A:633:VAL:N	2.52	0.43
1:A:752:PHE:CE2	1:A:754:THR:HG23	2.54	0.43
1:B:227:PHE:HB3	1:B:1256:ILE:HD11	1.99	0.43
1:A:889:TYR:CE1	1:A:893:LEU:HD21	2.54	0.42
1:B:585:LEU:N	1:B:586:PRO:CD	2.82	0.42
1:B:1233:ASP:HB3	1:B:1289:PHE:CE1	2.55	0.42
1:B:1166:LEU:O	1:B:1170:THR:HG23	2.18	0.42
1:B:1210:TRP:CZ3	1:B:1217:ARG:HB2	2.53	0.42
1:B:234:THR:O	1:B:234:THR:CG2	2.57	0.42
1:B:266:ASN:OD1	1:B:266:ASN:N	2.51	0.42
1:B:328:GLU:HG2	1:B:332:PHE:CE1	2.55	0.42
1:B:637:VAL:HG13	1:B:643:HIS:HB2	2.01	0.42
1:B:860:ASP:OD2	1:B:865:VAL:HG11	2.18	0.42
1:B:1170:THR:HB	1:B:1499:ARG:HD3	2.01	0.42
1:B:1390:LEU:HD23	1:B:1390:LEU:C	2.40	0.42
1:A:610:LEU:HD11	1:A:637:VAL:HG11	2.02	0.42
1:B:237:LYS:O	1:B:238:PRO:C	2.57	0.42
1:B:354:VAL:HB	1:B:355:PRO:HD2	2.02	0.42
1:A:465:ILE:HG21	1:A:501:LEU:CD1	2.50	0.42
1:A:839:VAL:O	1:A:839:VAL:HG13	2.20	0.42
1:A:1166:LEU:O	1:A:1170:THR:HG23	2.19	0.42
1:A:1210:TRP:CZ3	1:A:1217:ARG:HB2	2.55	0.42
1:B:1184:THR:HG22	1:B:1185:GLN:N	2.34	0.42
1:A:585:LEU:N	1:A:586:PRO:HD3	2.35	0.42
1:B:259:ALA:HB1	1:B:346:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:736:GLU:OE1	1:B:1130:GLN:NE2	2.52	0.42
1:B:363:ILE:HD13	1:B:393:TRP:CZ3	2.55	0.42
1:A:309:TYR:CE1	1:A:346:LEU:HD21	2.55	0.42
1:B:1297:ARG:HD2	1:B:1309:ILE:CG2	2.50	0.42
1:B:1449:GLU:C	1:B:1451:THR:H	2.21	0.42
1:A:256:THR:CG2	1:A:344:ARG:HD2	2.50	0.41
1:A:1235:CYS:HB2	1:A:1246:MET:HB2	2.02	0.41
1:B:285:ALA:HB2	1:B:305:LEU:CD1	2.50	0.41
1:B:514:THR:HG21	1:B:633:VAL:CG2	2.45	0.41
1:B:694:THR:HG22	1:B:744:ILE:HG13	2.02	0.41
1:A:1112:LEU:O	1:A:1113:PRO:C	2.59	0.41
1:B:432:ARG:N	1:B:433:PRO:CD	2.83	0.41
1:A:430:ASN:O	1:A:432:ARG:CG	2.68	0.41
1:A:738:LYS:O	1:A:741:CYS:N	2.54	0.41
1:B:436:HIS:HB2	1:B:559:TYR:HB2	2.01	0.41
1:B:1421:THR:HG22	1:B:1422:ALA:N	2.35	0.41
1:A:627:PRO:HB3	1:A:664:LEU:HD11	2.02	0.41
1:A:731:LEU:O	1:A:733:VAL:N	2.53	0.41
1:A:828:HIS:O	1:A:831:THR:HG22	2.20	0.41
1:A:883:LYS:O	1:A:886:VAL:HG13	2.20	0.41
1:B:611:THR:OG1	1:B:646:ARG:NH1	2.51	0.41
1:B:640:SER:O	1:B:644:ARG:CB	2.69	0.41
1:B:693:TRP:CH2	1:B:707:LEU:HD11	2.56	0.41
1:B:1333:THR:HG21	1:B:1381:MET:N	2.35	0.41
1:A:1233:ASP:HB3	1:A:1289:PHE:CE1	2.56	0.41
1:A:1382:GLN:O	1:A:1382:GLN:HG3	2.21	0.41
1:B:308:GLN:HB3	1:B:462:THR:HB	2.03	0.41
1:B:640:SER:O	1:B:644:ARG:HB2	2.21	0.41
1:A:473:VAL:HG21	1:A:487:ALA:HB2	2.03	0.41
1:B:733:VAL:O	1:B:736:GLU:HG2	2.21	0.41
1:A:315:ARG:HD2	1:A:315:ARG:O	2.21	0.41
1:A:1251:ASP:OD1	1:A:1253:VAL:HG12	2.20	0.41
1:B:883:LYS:O	1:B:886:VAL:CG1	2.69	0.41
1:B:1387:ARG:HG3	1:B:1387:ARG:O	2.20	0.41
1:B:387:ALA:HB1	1:B:388:PRO:HD2	2.01	0.41
1:B:1245:LEU:O	1:B:1256:ILE:HA	2.21	0.41
1:B:889:TYR:CD1	1:B:982:GLN:OE1	2.74	0.40
1:B:1290:GLU:OE2	1:B:1334:SER:N	2.55	0.40
1:B:966:ILE:HG12	1:B:1112:LEU:HD11	2.02	0.40
1:A:1389:LEU:HD23	1:A:1389:LEU:C	2.41	0.40
1:A:326:ILE:CG2	1:A:374:ILE:HD12	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:ILE:O	1:A:734:ILE:HG23	2.21	0.40
1:A:1205:ASN:O	1:A:1205:ASN:OD1	2.40	0.40
1:A:1237:ILE:C	1:A:1237:ILE:HD12	2.42	0.40
1:A:1297:ARG:HD3	1:A:1309:ILE:CG2	2.52	0.40
1:A:235:THR:CG2	1:A:864:ILE:HD12	2.52	0.40
1:A:432:ARG:HB2	1:A:433:PRO:HD3	2.03	0.40
1:A:768:CYS:O	1:A:772:THR:HG23	2.22	0.40
1:A:1249:SER:HB2	1:A:1251:ASP:OD1	2.22	0.40
1:B:324:PRO:O	1:B:365:VAL:HG12	2.21	0.40
1:B:1450:LEU:O	1:B:1451:THR:HB	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	A	1059/1504 (70%)	975 (92%)	82 (8%)	2 (0%)	47 81
1	B	1057/1504 (70%)	979 (93%)	74 (7%)	4 (0%)	34 72
All	All	2116/3008 (70%)	1954 (92%)	156 (7%)	6 (0%)	41 75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	431	PHE
1	B	733	VAL
1	B	1239	GLU
1	A	314	ILE
1	B	732	SER
1	B	1450	LEU

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	948/1294 (73%)	940 (99%)	8 (1%)	81 91
1	B	947/1294 (73%)	934 (99%)	13 (1%)	67 85
All	All	1895/2588 (73%)	1874 (99%)	21 (1%)	73 88

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	ASP
1	A	283	LEU
1	A	317	ARG
1	A	332	PHE
1	A	493	ARG
1	A	792	TRP
1	A	1222	SER
1	A	1373	ARG
1	B	229	ASP
1	B	283	LEU
1	B	369	ASN
1	B	554	CYS
1	B	603	SER
1	B	683	GLN
1	B	710	ASP
1	B	792	TRP
1	B	1217	ARG
1	B	1295	ASN
1	B	1305	ARG
1	B	1335	ASP
1	B	1484	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	555	HIS

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Mol	Chain	Res	Type
1	B	774	HIS
1	B	1382	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1079/1504 (71%)	0.32	56 (5%)	27	24	78, 140, 209, 261	0
1	B	1079/1504 (71%)	0.22	27 (2%)	57	51	80, 134, 209, 262	0
All	All	2158/3008 (71%)	0.27	83 (3%)	40	36	78, 138, 209, 262	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	989	GLU	5.5
1	A	1432	ALA	5.2
1	A	1431	PHE	4.6
1	A	1277	HIS	4.5
1	B	1110	PRO	4.4
1	A	1445	PHE	4.4
1	A	1430	VAL	4.4
1	A	730	GLY	4.3
1	A	1428	LEU	4.0
1	A	288	ASP	4.0
1	A	1400	LEU	4.0
1	B	889	TYR	3.9
1	A	289	PRO	3.9
1	A	428	LYS	3.9
1	A	731	LEU	3.7
1	B	271	PRO	3.7
1	B	982	GLN	3.4
1	A	1180	ILE	3.3
1	A	1414	SER	3.2
1	B	1233	ASP	3.1
1	A	1429	PRO	3.1
1	A	292	PRO	3.1
1	A	1479	ILE	3.1
1	A	290	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1112	LEU	3.0
1	A	1409	LEU	3.0
1	A	1442	VAL	3.0
1	A	265	LEU	3.0
1	A	1179	LEU	2.9
1	B	288	ASP	2.9
1	A	1433	VAL	2.9
1	A	889	TYR	2.8
1	A	1189	MET	2.8
1	B	1400	LEU	2.7
1	B	1284	ASN	2.7
1	A	1441	LYS	2.7
1	B	1446	ASP	2.6
1	A	416	GLU	2.6
1	B	1398	ILE	2.6
1	A	1089	ALA	2.6
1	B	1409	LEU	2.5
1	A	1473	PHE	2.5
1	B	292	PRO	2.5
1	A	1493	TYR	2.4
1	A	1480	LEU	2.4
1	A	426	TYR	2.4
1	A	452	LEU	2.4
1	A	1489	TYR	2.4
1	A	1352	ARG	2.4
1	B	1153	ARG	2.4
1	A	1392	ALA	2.4
1	A	1494	SER	2.4
1	A	297	ALA	2.4
1	B	1454	GLU	2.3
1	A	357	PRO	2.3
1	B	1448	ASN	2.3
1	A	1443	PHE	2.3
1	A	1451	THR	2.3
1	B	413	GLU	2.3
1	B	1154	ASN	2.3
1	B	851	ALA	2.2
1	B	1414	SER	2.2
1	A	982	GLN	2.2
1	B	1397	LYS	2.2
1	A	990	ILE	2.2
1	A	1399	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	363	ILE	2.2
1	A	1390	LEU	2.2
1	A	1173	TRP	2.2
1	B	385	LEU	2.2
1	A	491	GLY	2.1
1	A	1110	PRO	2.1
1	B	1352	ARG	2.1
1	A	970	ILE	2.1
1	B	1151	ARG	2.1
1	A	1367	LYS	2.1
1	A	1454	GLU	2.1
1	B	1227	GLU	2.1
1	A	1492	LEU	2.0
1	B	1100	GLY	2.0
1	A	394	ASP	2.0
1	B	621	ASP	2.0
1	B	986	LEU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.