Full wwPDB X-ray Structure Validation Report (i)

Dec 28, 2016 – 12:00 AM EST

PDB ID	:	5TRC
Title	:	Crystal structure of phosphorylated AC3-AC5 domains of yeast acetyl-CoA carboxylase
Authors	:	Wei, J.; Tong, L.
Deposited on	:	2016-10-26
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

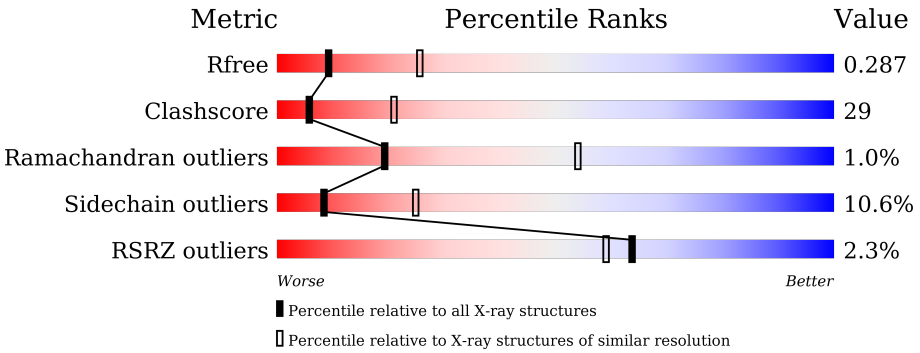
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	474	2% 48% 37% 5% 10%
1	B	474	2% 37% 43% 5% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6628 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 Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	P	S	0	0	0
			3414	2178	581	648	1	6			
1	B	398	Total	C	N	O	P	S	0	0	0
			3212	2051	549	605	1	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1504	HIS	-	expression tag	UNP Q00955
A	1505	HIS	-	expression tag	UNP Q00955
A	1506	HIS	-	expression tag	UNP Q00955
A	1507	HIS	-	expression tag	UNP Q00955
A	1508	HIS	-	expression tag	UNP Q00955
A	1509	HIS	-	expression tag	UNP Q00955
B	1504	HIS	-	expression tag	UNP Q00955
B	1505	HIS	-	expression tag	UNP Q00955
B	1506	HIS	-	expression tag	UNP Q00955
B	1507	HIS	-	expression tag	UNP Q00955
B	1508	HIS	-	expression tag	UNP Q00955
B	1509	HIS	-	expression tag	UNP Q00955

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

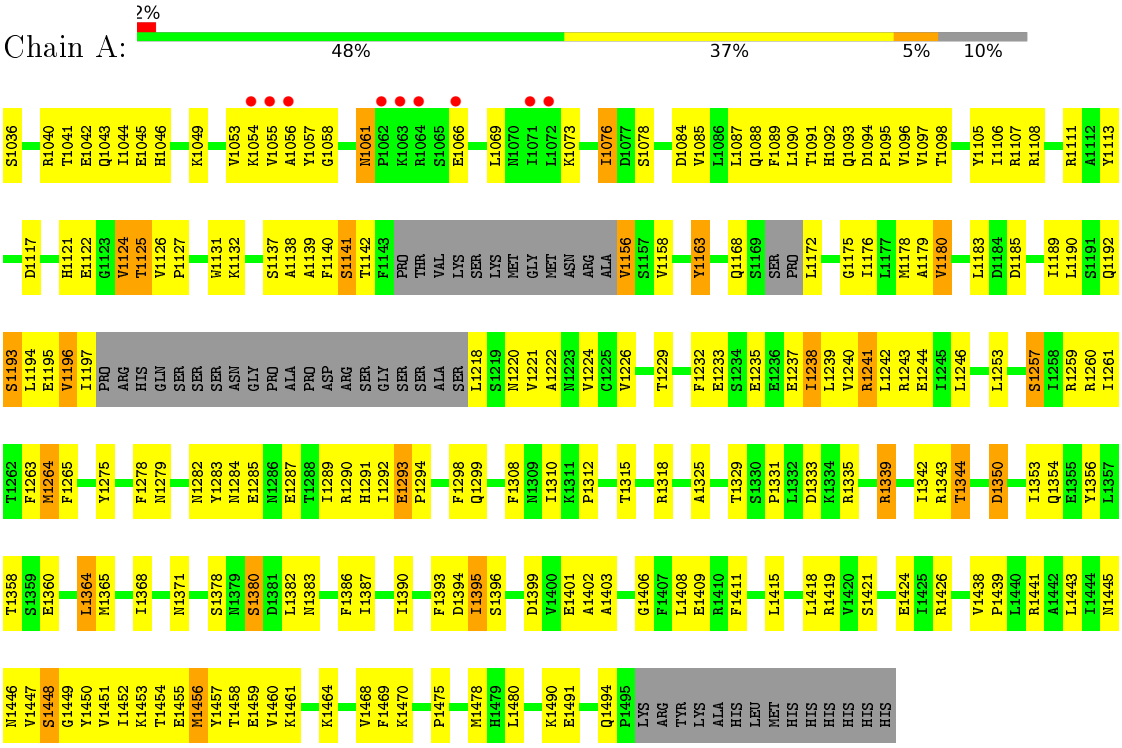
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

3 Residue-property plots (i)

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

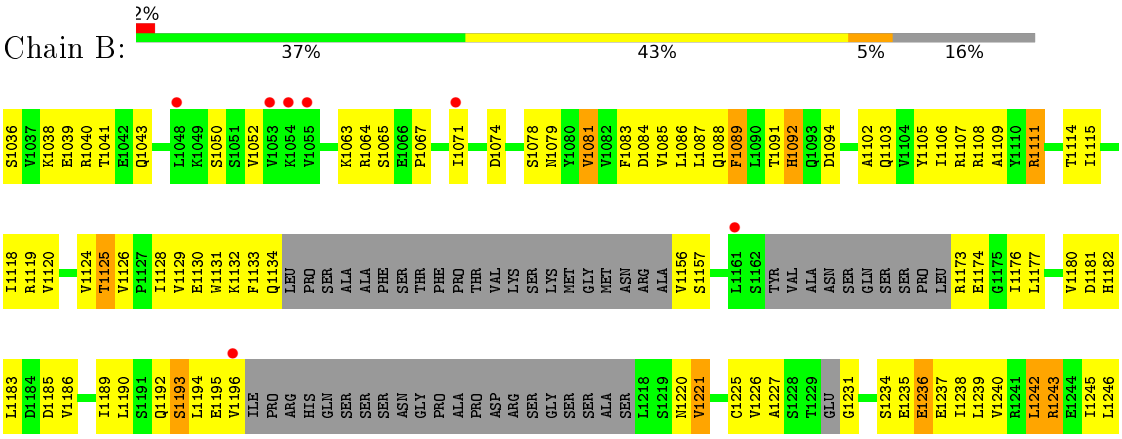
- Molecule 1: Acetyl-CoA carboxylase

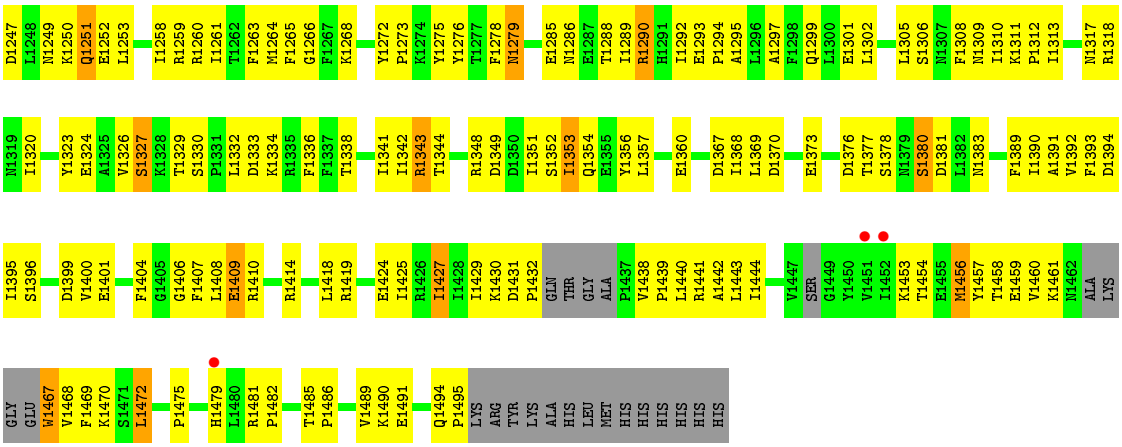
Chain A:



- Molecule 1: Acetyl-CoA carboxylase

Chain B:




D1247 L1248 N1249 K1250 Q1251 E1252 L1253 I1258 R1259 R1260 I1261 T1262 F1263 M1264 F1265 G1266 F1267 K1268 Y1272 P1273 K1274 Y1275 Y1276 T1277 F1278 N1279 E1285 N1286 E1287 T1288 I1289 R1290 H1291 I1292 E1293 P1294 A1295 L1296 A1297 F1298 Q1299 L1300 E1301 L1302 L1305 S1306 N1307 F1308 N1309 I1310 K1311 P1312 I1313 N1317 R1318
N1319 I1320 Y1323 E1324 A1325 V1326 S1327 K1328 T1329 S1330 P1331 L1332 D1333 K1334 R1335 F1336 F1337 T1338 I1341 I1342 R1343 T1344 R1348 D1349 D1350 I1351 S1352 I1353 Q1354 E1355 Y1356 L1357 E1360 D1367 I1368 L1369 D1370 E1373 D1376 T1377 S1378 N1379 S1380 D1381 L1382 N1383 F1389 I1390 A1391 V1392 F1393 D1394
I1395 S1396 D1399 V1400 E1401 F1404 G1405 G1406 F1407 L1408 E1409 R1410 R1414 L1418 R1419 E1424 I1425 R1426 I1427 I1428 I1429 K1430 D1431 P1432 GLN THR GLY ALA P1437 V1438 P1439 L1440 R1441 A1442 L1443 I1444 V1447 SER G1449 Y1450 V1451 I1452 K1453 T1454 E1455 M1456 Y1457 T1458 E1459 V1460 K1461 N1462 ALA LYS
GLY GLU W1467 V1468 F1469 K1470 S1471 L1472 P1475 H1479 L1480 R1481 P1482 T1485 P1486 V1489 K1490 E1491 Q1494 P1495 LYS ARG TYR LYS ALA HIS LEU MET HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.43Å 93.19Å 110.94Å 90.00° 99.57° 90.00°	Depositor
Resolution (Å)	46.57 – 2.90 46.57 – 2.88	Depositor EDS
% Data completeness (in resolution range)	97.5 (46.57-2.90) 97.5 (46.57-2.88)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.287 0.226 , 0.287	Depositor DCC
R_{free} test set	1252 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	82.6	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6628	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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

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

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	0.61	0/3470	0.71	1/4703 (0.0%)
1	B	0.53	0/3260	0.69	0/4410
All	All	0.57	0/6730	0.70	1/9113 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1293	GLU	C-N-CD	5.04	138.98	128.40

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	3414	0	3409	166	0
1	B	3212	0	3213	221	0
2	A	1	0	0	1	0
2	B	1	0	0	1	0
All	All	6628	0	6622	383	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 29.

All (383) 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:A:1275:TYR:O	1:A:1290:ARG:O	1.66	1.14
1:B:1221:VAL:HG11	1:B:1260:ARG:NH1	1.70	1.07
1:A:1445:ASN:OD1	1:A:1447:VAL:HG22	1.59	1.01
1:B:1221:VAL:HG13	1:B:1260:ARG:CG	1.97	0.94
1:A:1189:ILE:O	1:A:1193:SER:OG	1.85	0.94
1:B:1221:VAL:HG13	1:B:1260:ARG:HG3	1.49	0.93
1:B:1221:VAL:CG1	1:B:1260:ARG:HG3	2.00	0.89
1:B:1482:PRO:O	1:B:1485:THR:HG22	1.73	0.88
1:B:1313:ILE:HD11	1:B:1324:GLU:HB2	1.56	0.88
1:B:1305:LEU:HD12	1:B:1310:ILE:HD11	1.55	0.88
1:B:1221:VAL:HG11	1:B:1260:ARG:CZ	2.06	0.85
1:B:1275:TYR:O	1:B:1290:ARG:O	1.96	0.84
1:B:1373:GLU:OE2	1:B:1414:ARG:NH2	2.12	0.83
1:B:1106:ILE:HD11	1:B:1177:LEU:HD22	1.59	0.83
1:A:1044:ILE:HD12	1:A:1085:VAL:HG12	1.63	0.80
1:B:1088:GLN:OE1	1:B:1268:LYS:HG2	1.81	0.80
1:A:1421:SER:O	1:A:1446:ASN:HB3	1.83	0.78
1:B:1088:GLN:HE21	1:B:1089:PHE:HE1	1.29	0.78
1:B:1406:GLY:HA2	1:B:1409:GLU:HG3	1.64	0.78
1:A:1445:ASN:CG	1:A:1447:VAL:HG22	2.04	0.77
1:B:1272:TYR:O	1:B:1318:ARG:NH2	2.18	0.75
1:B:1461:LYS:HG2	1:B:1467:TRP:CD1	2.22	0.75
1:B:1305:LEU:CD1	1:B:1310:ILE:HD11	2.18	0.74
1:A:1408:LEU:O	1:A:1411:PHE:N	2.18	0.73
1:A:1329:THR:CG2	1:A:1494:GLN:HG2	2.19	0.73
1:B:1221:VAL:HG13	1:B:1260:ARG:HG2	1.70	0.73
1:A:1448:SER:O	1:A:1450:TYR:N	2.21	0.72
1:A:1108:ARG:NH1	2:A:1601:CL:CL	2.60	0.72
1:A:1117:ASP:OD1	1:A:1132:LYS:HE2	1.89	0.71
1:A:1045:GLU:HG3	1:A:1089:PHE:HE2	1.54	0.71
1:A:1141:SER:OG	1:A:1426:ARG:NH1	2.24	0.70
1:B:1039:GLU:O	1:B:1043:GLN:HG3	1.90	0.70
1:B:1063:LYS:HE2	1:B:1064:ARG:HG3	1.71	0.70
1:A:1421:SER:O	1:A:1446:ASN:CB	2.39	0.69
1:A:1113:TYR:OH	1:A:1158:VAL:HG23	1.93	0.69
1:B:1341:ILE:CG2	1:B:1390:ILE:HD11	2.22	0.69
1:B:1380:SER:HB2	1:B:1383:ASN:HD21	1.58	0.69
1:A:1045:GLU:HG3	1:A:1089:PHE:CE2	2.28	0.69
1:A:1342:ILE:HD11	1:A:1364:LEU:HD12	1.74	0.69
1:A:1329:THR:HG23	1:A:1494:GLN:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1291:HIS:CD2	1:A:1318:ARG:HG2	2.29	0.68
1:B:1040:ARG:NH1	1:B:1084:ASP:OD2	2.26	0.68
1:B:1343:ARG:HG2	1:B:1343:ARG:HH11	1.56	0.68
1:A:1126:VAL:CG2	1:A:1127:PRO:HD2	2.24	0.67
1:B:1036:SER:HA	1:B:1039:GLU:OE1	1.95	0.67
1:A:1315:THR:HB	1:A:1371:ASN:HD21	1.60	0.67
1:A:1315:THR:HB	1:A:1371:ASN:ND2	2.10	0.67
1:B:1313:ILE:CD1	1:B:1324:GLU:HB2	2.23	0.67
1:B:1461:LYS:HG2	1:B:1467:TRP:HD1	1.58	0.66
1:A:1293:GLU:OE2	1:A:1294:PRO:HD2	1.95	0.66
1:B:1109:ALA:O	1:B:1295:ALA:HB1	1.96	0.66
1:B:1220:ASN:O	1:B:1259:ARG:N	2.29	0.65
1:A:1126:VAL:HG22	1:A:1127:PRO:HD2	1.78	0.65
1:A:1339:ARG:HH11	1:A:1339:ARG:HG2	1.62	0.65
1:A:1350:ASP:N	1:A:1350:ASP:OD1	2.28	0.65
1:B:1299:GLN:OE1	1:B:1390:ILE:HD13	1.98	0.64
1:B:1109:ALA:O	1:B:1295:ALA:CB	2.46	0.64
1:A:1232:PHE:HE2	1:A:1241:ARG:HG3	1.63	0.64
1:A:1106:ILE:HD13	1:A:1131:TRP:CE3	2.33	0.64
1:B:1040:ARG:NH2	1:B:1084:ASP:OD2	2.30	0.63
1:B:1469:PHE:O	1:B:1479:HIS:O	2.16	0.63
1:B:1221:VAL:CG1	1:B:1260:ARG:NH1	2.55	0.63
1:B:1369:LEU:O	1:B:1373:GLU:HG3	1.98	0.63
1:A:1121:HIS:CE1	1:A:1196:VAL:HG11	2.34	0.63
1:A:1445:ASN:OD1	1:A:1447:VAL:CG2	2.43	0.63
1:B:1174:GLU:H	1:B:1220:ASN:ND2	1.97	0.63
1:A:1044:ILE:HD12	1:A:1085:VAL:CG1	2.28	0.62
1:B:1309:ASN:N	1:B:1326:VAL:O	2.31	0.62
1:B:1288:THR:HG22	1:B:1312:PRO:HD3	1.80	0.62
1:B:1174:GLU:O	1:B:1220:ASN:ND2	2.34	0.61
1:B:1344:THR:HG22	1:B:1356:TYR:OH	2.00	0.61
1:A:1088:GLN:HG3	1:A:1089:PHE:CD1	2.35	0.61
1:A:1457:TYR:CD2	1:A:1469:PHE:HB3	2.35	0.61
1:B:1440:LEU:HD23	1:B:1458:THR:HG22	1.81	0.61
1:B:1106:ILE:HD11	1:B:1177:LEU:CD2	2.28	0.61
1:B:1460:VAL:HG12	1:B:1461:LYS:H	1.65	0.61
1:B:1460:VAL:O	1:B:1468:VAL:N	2.23	0.61
1:B:1376:ASP:OD1	1:B:1378:SER:HB3	2.01	0.61
1:B:1408:LEU:HD12	1:B:1444:ILE:CG2	2.30	0.61
1:B:1342:ILE:HD12	1:B:1389:PHE:CZ	2.36	0.61
1:B:1272:TYR:CG	1:B:1273:PRO:HD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1234:SER:O	1:B:1238:ILE:HG13	2.01	0.60
1:A:1221:VAL:HG22	1:A:1260:ARG:HG3	1.83	0.60
1:A:1358:THR:OG1	1:A:1403:ALA:HB1	2.01	0.60
1:B:1242:LEU:HD21	1:B:1263:PHE:CD1	2.36	0.60
1:B:1108:ARG:NH1	2:B:1601:CL:CL	2.71	0.60
1:A:1226:VAL:O	1:A:1226:VAL:HG12	2.01	0.60
1:A:1278:PHE:CE2	1:A:1285:GLU:HB2	2.37	0.60
1:B:1289:ILE:HG13	1:B:1289:ILE:O	2.01	0.60
1:A:1226:VAL:HG11	1:A:1265:PHE:CE2	2.36	0.60
1:B:1289:ILE:HD11	1:B:1292:ILE:CG2	2.32	0.60
1:B:1087:LEU:HD12	1:B:1266:GLY:CA	2.32	0.59
1:A:1408:LEU:HD22	1:A:1415:LEU:HD11	1.84	0.59
1:B:1189:ILE:O	1:B:1193:SER:OG	2.20	0.59
1:A:1124:VAL:HG13	1:A:1192:GLN:HG2	1.85	0.59
1:A:1343:ARG:HH11	1:A:1343:ARG:HG3	1.68	0.59
1:B:1443:LEU:HD22	1:B:1457:TYR:HE1	1.68	0.58
1:A:1445:ASN:OD1	1:A:1447:VAL:HG13	2.02	0.58
1:A:1282:ASN:O	1:A:1284:ASN:N	2.30	0.58
1:A:1406:GLY:HA2	1:A:1409:GLU:OE1	2.03	0.58
1:A:1196:VAL:O	1:A:1196:VAL:HG12	2.04	0.58
1:A:1342:ILE:CD1	1:A:1364:LEU:HD12	2.34	0.58
1:B:1041:THR:HA	1:B:1085:VAL:HG11	1.85	0.58
1:B:1108:ARG:O	1:B:1111:ARG:HB2	2.04	0.58
1:B:1301:GLU:OE1	1:B:1441:ARG:NH2	2.37	0.58
1:A:1289:ILE:HG13	1:A:1289:ILE:O	2.03	0.58
1:A:1353:ILE:CD1	1:A:1394:ASP:HB3	2.34	0.58
1:A:1353:ILE:HD11	1:A:1394:ASP:HB3	1.86	0.58
1:A:1447:VAL:O	1:A:1448:SER:HB2	2.04	0.58
1:A:1344:THR:HB	1:A:1356:TYR:OH	2.04	0.57
1:B:1491:GLU:O	1:B:1494:GLN:HG3	2.04	0.57
1:B:1106:ILE:CD1	1:B:1177:LEU:HD22	2.32	0.57
1:B:1091:THR:HG21	1:B:1227:ALA:HB2	1.85	0.57
1:B:1408:LEU:HD12	1:B:1444:ILE:HG21	1.87	0.57
1:B:1235:GLU:OE2	1:B:1276:TYR:OH	2.20	0.57
1:B:1443:LEU:HD22	1:B:1457:TYR:CE1	2.39	0.57
1:A:1458:THR:HG22	1:A:1459:GLU:H	1.69	0.57
1:A:1156:VAL:HG12	1:A:1163:TYR:O	2.05	0.57
1:B:1052:VAL:HG22	1:B:1067:PRO:CA	2.35	0.56
1:A:1175:GLY:HA2	1:A:1221:VAL:O	2.06	0.56
1:A:1401:GLU:HB2	1:A:1456:MET:SD	2.44	0.56
1:B:1089:PHE:CD1	1:B:1089:PHE:N	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:ASP:O	1:A:1189:ILE:HG12	2.05	0.56
1:B:1124:VAL:HG22	1:B:1192:GLN:CD	2.26	0.56
1:B:1128:ILE:CD1	1:B:1193:SER:HB3	2.36	0.56
1:B:1341:ILE:HG23	1:B:1390:ILE:HD11	1.86	0.56
1:A:1399:ASP:O	1:A:1402:ALA:HB3	2.06	0.56
1:A:1232:PHE:CE2	1:A:1241:ARG:HG3	2.40	0.56
1:B:1353:ILE:HG21	1:B:1394:ASP:OD1	2.06	0.56
1:A:1091:THR:HG21	1:A:1180:VAL:O	2.06	0.56
1:A:1491:GLU:HB3	1:A:1494:GLN:NE2	2.21	0.56
1:B:1243:ARG:HA	1:B:1246:LEU:HD12	1.87	0.55
1:A:1088:GLN:HE21	1:A:1089:PHE:HE1	1.53	0.55
1:A:1194:LEU:O	1:A:1197:ILE:HG23	2.06	0.55
1:A:1257:SER:O	1:A:1257:SER:OG	2.23	0.55
1:B:1356:TYR:CZ	1:B:1360:GLU:HG3	2.41	0.55
1:B:1114:THR:O	1:B:1133:PHE:HA	2.07	0.55
1:B:1040:ARG:HH12	1:B:1084:ASP:CG	2.10	0.55
1:B:1242:LEU:HA	1:B:1245:ILE:HD12	1.88	0.55
1:A:1040:ARG:HA	1:A:1043:GLN:HB2	1.89	0.55
1:B:1052:VAL:CG2	1:B:1067:PRO:HB3	2.37	0.55
1:B:1285:GLU:OE2	1:B:1290:ARG:CD	2.55	0.55
1:A:1194:LEU:HD11	1:A:1253:LEU:HD23	1.88	0.54
1:A:1339:ARG:NH1	1:A:1339:ARG:HG2	2.21	0.54
1:A:1441:ARG:HG3	1:A:1469:PHE:HE1	1.72	0.54
1:A:1057:TYR:CE1	1:B:1040:ARG:HB3	2.43	0.54
1:B:1052:VAL:HG22	1:B:1067:PRO:HA	1.89	0.54
1:B:1102:ALA:HB1	1:B:1177:LEU:HD23	1.89	0.54
1:A:1235:GLU:O	1:A:1238:ILE:N	2.41	0.54
1:B:1089:PHE:HD1	1:B:1089:PHE:H	1.55	0.54
1:B:1425:ILE:HB	1:B:1442:ALA:HB3	1.90	0.54
1:A:1354:GLN:HB2	1:A:1395:ILE:HD11	1.90	0.54
1:A:1395:ILE:HG12	1:A:1396:SER:H	1.72	0.54
1:B:1289:ILE:CD1	1:B:1292:ILE:CG2	2.86	0.53
1:B:1194:LEU:O	1:B:1196:VAL:N	2.41	0.53
1:A:1342:ILE:CG1	1:A:1364:LEU:HD12	2.38	0.53
1:B:1310:ILE:CG2	1:B:1311:LYS:N	2.71	0.53
1:B:1354:GLN:N	1:B:1395:ILE:HD11	2.24	0.53
1:B:1395:ILE:HG22	1:B:1400:VAL:HG23	1.91	0.52
1:B:1460:VAL:HG21	1:B:1470:LYS:HD2	1.91	0.52
1:A:1049:LYS:O	1:A:1053:VAL:HG23	2.09	0.52
1:B:1406:GLY:CA	1:B:1409:GLU:HG3	2.36	0.52
1:B:1088:GLN:HG3	1:B:1089:PHE:CD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1391:ALA:HB3	1:B:1393:PHE:CZ	2.44	0.52
1:A:1058:GLY:HA2	1:B:1040:ARG:HG2	1.90	0.52
1:B:1182:HIS:HE2	1:B:1231:GLY:N	2.08	0.52
1:B:1279:ASN:HD21	1:B:1286:ASN:HD22	1.57	0.52
1:B:1439:PRO:HG2	1:B:1459:GLU:HB2	1.92	0.52
1:B:1180:VAL:HG12	1:B:1189:ILE:HD12	1.92	0.52
1:B:1225:CYS:SG	1:B:1226:VAL:N	2.83	0.52
1:A:1178:MET:HE2	1:A:1193:SER:HB2	1.90	0.52
1:B:1341:ILE:HG21	1:B:1390:ILE:HD11	1.92	0.52
1:B:1460:VAL:HG12	1:B:1461:LYS:N	2.25	0.52
1:A:1055:VAL:HG12	1:A:1061:ASN:HB3	1.92	0.52
1:A:1158:VAL:HG11	1:A:1298:PHE:HD2	1.75	0.52
1:A:1458:THR:HG22	1:A:1459:GLU:N	2.23	0.52
1:A:1395:ILE:CG1	1:A:1396:SER:H	2.22	0.51
1:B:1086:LEU:HG	1:B:1086:LEU:O	2.08	0.51
1:B:1064:ARG:O	1:B:1065:SER:OG	2.25	0.51
1:B:1106:ILE:HD12	1:B:1131:TRP:CZ3	2.45	0.51
1:B:1156:VAL:HG13	1:B:1157:SEP:N	2.25	0.51
1:B:1357:LEU:HD22	1:B:1427:ILE:HD11	1.92	0.51
1:A:1055:VAL:HG22	1:A:1056:ALA:N	2.26	0.51
1:B:1289:ILE:CD1	1:B:1292:ILE:HG22	2.40	0.51
1:B:1293:GLU:OE2	1:B:1294:PRO:HD2	2.10	0.51
1:B:1285:GLU:OE2	1:B:1290:ARG:HD2	2.11	0.51
1:B:1338:THR:HG21	1:B:1368:ILE:HG12	1.92	0.51
1:B:1180:VAL:HB	1:B:1185:ASP:CB	2.41	0.50
1:B:1124:VAL:HG23	1:B:1125:THR:OG1	2.10	0.50
1:B:1334:LYS:O	1:B:1380:SER:HA	2.11	0.50
1:B:1440:LEU:CD2	1:B:1458:THR:HG22	2.42	0.50
1:B:1489:VAL:CG1	1:B:1490:LYS:N	2.75	0.50
1:A:1045:GLU:CG	1:A:1089:PHE:HE2	2.21	0.50
1:B:1132:LYS:HA	1:B:1173:ARG:O	2.11	0.50
1:B:1220:ASN:O	1:B:1258:ILE:HA	2.11	0.50
1:B:1236:GLU:O	1:B:1240:VAL:HG12	2.12	0.50
1:B:1353:ILE:HD12	1:B:1353:ILE:H	1.75	0.50
1:A:1113:TYR:CZ	1:A:1158:VAL:HG23	2.46	0.50
1:A:1353:ILE:HD13	1:A:1395:ILE:N	2.26	0.50
1:B:1369:LEU:HD22	1:B:1418:LEU:HD12	1.94	0.50
1:B:1429:ILE:HB	1:B:1438:VAL:HG13	1.94	0.50
1:A:1240:VAL:O	1:A:1244:GLU:HG3	2.12	0.49
1:B:1194:LEU:HD11	1:B:1253:LEU:HD23	1.94	0.49
1:A:1092:HIS:ND1	1:A:1093:GLN:N	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1128:ILE:CG2	1:B:1176:ILE:HG23	2.41	0.49
1:B:1071:ILE:N	1:B:1071:ILE:HD12	2.27	0.49
1:B:1265:PHE:N	1:B:1265:PHE:CD1	2.78	0.49
1:A:1441:ARG:HG3	1:A:1469:PHE:CE1	2.48	0.49
1:B:1183:LEU:HD12	1:B:1186:VAL:HG21	1.93	0.49
1:B:1391:ALA:HB3	1:B:1393:PHE:CE2	2.47	0.49
1:A:1220:ASN:N	1:A:1257:SER:O	2.41	0.49
1:B:1481:ARG:HG3	1:B:1481:ARG:HH11	1.77	0.49
1:B:1301:GLU:CD	1:B:1441:ARG:HH22	2.16	0.49
1:A:1329:THR:HG21	1:A:1494:GLN:OE1	2.13	0.48
1:B:1074:ASP:O	1:B:1078:SER:HB2	2.13	0.48
1:A:1246:LEU:HD13	1:A:1283:TYR:HB3	1.95	0.48
1:B:1126:VAL:HG21	1:B:1189:ILE:HD13	1.94	0.48
1:B:1194:LEU:CD2	1:B:1258:ILE:HD11	2.43	0.48
1:B:1260:ARG:HB3	1:B:1279:ASN:HB3	1.95	0.48
1:B:1468:VAL:HG12	1:B:1469:PHE:N	2.27	0.48
1:B:1089:PHE:O	1:B:1092:HIS:HB3	2.14	0.48
1:B:1489:VAL:HG12	1:B:1490:LYS:N	2.28	0.48
1:A:1278:PHE:CD2	1:A:1285:GLU:HA	2.48	0.48
1:A:1283:TYR:CD1	1:A:1283:TYR:N	2.82	0.48
1:B:1174:GLU:H	1:B:1220:ASN:HD21	1.62	0.48
1:B:1260:ARG:HG3	1:B:1260:ARG:HH11	1.78	0.48
1:B:1393:PHE:O	1:B:1430:LYS:N	2.41	0.48
1:A:1364:LEU:HD13	1:A:1387:ILE:HG12	1.94	0.47
1:B:1242:LEU:HD21	1:B:1263:PHE:CE1	2.49	0.47
1:B:1258:ILE:O	1:B:1258:ILE:HG22	2.14	0.47
1:B:1102:ALA:O	1:B:1106:ILE:HG12	2.13	0.47
1:B:1272:TYR:CD1	1:B:1273:PRO:HD2	2.49	0.47
1:B:1395:ILE:CG2	1:B:1396:SER:N	2.78	0.47
1:B:1441:ARG:HG2	1:B:1469:PHE:HE1	1.79	0.47
1:B:1089:PHE:HD1	1:B:1089:PHE:N	2.11	0.47
1:B:1239:LEU:HD21	1:B:1276:TYR:CD1	2.50	0.47
1:B:1264:MET:HG2	1:B:1264:MET:O	2.14	0.47
1:B:1401:GLU:HB2	1:B:1456:MET:SD	2.55	0.47
1:A:1069:LEU:O	1:A:1073:LYS:HG2	2.15	0.47
1:A:1087:LEU:HD11	1:A:1264:MET:HE2	1.96	0.47
1:A:1408:LEU:HD22	1:A:1415:LEU:CD1	2.45	0.47
1:B:1085:VAL:O	1:B:1085:VAL:HG12	2.14	0.47
1:A:1395:ILE:HD11	1:A:1399:ASP:HB3	1.97	0.47
1:B:1081:VAL:HG12	1:B:1344:THR:O	2.14	0.47
1:A:1090:LEU:HB3	1:A:1179:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:ALA:O	1:A:1261:ILE:HA	2.14	0.46
1:A:1468:VAL:HG12	1:A:1469:PHE:O	2.16	0.46
1:A:1041:THR:HG23	1:A:1088:GLN:NE2	2.31	0.46
1:A:1448:SER:C	1:A:1450:TYR:H	2.18	0.46
1:A:1460:VAL:HG21	1:A:1470:LYS:HD3	1.97	0.46
1:B:1343:ARG:HG2	1:B:1343:ARG:NH1	2.28	0.46
1:A:1138:ALA:CB	1:A:1461:LYS:HE2	2.46	0.46
1:B:1180:VAL:HB	1:B:1185:ASP:HB3	1.98	0.46
1:B:1468:VAL:CG1	1:B:1469:PHE:N	2.79	0.46
1:A:1456:MET:HB2	1:A:1456:MET:HE3	1.69	0.46
1:B:1264:MET:C	1:B:1265:PHE:HD1	2.19	0.46
1:B:1310:ILE:HG22	1:B:1311:LYS:N	2.31	0.46
1:A:1279:ASN:O	1:A:1283:TYR:HA	2.17	0.46
1:B:1124:VAL:HG22	1:B:1192:GLN:OE1	2.15	0.46
1:B:1081:VAL:HG12	1:B:1344:THR:C	2.36	0.45
1:B:1249:ASN:OD1	1:B:1252:GLU:HB2	2.16	0.45
1:B:1279:ASN:OD1	1:B:1279:ASN:N	2.49	0.45
1:B:1308:PHE:HA	1:B:1327:SER:HA	1.98	0.45
1:B:1431:ASP:HA	1:B:1432:PRO:HD2	1.78	0.45
1:A:1454:THR:OG1	1:A:1454:THR:O	2.33	0.45
1:B:1260:ARG:HA	1:B:1278:PHE:O	2.17	0.45
1:A:1382:LEU:HA	1:A:1382:LEU:HD23	1.64	0.45
1:B:1239:LEU:HD21	1:B:1276:TYR:CE1	2.51	0.45
1:B:1333:ASP:OD1	1:B:1490:LYS:HE2	2.16	0.45
1:A:1380:SER:HB2	1:A:1383:ASN:HD21	1.81	0.45
1:A:1264:MET:HB2	1:A:1264:MET:HE2	1.65	0.45
1:A:1342:ILE:HG13	1:A:1364:LEU:HD12	1.98	0.45
1:B:1183:LEU:O	1:B:1186:VAL:HG23	2.15	0.45
1:B:1395:ILE:O	1:B:1429:ILE:HG23	2.16	0.45
1:A:1308:PHE:HB3	1:A:1325:ALA:HB1	1.97	0.45
1:A:1329:THR:CG2	1:A:1494:GLN:CG	2.92	0.45
1:B:1180:VAL:HG23	1:B:1181:ASP:N	2.30	0.45
1:B:1348:ARG:HH11	1:B:1348:ARG:HG3	1.82	0.45
1:A:1108:ARG:O	1:A:1111:ARG:NH1	2.49	0.45
1:A:1264:MET:HE3	1:A:1275:TYR:CE2	2.52	0.45
1:B:1040:ARG:CZ	1:B:1084:ASP:OD2	2.64	0.45
1:B:1180:VAL:HG12	1:B:1189:ILE:CD1	2.47	0.45
1:B:1351:ILE:CG2	1:B:1352:SER:N	2.79	0.45
1:A:1084:ASP:OD1	1:A:1085:VAL:N	2.50	0.44
1:A:1451:VAL:HG13	1:A:1452:ILE:N	2.32	0.44
1:B:1092:HIS:NE2	1:B:1094:ASP:HB3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1109:ALA:O	1:B:1295:ALA:HB3	2.17	0.44
1:A:1339:ARG:HH11	1:A:1339:ARG:CG	2.29	0.44
1:B:1124:VAL:HG13	1:B:1192:GLN:HG3	1.98	0.44
1:B:1289:ILE:HD12	1:B:1292:ILE:HG22	1.99	0.44
1:A:1041:THR:OG1	1:A:1085:VAL:HG22	2.17	0.44
1:A:1183:LEU:HD23	1:A:1232:PHE:CZ	2.52	0.44
1:B:1084:ASP:N	1:B:1084:ASP:OD1	2.48	0.44
1:A:1176:ILE:HG21	1:A:1178:MET:HE2	1.99	0.44
1:B:1107:ARG:NH2	1:B:1118:ILE:HD12	2.31	0.44
1:A:1315:THR:CG2	1:A:1371:ASN:HD22	2.30	0.44
1:A:1418:LEU:O	1:A:1419:ARG:HB2	2.18	0.44
1:A:1438:VAL:HA	1:A:1439:PRO:HD2	1.55	0.44
1:A:1224:VAL:O	1:A:1263:PHE:HA	2.16	0.44
1:B:1424:GLU:HA	1:B:1442:ALA:O	2.18	0.44
1:B:1442:ALA:C	1:B:1443:LEU:HD12	2.38	0.44
1:A:1395:ILE:HG12	1:A:1399:ASP:HB2	1.98	0.44
1:B:1221:VAL:CG1	1:B:1260:ARG:CG	2.72	0.44
1:A:1395:ILE:CG1	1:A:1399:ASP:HB2	2.48	0.44
1:B:1408:LEU:HD12	1:B:1444:ILE:HG22	1.99	0.44
1:A:1076:ILE:HG12	1:A:1107:ARG:HB3	2.00	0.43
1:A:1106:ILE:CD1	1:A:1131:TRP:CE3	3.01	0.43
1:B:1348:ARG:HD2	1:B:1351:ILE:HD12	2.00	0.43
1:A:1054:LYS:NZ	1:A:1066:GLU:O	2.49	0.43
1:A:1195:GLU:C	1:A:1197:ILE:H	2.22	0.43
1:B:1180:VAL:CG1	1:B:1189:ILE:HD12	2.48	0.43
1:A:1395:ILE:HG12	1:A:1396:SER:N	2.34	0.43
1:B:1128:ILE:HD11	1:B:1193:SER:HB3	2.01	0.43
1:B:1356:TYR:CE2	1:B:1360:GLU:HG3	2.53	0.43
1:A:1190:LEU:O	1:A:1193:SER:OG	2.36	0.43
1:B:1249:ASN:O	1:B:1251:GLN:N	2.51	0.43
1:A:1364:LEU:CD2	1:A:1368:ILE:HG13	2.49	0.43
1:A:1246:LEU:HD13	1:A:1283:TYR:CB	2.48	0.43
1:A:1094:ASP:OD1	1:A:1096:VAL:HG23	2.18	0.43
1:A:1450:TYR:CD1	1:A:1450:TYR:N	2.86	0.43
1:A:1088:GLN:HG3	1:A:1089:PHE:CE1	2.54	0.43
1:A:1168:GLN:HG3	1:A:1168:GLN:O	2.19	0.43
1:A:1333:ASP:CG	1:A:1490:LYS:HD2	2.40	0.43
1:B:1285:GLU:OE2	1:B:1290:ARG:HD3	2.18	0.43
1:B:1342:ILE:HD13	1:B:1360:GLU:HB3	2.00	0.43
1:B:1439:PRO:CG	1:B:1459:GLU:HB2	2.49	0.43
1:A:1046:HIS:NE2	1:B:1050:SER:CB	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1381:ASP:OD1	1:B:1419:ARG:NH2	2.42	0.42
1:A:1386:PHE:HD1	1:A:1424:GLU:O	2.02	0.42
1:B:1481:ARG:NH1	1:B:1481:ARG:HG3	2.35	0.42
1:A:1218:LEU:O	1:A:1259:ARG:HD2	2.20	0.42
1:B:1460:VAL:O	1:B:1467:TRP:HA	2.19	0.42
1:B:1260:ARG:HG3	1:B:1260:ARG:NH1	2.34	0.42
1:A:1057:TYR:HE1	1:B:1040:ARG:HB3	1.83	0.42
1:B:1261:ILE:HD11	1:B:1263:PHE:CZ	2.54	0.42
1:A:1055:VAL:CG2	1:A:1056:ALA:N	2.82	0.42
1:A:1105:TYR:CE1	1:A:1264:MET:HE1	2.55	0.42
1:A:1126:VAL:HG22	1:A:1127:PRO:CD	2.47	0.42
1:A:1176:ILE:HG21	1:A:1178:MET:CE	2.50	0.42
1:A:1448:SER:C	1:A:1450:TYR:N	2.73	0.42
1:B:1404:PHE:O	1:B:1407:PHE:HB2	2.20	0.42
1:A:1092:HIS:CD2	1:A:1097:VAL:HG21	2.54	0.42
1:A:1287:GLU:HB3	1:A:1312:PRO:HG3	2.02	0.42
1:B:1243:ARG:NH1	1:B:1243:ARG:HG2	2.35	0.41
1:A:1096:VAL:O	1:A:1096:VAL:HG12	2.20	0.41
1:A:1299:GLN:NE2	1:A:1390:ILE:HD13	2.35	0.41
1:B:1083:PHE:CD1	1:B:1083:PHE:N	2.86	0.41
1:B:1494:GLN:HA	1:B:1495:PRO:HD2	1.76	0.41
1:B:1132:LYS:HG2	1:B:1174:GLU:HG2	2.01	0.41
1:A:1078:SER:O	1:A:1108:ARG:NH2	2.53	0.41
1:A:1390:ILE:HG22	1:A:1390:ILE:O	2.19	0.41
1:A:1451:VAL:CG1	1:A:1452:ILE:N	2.84	0.41
1:A:1455:GLU:OE1	1:A:1457:TYR:OH	2.32	0.41
1:B:1079:ASN:ND2	1:B:1392:VAL:HB	2.35	0.41
1:A:1041:THR:HG23	1:A:1088:GLN:HE22	1.85	0.41
1:A:1094:ASP:HA	1:A:1095:PRO:HD3	1.91	0.41
1:B:1038:LYS:HE2	1:B:1038:LYS:HB3	1.91	0.41
1:B:1336:PHE:CE1	1:B:1377:THR:HA	2.55	0.41
1:A:1343:ARG:HG3	1:A:1343:ARG:NH1	2.33	0.41
1:B:1317:ASN:HB3	1:B:1320:ILE:HD12	2.02	0.41
1:B:1336:PHE:N	1:B:1383:ASN:OD1	2.49	0.41
1:A:1125:THR:HB	1:A:1126:VAL:H	1.58	0.41
1:B:1120:VAL:HG22	1:B:1129:VAL:HG13	2.03	0.41
1:B:1243:ARG:O	1:B:1247:ASP:N	2.44	0.41
1:B:1332:LEU:HD23	1:B:1332:LEU:HA	1.77	0.41
1:B:1472:LEU:HD22	1:B:1472:LEU:HA	1.82	0.41
1:B:1395:ILE:HG22	1:B:1396:SER:N	2.35	0.41
1:B:1250:LYS:HA	1:B:1253:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1349:ASP:OD1	1:B:1349:ASP:N	2.52	0.41
1:B:1356:TYR:CZ	1:B:1360:GLU:CG	3.03	0.41
1:A:1139:ALA:HB3	1:A:1140:PHE:CD1	2.56	0.41
1:B:1087:LEU:HD12	1:B:1266:GLY:HA2	2.01	0.40
1:A:1443:LEU:HD12	1:A:1443:LEU:N	2.36	0.40
1:B:1302:LEU:HD21	1:B:1323:TYR:CE2	2.56	0.40
1:A:1395:ILE:CG1	1:A:1396:SER:N	2.83	0.40
1:B:1105:TYR:CZ	1:B:1264:MET:HE1	2.56	0.40
1:B:1289:ILE:HD11	1:B:1297:ALA:HB2	2.03	0.40
1:B:1348:ARG:NH1	1:B:1348:ARG:HG3	2.36	0.40
1:B:1485:THR:HA	1:B:1486:PRO:HD3	1.85	0.40
1:B:1036:SER:HB3	1:B:1040:ARG:HG3	2.04	0.40
1:A:1233:GLU:OE1	1:A:1233:GLU:HA	2.22	0.40
1:A:1242:LEU:O	1:A:1246:LEU:HG	2.22	0.40
1:A:1353:ILE:HG21	1:A:1393:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	417/474 (88%)	371 (89%)	40 (10%)	6 (1%)	14	44
1	B	381/474 (80%)	350 (92%)	29 (8%)	2 (0%)	34	71
All	All	798/948 (84%)	721 (90%)	69 (9%)	8 (1%)	19	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1449	GLY
1	B	1195	GLU
1	B	1475	PRO

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Mol	Chain	Res	Type
1	A	1378	SER
1	A	1331	PRO
1	A	1196	VAL
1	A	1475	PRO
1	A	1395	ILE

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	380/421 (90%)	340 (90%)	40 (10%)	8 25
1	B	359/421 (85%)	321 (89%)	38 (11%)	8 25
All	All	739/842 (88%)	661 (89%)	78 (11%)	8 25

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1036	SER
1	A	1042	GLU
1	A	1061	ASN
1	A	1076	ILE
1	A	1098	THR
1	A	1122	GLU
1	A	1124	VAL
1	A	1125	THR
1	A	1137	SER
1	A	1141	SER
1	A	1142	THR
1	A	1156	VAL
1	A	1163	TYR
1	A	1172	LEU
1	A	1180	VAL
1	A	1193	SER
1	A	1229	THR
1	A	1237	GLU

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Mol	Chain	Res	Type
1	A	1238	ILE
1	A	1239	LEU
1	A	1241	ARG
1	A	1243	ARG
1	A	1257	SER
1	A	1264	MET
1	A	1292	ILE
1	A	1310	ILE
1	A	1335	ARG
1	A	1339	ARG
1	A	1344	THR
1	A	1350	ASP
1	A	1360	GLU
1	A	1364	LEU
1	A	1365	MET
1	A	1380	SER
1	A	1448	SER
1	A	1453	LYS
1	A	1456	MET
1	A	1464	LYS
1	A	1478	MET
1	A	1480	LEU
1	B	1081	VAL
1	B	1089	PHE
1	B	1092	HIS
1	B	1103	GLN
1	B	1111	ARG
1	B	1115	ILE
1	B	1119	ARG
1	B	1125	THR
1	B	1130	GLU
1	B	1134	GLN
1	B	1190	LEU
1	B	1193	SER
1	B	1221	VAL
1	B	1236	GLU
1	B	1237	GLU
1	B	1242	LEU
1	B	1243	ARG
1	B	1251	GLN
1	B	1279	ASN
1	B	1290	ARG

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Mol	Chain	Res	Type
1	B	1306	SER
1	B	1327	SER
1	B	1329	THR
1	B	1330	SER
1	B	1343	ARG
1	B	1353	ILE
1	B	1367	ASP
1	B	1370	ASP
1	B	1380	SER
1	B	1399	ASP
1	B	1409	GLU
1	B	1410	ARG
1	B	1427	ILE
1	B	1453	LYS
1	B	1454	THR
1	B	1456	MET
1	B	1467	TRP
1	B	1472	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1061	ASN
1	A	1088	GLN
1	A	1121	HIS
1	A	1192	GLN
1	A	1371	ASN
1	B	1134	GLN
1	B	1220	ASN
1	B	1286	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)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	A	1157	1	7,9,10	1.41	1 (14%)	8,12,14	1.27	0
1	SEP	B	1157	1	7,9,10	1.70	3 (42%)	8,12,14	1.02	0

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
1	SEP	A	1157	1	-	0/5/8/10	0/0/0/0
1	SEP	B	1157	1	-	0/5/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1157	SEP	P-O2P	2.05	1.61	1.54
1	B	1157	SEP	P-O3P	2.42	1.63	1.54
1	B	1157	SEP	P-O1P	2.71	1.59	1.50
1	A	1157	SEP	P-O1P	3.02	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1157	SEP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	425/474 (89%)	0.16	9 (2%)	67	62	39, 77, 116, 143	0
1	B	397/474 (83%)	0.25	10 (2%)	61	55	59, 95, 126, 148	0
All	All	822/948 (86%)	0.21	19 (2%)	64	59	39, 86, 122, 148	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1054	LYS	5.0
1	A	1055	VAL	3.3
1	A	1072	LEU	3.2
1	B	1053	VAL	3.2
1	B	1054	LYS	3.0
1	A	1071	ILE	2.9
1	B	1161	LEU	2.9
1	B	1451	VAL	2.8
1	A	1066	GLU	2.8
1	B	1048	LEU	2.8
1	B	1055	VAL	2.6
1	A	1062	PRO	2.5
1	B	1196	VAL	2.3
1	B	1071	ILE	2.2
1	B	1479	HIS	2.1
1	A	1064	ARG	2.1
1	B	1452	ILE	2.1
1	A	1056	ALA	2.0
1	A	1063	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	SEP	B	1157	10/11	0.93	0.18	-	83,100,104,105	0
1	SEP	A	1157	10/11	0.97	0.21	-	55,65,71,75	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	B	1601	1/1	0.98	0.12	-2.07	76,76,76,76	0
2	CL	A	1601	1/1	0.94	0.09	-	71,71,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.