Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 12:21 PM JST

PDB ID	:	8WY1
Title	:	The structure of cyclization domain in cyclic beta-1,2-glucan synthase from Thermoanaerobacter italicus
Authors	:	Tanaka, N.; Saito, R.; Kobayashi, K.; Nakai, H.; Kamo, S.; Kuramochi, K.; Taguchi, H.; Nakajima, M.; Masaike, T.
Deposited on	:	2023-10-30
Resolution	:	3.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

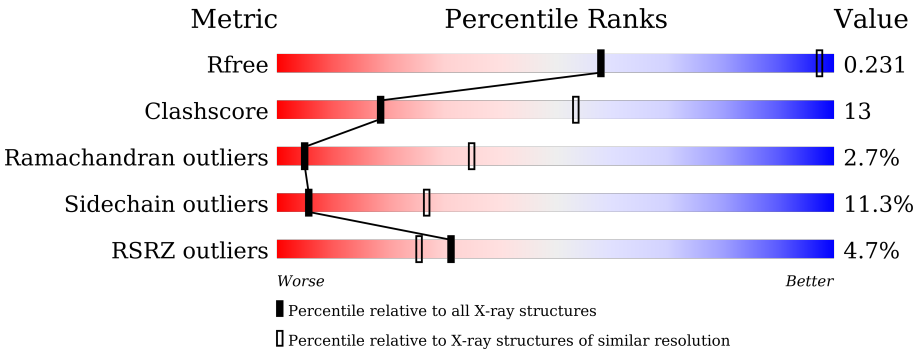
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.90 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}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	596	% 62% 32%
1	B	596	3% 60% 32%
1	C	596	5% 60% 31% 6%
1	D	596	9% 58% 33% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 18842 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 Glycosyltransferase 36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	574	Total	C	N	O	S	0	0	0
			4715	3047	772	881	15			
1	B	573	Total	C	N	O	S	0	0	0
			4706	3042	771	878	15			
1	C	573	Total	C	N	O	S	0	0	0
			4706	3042	771	878	15			
1	D	574	Total	C	N	O	S	0	0	0
			4715	3047	772	881	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1004	MET	-	initiating methionine	UNP D3T4C1
A	1592	LEU	-	expression tag	UNP D3T4C1
A	1593	GLU	-	expression tag	UNP D3T4C1
A	1594	HIS	-	expression tag	UNP D3T4C1
A	1595	HIS	-	expression tag	UNP D3T4C1
A	1596	HIS	-	expression tag	UNP D3T4C1
A	1597	HIS	-	expression tag	UNP D3T4C1
A	1598	HIS	-	expression tag	UNP D3T4C1
A	1599	HIS	-	expression tag	UNP D3T4C1
B	1004	MET	-	initiating methionine	UNP D3T4C1
B	1592	LEU	-	expression tag	UNP D3T4C1
B	1593	GLU	-	expression tag	UNP D3T4C1
B	1594	HIS	-	expression tag	UNP D3T4C1
B	1595	HIS	-	expression tag	UNP D3T4C1
B	1596	HIS	-	expression tag	UNP D3T4C1
B	1597	HIS	-	expression tag	UNP D3T4C1
B	1598	HIS	-	expression tag	UNP D3T4C1
B	1599	HIS	-	expression tag	UNP D3T4C1
C	1004	MET	-	initiating methionine	UNP D3T4C1
C	1592	LEU	-	expression tag	UNP D3T4C1
C	1593	GLU	-	expression tag	UNP D3T4C1

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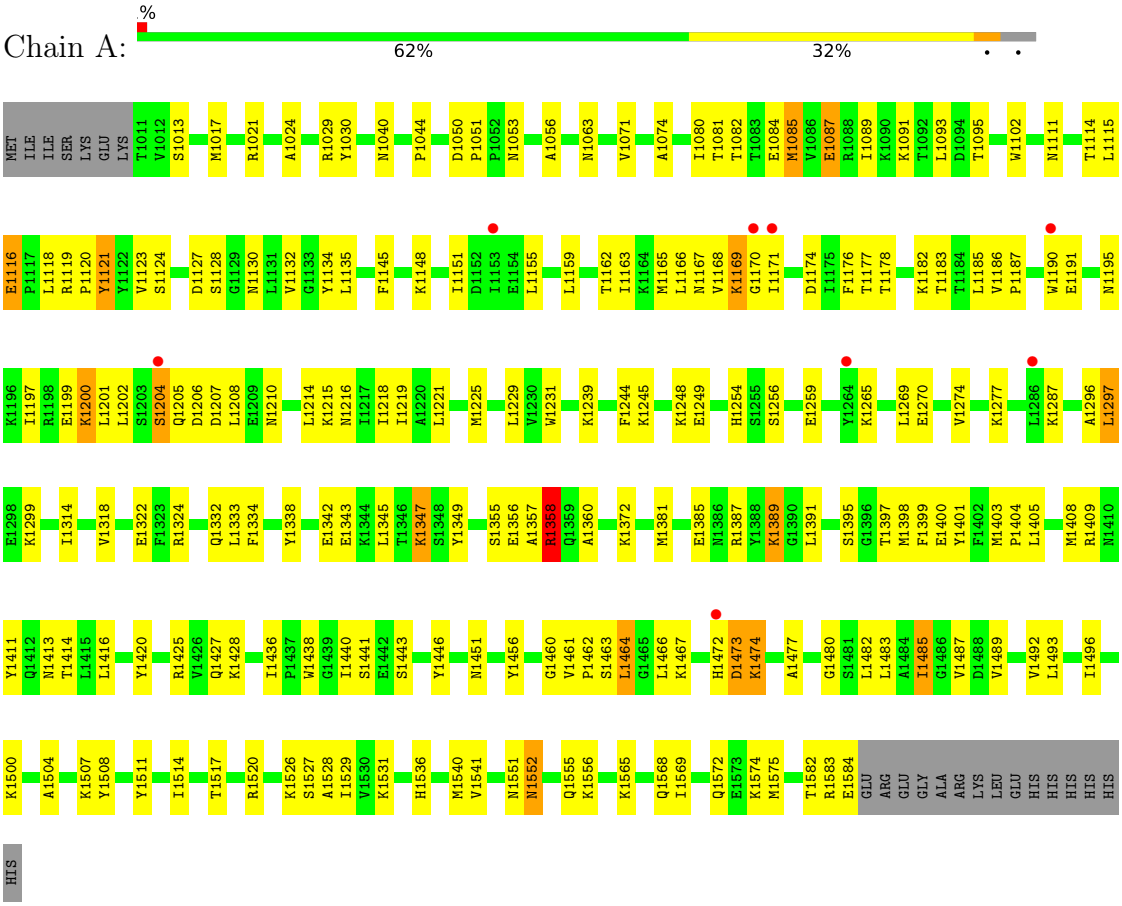
Chain	Residue	Modelled	Actual	Comment	Reference
C	1594	HIS	-	expression tag	UNP D3T4C1
C	1595	HIS	-	expression tag	UNP D3T4C1
C	1596	HIS	-	expression tag	UNP D3T4C1
C	1597	HIS	-	expression tag	UNP D3T4C1
C	1598	HIS	-	expression tag	UNP D3T4C1
C	1599	HIS	-	expression tag	UNP D3T4C1
D	1004	MET	-	initiating methionine	UNP D3T4C1
D	1592	LEU	-	expression tag	UNP D3T4C1
D	1593	GLU	-	expression tag	UNP D3T4C1
D	1594	HIS	-	expression tag	UNP D3T4C1
D	1595	HIS	-	expression tag	UNP D3T4C1
D	1596	HIS	-	expression tag	UNP D3T4C1
D	1597	HIS	-	expression tag	UNP D3T4C1
D	1598	HIS	-	expression tag	UNP D3T4C1
D	1599	HIS	-	expression tag	UNP D3T4C1

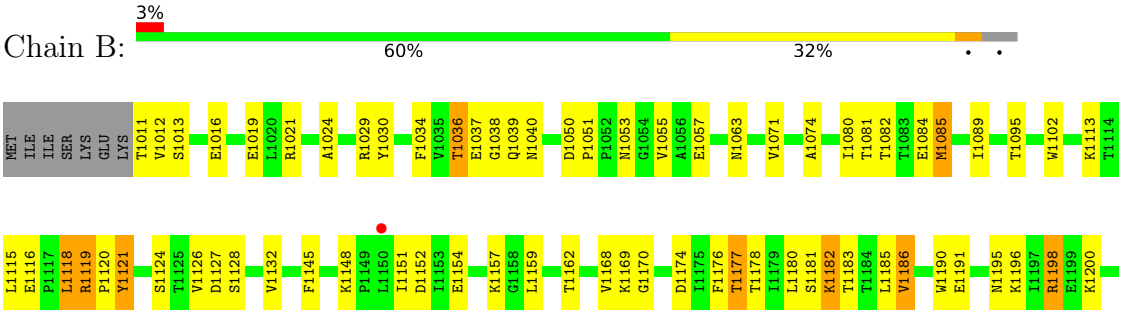
3 Residue-property plots (i)

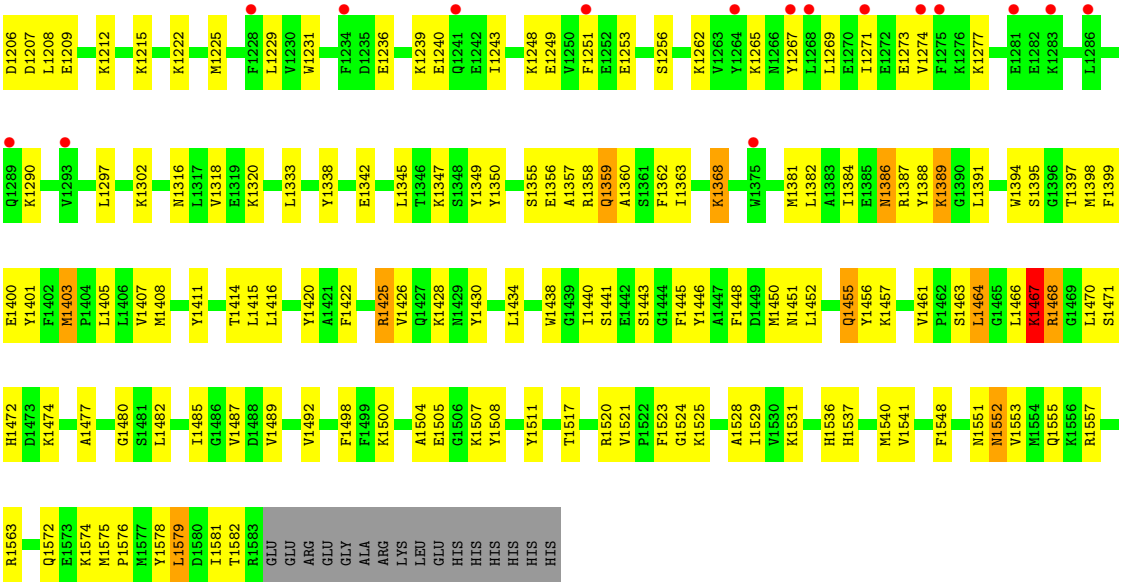
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycosyltransferase 36



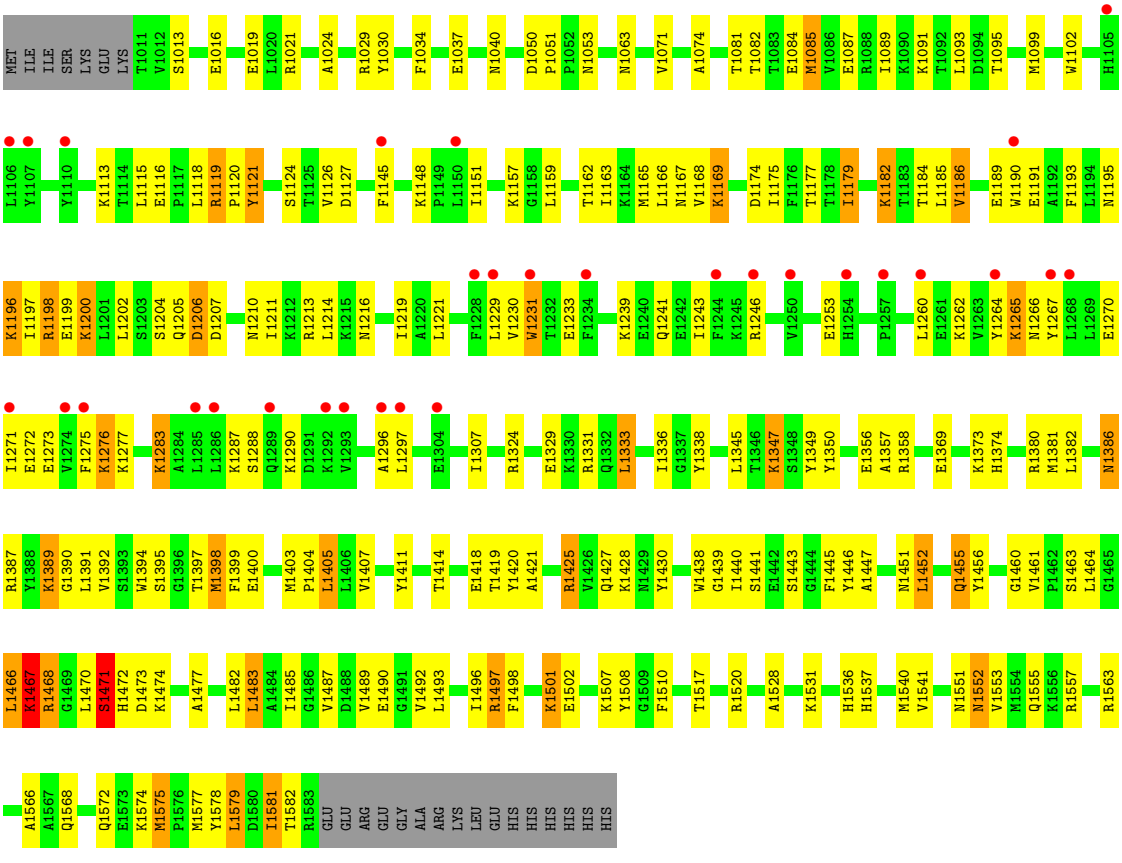
• Molecule 1: Glycosyltransferase 36





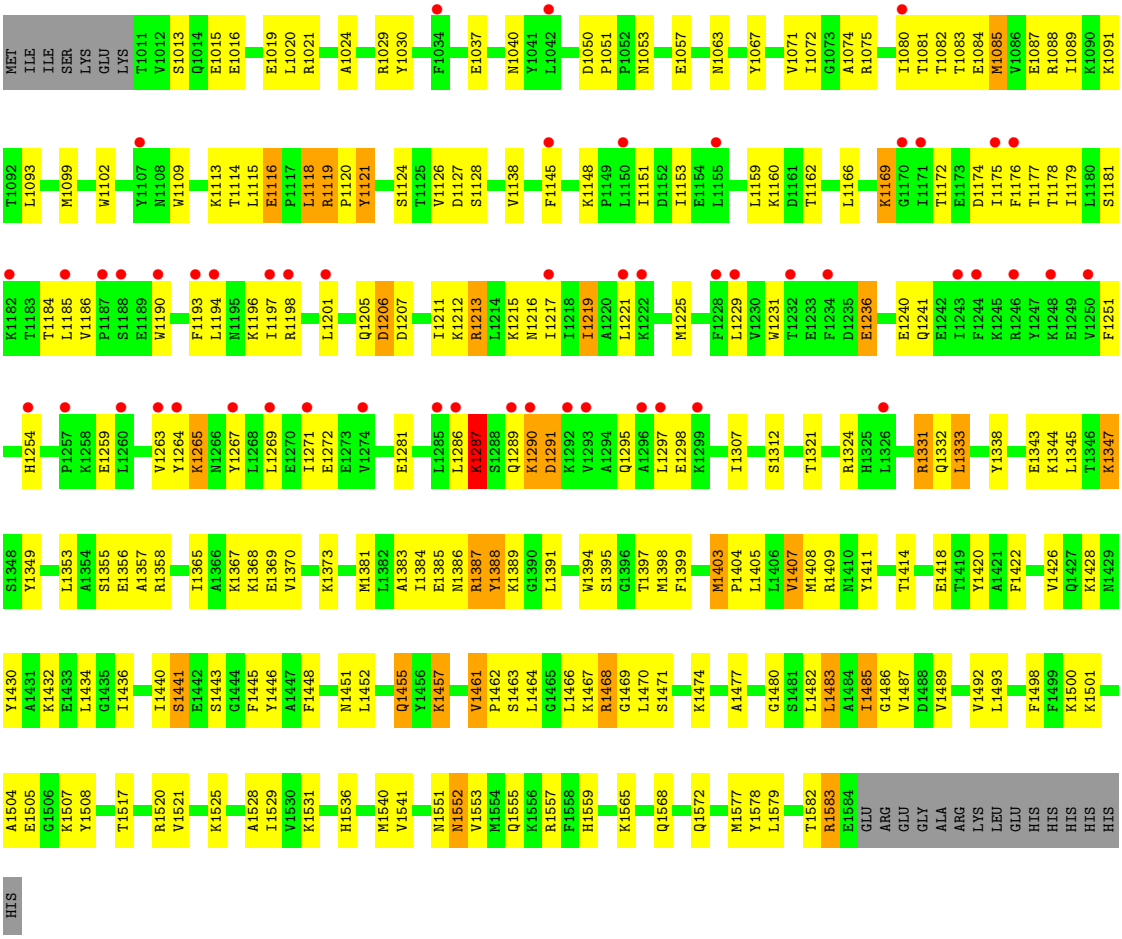
• Molecule 1: Glycosyltransferase 36

Chain C:



• Molecule 1: Glycosyltransferase 36

Chain D:


MET ILE ILE SER LYS GLU LYS T1011 Y1012 S1013 Q1014 E1015 E1016 E1019 L1020 R1021 A1024 R1029 Y1030 F1034 E1037 N1040 Y1041 L1042 D1050 P1051 P1052 N1053 E1057 N1063 Y1067 V1071 I1072 G1073 A1074 R1075 T1080 T1081 T1082 T1083 E1084 M1085 V1086 E1087 R1088 I1089 K1090 K1091
T1092 L1093 M1099 W1102 Y1107 N1108 W1109 K1113 T1114 L1115 E1116 P1117 L1118 R1119 P1120 Y1121 S1124 T1125 V1126 D1127 S1128 V1138 F1145 K1148 P1149 L1150 I1151 D1152 I1153 E1154 L1155 L1159 K1160 D1161 T1162 L1166 K1169 G1170 I1171 T1172 E1173 D1174 I1175 F1176 T1177 T1178 I1179 L1180 S1181
K1182 T1183 T1184 L1185 V1186 P1187 S1188 E1189 W1190 F1193 L1194 N1195 K1196 I1197 R1198 L1201 Q1205 D1206 D1207 I1211 K1212 R1213 L1214 K1215 N1216 I1217 I1218 I1219 A1220 L1221 K1222 M1225 F1228 L1229 V1230 W1231 T1232 E1233 F1234 D1235 E1236 E1240 Q1241 E1242 T1243 F1244 K1245 R1246 Y1247 K1248 E1249 V1250 F1251
H1254 P1257 K1258 E1259 L1260 V1263 Y1264 K1265 N1266 Y1267 L1268 L1269 E1270 I1271 E1272 E1273 V1274 E1281 L1285 L1286 K1287 S1288 Q1289 K1290 D1291 K1292 V1293 A1294 Q1295 A1296 L1297 E1298 K1299 I1307 S1312 T1321 R1324 H1325 L1326 R1331 Q1332 L1333 Y1338 E1343 K1344 L1345 T1346 K1347
S1348 Y1349 L1353 A1354 S1355 E1356 A1357 R1358 I1365 A1366 K1367 K1368 E1369 V1370 K1373 M1381 L1382 A1383 I1384 E1385 N1386 R1387 Y1388 K1389 G1390 L1391 W1394 S1395 G1396 T1397 M1398 F1399 M1403 P1404 L1405 L1406 V1407 M1408 R1409 N1410 Y1411 T1414 E1418 T1419 Y1420 A1421 F1422 V1426 Q1427 K1428 N1429
Y1430 A1431 K1432 E1433 L1434 G1435 I1436 I1440 S1441 E1442 S1443 G1444 F1445 Y1446 A1447 F1448 N1451 L1452 Q1455 Y1456 K1457 V1461 P1462 S1463 L1464 G1465 L1466 K1467 R1468 G1469 L1470 S1471 K1474 A1477 G1480 S1481 L1482 L1483 A1484 I1485 G1486 V1487 D1488 V1489 V1492 L1493 F1498 F1499 K1500 K1501
A1504 E1505 G1506 K1507 Y1508 T1517 R1520 V1521 K1525 A1528 I1529 V1530 K1531 H1536 M1540 V1541 N1551 N1552 V1553 M1554 Q1555 K1556 R1557 F1588 H1559 K1565 Q1568 Q1572 M1577 Y1578 L1579 T1582 R1583 E1584 GLU ARG GLU GLY ALA ARG LYS LEU GLU HIS HIS HIS HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	172.72Å 172.72Å 395.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.60 – 3.90 89.60 – 3.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (89.60-3.90) 100.0 (89.60-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 3.89Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.198 , 0.232 0.204 , 0.231	Depositor DCC
R_{free} test set	2738 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	104.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 104.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18842	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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	0.69	0/4814	0.90	1/6485 (0.0%)
1	B	0.70	0/4805	0.91	0/6473
1	C	0.70	0/4805	0.90	1/6473 (0.0%)
1	D	0.69	0/4814	0.90	0/6485
All	All	0.70	0/19238	0.90	2/25916 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1398	MET	CA-CB-CG	-6.50	102.25	113.30
1	A	1358	ARG	NE-CZ-NH1	-6.21	117.19	120.30

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	4715	0	4756	104	0
1	B	4706	0	4750	143	0
1	C	4706	0	4750	153	0
1	D	4715	0	4756	119	0
All	All	18842	0	19012	499	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 13.

All (499) 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:1036:THR:HG23	1:B:1039:GLN:HG2	1.40	1.00
1:C:1050:ASP:HB3	1:C:1051:PRO:HD3	1.51	0.93
1:B:1387:ARG:HB3	1:C:1387:ARG:HB3	1.52	0.89
1:A:1050:ASP:HB3	1:A:1051:PRO:HD3	1.59	0.83
1:B:1395:SER:OG	1:B:1400:GLU:OE2	1.99	0.78
1:B:1050:ASP:HB3	1:B:1051:PRO:HD3	1.65	0.77
1:B:1151:ILE:HD11	1:B:1225:MET:HG3	1.65	0.77
1:D:1213:ARG:HG3	1:D:1217:ILE:HD12	1.68	0.74
1:D:1050:ASP:HB3	1:D:1051:PRO:HD3	1.70	0.73
1:C:1169:LYS:HG2	1:C:1204:SER:HB2	1.69	0.72
1:B:1579:LEU:HD21	1:C:1581:ILE:HD13	1.72	0.72
1:C:1394:TRP:HD1	1:C:1467:LYS:HG2	1.55	0.72
1:B:1196:LYS:HE3	1:B:1200:LYS:HD3	1.71	0.71
1:B:1461:VAL:HB	1:B:1464:LEU:HD12	1.73	0.70
1:B:1063:ASN:OD1	1:B:1536:HIS:HB3	1.90	0.70
1:C:1051:PRO:HB3	1:C:1452:LEU:HD12	1.74	0.70
1:B:1581:ILE:HD11	1:C:1382:LEU:HG	1.72	0.70
1:B:1119:ARG:HB3	1:B:1120:PRO:HD3	1.73	0.69
1:C:1267:TYR:O	1:C:1271:ILE:HG13	1.91	0.69
1:B:1382:LEU:HG	1:C:1581:ILE:HD11	1.75	0.69
1:A:1461:VAL:HB	1:A:1464:LEU:HD12	1.76	0.68
1:D:1430:TYR:O	1:D:1434:LEU:HG	1.94	0.67
1:D:1461:VAL:HG13	1:D:1464:LEU:HD12	1.77	0.67
1:D:1559:HIS:O	1:D:1565:LYS:HD3	1.95	0.66
1:A:1063:ASN:OD1	1:A:1536:HIS:HB3	1.96	0.66
1:C:1394:TRP:CD1	1:C:1467:LYS:HG2	2.31	0.66
1:C:1231:TRP:HH2	1:C:1260:LEU:HD22	1.60	0.65
1:D:1241:GLN:OE1	1:D:1286:LEU:HG	1.94	0.65
1:D:1063:ASN:OD1	1:D:1536:HIS:HB3	1.96	0.65
1:C:1470:LEU:HD13	1:D:1470:LEU:HB3	1.77	0.65
1:C:1151:ILE:HG13	1:C:1229:LEU:HD11	1.79	0.64
1:D:1500:LYS:HG2	1:D:1505:GLU:HB2	1.80	0.64
1:B:1578:TYR:HA	1:C:1382:LEU:O	1.98	0.64
1:A:1395:SER:OG	1:A:1400:GLU:OE2	2.11	0.64
1:D:1462:PRO:HG3	1:D:1470:LEU:O	1.98	0.63
1:C:1204:SER:OG	1:C:1206:ASP:OD1	2.17	0.63
1:B:1398:MET:HE2	1:B:1480:GLY:O	1.98	0.63
1:C:1536:HIS:CD2	1:C:1537:HIS:CD2	2.87	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1398:MET:HE2	1:A:1480:GLY:O	1.99	0.63
1:C:1082:THR:HG23	1:C:1145:PHE:HB3	1.81	0.62
1:D:1166:LEU:HD11	1:D:1213:ARG:HG2	1.82	0.62
1:C:1063:ASN:OD1	1:C:1536:HIS:HB3	1.99	0.62
1:A:1050:ASP:HB2	1:A:1531:LYS:HB2	1.82	0.62
1:D:1265:LYS:HE3	1:D:1297:LEU:HD21	1.80	0.62
1:D:1398:MET:HE2	1:D:1480:GLY:O	1.98	0.62
1:C:1050:ASP:HB3	1:C:1051:PRO:CD	2.28	0.61
1:B:1536:HIS:CD2	1:B:1537:HIS:CD2	2.88	0.61
1:B:1394:TRP:O	1:B:1466:LEU:O	2.18	0.60
1:C:1231:TRP:CH2	1:C:1260:LEU:HD22	2.35	0.60
1:D:1050:ASP:HB2	1:D:1531:LYS:HG3	1.83	0.60
1:D:1446:TYR:CD1	1:D:1528:ALA:HB1	2.37	0.59
1:D:1216:ASN:HA	1:D:1219:ILE:HB	1.84	0.59
1:B:1576:PRO:HG2	1:C:1581:ILE:HD12	1.83	0.59
1:D:1485:ILE:HA	1:D:1492:VAL:HG21	1.85	0.59
1:D:1201:LEU:HD22	1:D:1211:ILE:HG23	1.83	0.59
1:C:1199:GLU:HA	1:C:1202:LEU:HD12	1.84	0.59
1:C:1126:VAL:HG22	1:C:1357:ALA:HB2	1.83	0.59
1:A:1082:THR:HG23	1:A:1145:PHE:HB3	1.83	0.59
1:B:1265:LYS:HE3	1:B:1297:LEU:HD21	1.84	0.58
1:C:1446:TYR:CD1	1:C:1528:ALA:HB1	2.38	0.58
1:A:1358:ARG:NH1	1:A:1401:TYR:O	2.36	0.58
1:B:1582:THR:CG2	1:C:1380:ARG:H	2.16	0.58
1:D:1267:TYR:O	1:D:1271:ILE:HG13	2.03	0.58
1:C:1394:TRP:O	1:C:1467:LYS:HG3	2.03	0.58
1:D:1385:GLU:HB3	1:D:1422:PHE:HE1	1.68	0.58
1:A:1114:THR:OG1	1:A:1116:GLU:HB2	2.02	0.58
1:D:1082:THR:HG23	1:D:1145:PHE:HB3	1.86	0.58
1:B:1119:ARG:O	1:B:1121:TYR:N	2.36	0.58
1:C:1460:GLY:N	1:C:1468:ARG:HH21	2.02	0.58
1:B:1582:THR:HG23	1:C:1380:ARG:H	1.68	0.58
1:A:1472:HIS:O	1:A:1473:ASP:C	2.42	0.58
1:C:1411:TYR:HB2	1:C:1414:THR:HG21	1.86	0.57
1:C:1440:ILE:HD12	1:C:1440:ILE:H	1.69	0.57
1:A:1119:ARG:O	1:A:1121:TYR:N	2.37	0.57
1:C:1468:ARG:HD2	1:C:1471:SER:HB2	1.85	0.57
1:C:1485:ILE:HA	1:C:1492:VAL:HG21	1.85	0.57
1:D:1194:LEU:O	1:D:1198:ARG:HG2	2.04	0.57
1:B:1198:ARG:HD2	1:B:1215:LYS:HE3	1.85	0.57
1:D:1194:LEU:HD21	1:D:1221:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1482:LEU:HD13	1:A:1541:VAL:HG13	1.86	0.57
1:B:1082:THR:HG23	1:B:1145:PHE:HB3	1.87	0.57
1:B:1145:PHE:HA	1:B:1148:LYS:HB2	1.86	0.56
1:B:1355:SER:O	1:B:1358:ARG:HG3	2.04	0.56
1:C:1461:VAL:HB	1:C:1464:LEU:HD12	1.87	0.56
1:C:1119:ARG:O	1:C:1121:TYR:N	2.38	0.56
1:A:1187:PRO:O	1:A:1225:MET:HE1	2.06	0.56
1:A:1440:ILE:H	1:A:1440:ILE:HD12	1.70	0.56
1:A:1485:ILE:HA	1:A:1492:VAL:HG21	1.88	0.56
1:C:1145:PHE:HA	1:C:1148:LYS:HB2	1.88	0.56
1:A:1381:MET:O	1:A:1391:LEU:HA	2.06	0.56
1:C:1421:ALA:O	1:C:1425:ARG:HD2	2.05	0.56
1:C:1050:ASP:HB2	1:C:1531:LYS:HB2	1.88	0.56
1:A:1244:PHE:O	1:A:1248:LYS:HG3	2.06	0.55
1:D:1428:LYS:O	1:D:1432:LYS:HG3	2.05	0.55
1:A:1443:SER:HB3	1:A:1477:ALA:HB2	1.88	0.55
1:D:1353:LEU:O	1:D:1358:ARG:HD3	2.06	0.55
1:A:1151:ILE:CG1	1:A:1229:LEU:HD11	2.36	0.55
1:C:1186:VAL:HG22	1:C:1189:GLU:HG3	1.87	0.55
1:B:1456:TYR:O	1:B:1457:LYS:HG2	2.07	0.55
1:D:1445:PHE:CE1	1:D:1457:LYS:HG2	2.42	0.55
1:D:1387:ARG:HG2	1:D:1388:TYR:H	1.72	0.55
1:D:1448:PHE:HB3	1:D:1452:LEU:HA	1.89	0.55
1:A:1496:ILE:O	1:A:1500:LYS:HG2	2.07	0.55
1:C:1102:TRP:CZ2	1:C:1338:TYR:CD2	2.95	0.55
1:B:1124:SER:HB3	1:B:1127:ASP:HB2	1.89	0.55
1:A:1151:ILE:HG13	1:A:1229:LEU:HD11	1.87	0.54
1:B:1405:LEU:HD21	1:B:1420:TYR:CZ	2.41	0.54
1:A:1507:LYS:HD3	1:A:1508:TYR:CE2	2.43	0.54
1:C:1166:LEU:HD11	1:C:1213:ARG:HG2	1.90	0.54
1:C:1196:LYS:O	1:C:1200:LYS:HG3	2.08	0.54
1:A:1229:LEU:HD22	1:A:1231:TRP:CH2	2.42	0.54
1:A:1414:THR:HG21	1:A:1572:GLN:HA	1.89	0.54
1:D:1194:LEU:HD11	1:D:1221:LEU:HB3	1.88	0.54
1:B:1267:TYR:O	1:B:1271:ILE:HG13	2.07	0.54
1:A:1416:LEU:HB3	1:A:1420:TYR:CE2	2.44	0.53
1:D:1016:GLU:O	1:D:1019:GLU:HB3	2.08	0.53
1:D:1271:ILE:HB	1:D:1290:LYS:HE3	1.89	0.53
1:C:1168:VAL:HB	1:C:1210:ASN:HD21	1.74	0.53
1:D:1124:SER:HB3	1:D:1127:ASP:HB2	1.90	0.53
1:B:1440:ILE:HD12	1:B:1440:ILE:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1524:GLY:O	1:B:1525:LYS:HE3	2.08	0.53
1:C:1231:TRP:CZ3	1:C:1264:TYR:CE1	2.97	0.53
1:D:1145:PHE:HA	1:D:1148:LYS:HB2	1.90	0.53
1:C:1536:HIS:HD2	1:C:1537:HIS:CD2	2.27	0.53
1:D:1440:ILE:HD12	1:D:1440:ILE:H	1.73	0.53
1:B:1466:LEU:O	1:B:1467:LYS:HB3	2.09	0.53
1:D:1254:HIS:HB3	1:D:1259:GLU:HB3	1.91	0.53
1:A:1265:LYS:O	1:A:1269:LEU:HG	2.09	0.52
1:C:1496:ILE:HG23	1:C:1510:PHE:HZ	1.74	0.52
1:D:1443:SER:HB3	1:D:1477:ALA:HB2	1.90	0.52
1:B:1185:LEU:HD21	1:B:1190:TRP:CD2	2.44	0.52
1:D:1482:LEU:HD13	1:D:1541:VAL:HG13	1.90	0.52
1:B:1446:TYR:CD1	1:B:1528:ALA:HB1	2.44	0.52
1:B:1507:LYS:HD3	1:B:1508:TYR:CE2	2.45	0.52
1:C:1483:LEU:HD11	1:C:1540:MET:SD	2.50	0.52
1:B:1229:LEU:HD22	1:B:1231:TRP:CH2	2.45	0.52
1:C:1443:SER:HB3	1:C:1477:ALA:HB2	1.92	0.52
1:C:1445:PHE:CZ	1:C:1455:GLN:HB2	2.44	0.52
1:D:1489:VAL:O	1:D:1493:LEU:HG	2.09	0.52
1:A:1124:SER:HB3	1:A:1127:ASP:HB2	1.92	0.52
1:A:1489:VAL:O	1:A:1493:LEU:HG	2.09	0.52
1:B:1578:TYR:HB3	1:C:1381:MET:CE	2.40	0.52
1:A:1446:TYR:CD1	1:A:1528:ALA:HB1	2.44	0.52
1:B:1430:TYR:O	1:B:1434:LEU:HG	2.09	0.52
1:D:1075:ARG:HH21	1:D:1082:THR:HG1	1.58	0.52
1:D:1483:LEU:HD11	1:D:1540:MET:SD	2.50	0.52
1:C:1507:LYS:HD3	1:C:1508:TYR:CE2	2.44	0.51
1:A:1395:SER:O	1:A:1460:GLY:HA3	2.11	0.51
1:C:1119:ARG:HB3	1:C:1120:PRO:HD3	1.92	0.51
1:D:1365:ILE:HG12	1:D:1370:VAL:HG23	1.92	0.51
1:A:1087:GLU:HG3	1:A:1091:LYS:HD2	1.91	0.51
1:B:1358:ARG:NH1	1:B:1401:TYR:O	2.44	0.51
1:C:1231:TRP:CH2	1:C:1264:TYR:HE1	2.28	0.51
1:B:1038:GLY:O	1:B:1113:LYS:HD2	2.10	0.51
1:B:1578:TYR:HB3	1:C:1381:MET:HE3	1.92	0.51
1:A:1403:MET:HG3	1:A:1540:MET:CE	2.41	0.51
1:C:1016:GLU:O	1:C:1019:GLU:HB3	2.11	0.51
1:B:1384:ILE:HD11	1:C:1579:LEU:HD21	1.93	0.51
1:A:1254:HIS:HB3	1:A:1259:GLU:HB3	1.93	0.51
1:D:1461:VAL:CG1	1:D:1464:LEU:HD12	2.41	0.51
1:B:1553:VAL:HG22	1:B:1557:ARG:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1392:VAL:CG2	1:C:1466:LEU:HG	2.41	0.50
1:D:1414:THR:HG21	1:D:1572:GLN:HA	1.94	0.50
1:A:1270:GLU:O	1:A:1274:VAL:HG23	2.11	0.50
1:B:1011:THR:HG22	1:B:1012:VAL:H	1.76	0.50
1:A:1050:ASP:HB2	1:A:1531:LYS:CB	2.41	0.50
1:D:1507:LYS:HD3	1:D:1508:TYR:CZ	2.46	0.50
1:A:1089:ILE:HG22	1:A:1093:LEU:HD12	1.93	0.50
1:A:1414:THR:CG2	1:A:1572:GLN:HA	2.41	0.50
1:C:1398:MET:SD	1:C:1439:GLY:HA2	2.51	0.50
1:B:1050:ASP:CB	1:B:1051:PRO:HD3	2.40	0.50
1:B:1536:HIS:HD2	1:B:1537:HIS:CD2	2.30	0.50
1:D:1446:TYR:CG	1:D:1528:ALA:HB1	2.47	0.50
1:A:1081:THR:OG1	1:A:1084:GLU:HB2	2.12	0.50
1:B:1384:ILE:HD11	1:C:1579:LEU:HD11	1.93	0.50
1:B:1415:LEU:HA	1:B:1575:MET:HG2	1.94	0.50
1:D:1231:TRP:CE3	1:D:1251:PHE:CD1	2.99	0.50
1:A:1185:LEU:HD21	1:A:1190:TRP:CD2	2.47	0.50
1:C:1163:ILE:HD11	1:C:1214:LEU:HD11	1.94	0.50
1:C:1553:VAL:HG22	1:C:1557:ARG:HD2	1.93	0.50
1:A:1191:GLU:O	1:A:1195:ASN:ND2	2.45	0.49
1:C:1231:TRP:HZ3	1:C:1264:TYR:CE1	2.30	0.49
1:A:1225:MET:HG3	1:A:1229:LEU:HD12	1.94	0.49
1:A:1347:LYS:O	1:A:1349:TYR:CE1	2.65	0.49
1:B:1102:TRP:CZ2	1:B:1338:TYR:CD2	3.00	0.49
1:B:1466:LEU:O	1:B:1467:LYS:HD2	2.12	0.49
1:C:1428:LYS:HG2	1:C:1438:TRP:CG	2.47	0.49
1:C:1470:LEU:O	1:C:1472:HIS:N	2.45	0.49
1:A:1296:ALA:HA	1:A:1299:LYS:HD3	1.93	0.49
1:B:1414:THR:CG2	1:B:1572:GLN:HA	2.42	0.49
1:D:1179:ILE:HD12	1:D:1179:ILE:H	1.76	0.49
1:D:1565:LYS:HE2	1:D:1568:GLN:HE22	1.75	0.49
1:B:1050:ASP:HB3	1:B:1051:PRO:CD	2.38	0.49
1:B:1382:LEU:O	1:C:1578:TYR:HA	2.13	0.49
1:D:1265:LYS:O	1:D:1269:LEU:HG	2.13	0.49
1:B:1485:ILE:HA	1:B:1492:VAL:HG21	1.94	0.49
1:D:1403:MET:HB3	1:D:1404:PRO:HD3	1.93	0.49
1:C:1089:ILE:HG22	1:C:1093:LEU:HD12	1.93	0.49
1:C:1482:LEU:HD13	1:C:1541:VAL:HG13	1.95	0.49
1:A:1216:ASN:HA	1:A:1219:ILE:HB	1.94	0.49
1:A:1411:TYR:HB2	1:A:1414:THR:HG21	1.95	0.49
1:B:1387:ARG:HB3	1:C:1387:ARG:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1102:TRP:CZ2	1:D:1338:TYR:CD2	3.00	0.49
1:C:1468:ARG:HD2	1:C:1471:SER:CB	2.42	0.49
1:D:1153:ILE:HG12	1:D:1184:THR:HA	1.94	0.49
1:D:1552:ASN:O	1:D:1555:GLN:HB2	2.13	0.49
1:B:1152:ASP:OD1	1:B:1154:GLU:HB2	2.13	0.48
1:B:1191:GLU:O	1:B:1195:ASN:ND2	2.46	0.48
1:B:1036:THR:HG23	1:B:1039:GLN:CG	2.29	0.48
1:B:1036:THR:OG1	1:B:1038:GLY:N	2.44	0.48
1:B:1081:THR:OG1	1:B:1084:GLU:HB2	2.13	0.48
1:B:1388:TYR:CZ	1:B:1425:ARG:NH1	2.81	0.48
1:B:1445:PHE:HE1	1:B:1457:LYS:HG3	1.77	0.48
1:D:1553:VAL:HG22	1:D:1557:ARG:HD2	1.95	0.48
1:C:1382:LEU:HD22	1:C:1390:GLY:C	2.34	0.48
1:D:1126:VAL:HG22	1:D:1357:ALA:HB2	1.96	0.48
1:D:1385:GLU:HB3	1:D:1422:PHE:CE1	2.48	0.48
1:A:1102:TRP:CZ2	1:A:1338:TYR:CD2	3.02	0.48
1:A:1428:LYS:HG2	1:A:1438:TRP:CG	2.48	0.48
1:A:1552:ASN:O	1:A:1555:GLN:HB2	2.13	0.48
1:A:1050:ASP:HB3	1:A:1051:PRO:CD	2.36	0.48
1:B:1016:GLU:O	1:B:1019:GLU:HB3	2.12	0.48
1:C:1124:SER:HB3	1:C:1127:ASP:HB2	1.95	0.48
1:C:1169:LYS:N	1:C:1206:ASP:OD2	2.46	0.48
1:C:1185:LEU:HD21	1:C:1190:TRP:CD2	2.48	0.48
1:C:1265:LYS:HB3	1:C:1265:LYS:HE3	1.49	0.48
1:A:1095:THR:HG23	1:A:1115:LEU:HD11	1.95	0.48
1:D:1409:ARG:NH1	1:D:1411:TYR:OH	2.46	0.48
1:A:1405:LEU:HD21	1:A:1420:TYR:CZ	2.48	0.48
1:B:1414:THR:HG21	1:B:1572:GLN:HA	1.96	0.48
1:B:1470:LEU:O	1:B:1472:HIS:N	2.47	0.48
1:B:1504:ALA:HA	1:B:1529:ILE:HD13	1.96	0.48
1:B:1443:SER:HB3	1:B:1477:ALA:HB2	1.95	0.48
1:D:1267:TYR:CE2	1:D:1271:ILE:HD11	2.49	0.48
1:A:1200:LYS:HE2	1:A:1200:LYS:HB3	1.71	0.47
1:C:1169:LYS:HG2	1:C:1204:SER:CB	2.40	0.47
1:D:1119:ARG:O	1:D:1121:TYR:N	2.37	0.47
1:D:1347:LYS:O	1:D:1349:TYR:CE2	2.67	0.47
1:D:1517:THR:OG1	1:D:1520:ARG:NH2	2.47	0.47
1:B:1265:LYS:O	1:B:1269:LEU:HG	2.13	0.47
1:B:1428:LYS:HG2	1:B:1438:TRP:CG	2.49	0.47
1:A:1389:LYS:HG3	1:A:1575:MET:HE1	1.96	0.47
1:A:1245:LYS:HG2	1:A:1248:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1236:GLU:O	1:B:1240:GLU:HG2	2.15	0.47
1:C:1191:GLU:O	1:C:1195:ASN:ND2	2.47	0.47
1:A:1443:SER:CB	1:A:1477:ALA:HB2	2.43	0.47
1:B:1362:PHE:CD2	1:B:1408:MET:HE1	2.49	0.47
1:D:1394:TRP:CD1	1:D:1467:LYS:HD3	2.49	0.47
1:A:1507:LYS:HD3	1:A:1508:TYR:CZ	2.49	0.47
1:A:1517:THR:OG1	1:A:1520:ARG:NH2	2.48	0.47
1:A:1119:ARG:HB3	1:A:1120:PRO:HD3	1.95	0.47
1:C:1179:ILE:HA	1:C:1182:LYS:NZ	2.30	0.47
1:D:1225:MET:HG3	1:D:1229:LEU:HD12	1.97	0.47
1:A:1355:SER:O	1:A:1357:ALA:N	2.48	0.47
1:B:1426:VAL:HG11	1:B:1463:SER:HB2	1.96	0.47
1:C:1382:LEU:HD23	1:C:1382:LEU:HA	1.74	0.47
1:D:1521:VAL:HG11	1:D:1525:LYS:O	2.13	0.47
1:C:1275:PHE:CZ	1:C:1283:LYS:HE3	2.50	0.47
1:C:1414:THR:HG21	1:C:1572:GLN:HA	1.96	0.47
1:D:1072:ILE:HD11	1:D:1138:VAL:HG13	1.96	0.47
1:A:1413:ASN:HB2	1:A:1574:LYS:HE2	1.96	0.46
1:B:1212:LYS:HE2	1:B:1212:LYS:HA	1.96	0.46
1:B:1482:LEU:HD13	1:B:1541:VAL:HG13	1.97	0.46
1:C:1552:ASN:O	1:C:1555:GLN:HB2	2.15	0.46
1:A:1197:ILE:CG2	1:A:1218:ILE:HD11	2.46	0.46
1:D:1169:LYS:HG3	1:D:1206:ASP:HB2	1.97	0.46
1:D:1445:PHE:CZ	1:D:1455:GLN:HB2	2.50	0.46
1:B:1517:THR:OG1	1:B:1520:ARG:NH2	2.48	0.46
1:C:1347:LYS:O	1:C:1349:TYR:CE2	2.68	0.46
1:A:1201:LEU:HB3	1:A:1215:LYS:HE3	1.96	0.46
1:D:1236:GLU:O	1:D:1240:GLU:HG2	2.16	0.46
1:D:1381:MET:O	1:D:1391:LEU:HA	2.15	0.46
1:D:1411:TYR:HB2	1:D:1414:THR:HG21	1.98	0.46
1:A:1472:HIS:O	1:A:1474:LYS:N	2.49	0.46
1:C:1331:ARG:HB3	1:C:1333:LEU:HB2	1.98	0.46
1:C:1395:SER:OG	1:C:1400:GLU:OE1	2.29	0.46
1:C:1445:PHE:CE1	1:C:1455:GLN:HB2	2.51	0.46
1:C:1471:SER:O	1:C:1472:HIS:HB3	2.15	0.46
1:D:1263:VAL:CG1	1:D:1263:VAL:O	2.64	0.46
1:A:1358:ARG:HH12	1:A:1420:TYR:HE1	1.61	0.46
1:B:1040:ASN:HB2	1:B:1115:LEU:HD21	1.98	0.46
1:B:1231:TRP:CE2	1:B:1251:PHE:HB3	2.50	0.46
1:C:1324:ARG:HG3	1:C:1369:GLU:OE2	2.16	0.46
1:C:1517:THR:OG1	1:C:1520:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1169:LYS:CG	1:D:1206:ASP:HB2	2.46	0.46
1:B:1422:PHE:O	1:B:1425:ARG:HG2	2.15	0.46
1:C:1087:GLU:HG3	1:C:1091:LYS:HD2	1.97	0.46
1:D:1263:VAL:O	1:D:1263:VAL:HG12	2.15	0.46
1:C:1095:THR:HG23	1:C:1115:LEU:HD11	1.98	0.46
1:C:1266:ASN:O	1:C:1270:GLU:HB3	2.16	0.46
1:D:1264:TYR:O	1:D:1297:LEU:HD22	2.15	0.46
1:C:1501:LYS:HG3	1:C:1502:GLU:N	2.31	0.46
1:B:1185:LEU:HD21	1:B:1190:TRP:CE3	2.51	0.45
1:C:1489:VAL:O	1:C:1493:LEU:HG	2.17	0.45
1:D:1229:LEU:HD22	1:D:1231:TRP:CH2	2.50	0.45
1:D:1559:HIS:O	1:D:1565:LYS:CD	2.62	0.45
1:A:1171:ILE:HG21	1:A:1214:LEU:CD2	2.46	0.45
1:C:1081:THR:OG1	1:C:1084:GLU:HB2	2.15	0.45
1:B:1389:LYS:HG3	1:B:1575:MET:HE1	1.99	0.45
1:B:1521:VAL:HG11	1:B:1525:LYS:O	2.17	0.45
1:A:1428:LYS:HG2	1:A:1438:TRP:CD1	2.51	0.45
1:A:1504:ALA:HA	1:A:1529:ILE:HD13	1.97	0.45
1:C:1336:ILE:HA	1:C:1350:TYR:CE2	2.51	0.45
1:A:1403:MET:HG3	1:A:1540:MET:HE2	1.98	0.45
1:A:1552:ASN:O	1:A:1556:LYS:HG3	2.17	0.45
1:B:1381:MET:HE3	1:B:1381:MET:HB3	1.95	0.45
1:C:1271:ILE:O	1:C:1275:PHE:HB2	2.16	0.45
1:D:1185:LEU:HD21	1:D:1190:TRP:CD2	2.51	0.45
1:A:1504:ALA:HB2	1:A:1514:ILE:HD11	1.99	0.45
1:B:1071:VAL:O	1:B:1074:ALA:HB3	2.17	0.45
1:B:1355:SER:O	1:B:1357:ALA:N	2.49	0.45
1:B:1368:LYS:HE3	1:B:1563:ARG:HG2	1.99	0.45
1:C:1428:LYS:HG2	1:C:1438:TRP:CD1	2.52	0.45
1:C:1447:ALA:O	1:C:1455:GLN:HG2	2.17	0.45
1:D:1087:GLU:HG2	1:D:1091:LYS:HD2	1.97	0.45
1:C:1243:ILE:HD11	1:C:1270:GLU:HG2	1.97	0.45
1:C:1443:SER:C	1:C:1456:TYR:HD1	2.21	0.45
1:D:1193:PHE:O	1:D:1197:ILE:HG12	2.17	0.45
1:B:1428:LYS:HG2	1:B:1438:TRP:CD1	2.52	0.45
1:B:1581:ILE:CD1	1:C:1382:LEU:HG	2.42	0.45
1:C:1386:ASN:HB2	1:C:1387:ARG:H	1.68	0.44
1:D:1081:THR:OG1	1:D:1084:GLU:HB2	2.16	0.44
1:B:1080:ILE:HD12	1:B:1085:MET:HA	1.99	0.44
1:B:1195:ASN:OD1	1:B:1222:LYS:NZ	2.29	0.44
1:D:1430:TYR:CD2	1:D:1461:VAL:HB	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1448:PHE:HB3	1:B:1452:LEU:HA	1.99	0.44
1:C:1470:LEU:O	1:C:1471:SER:C	2.55	0.44
1:B:1443:SER:C	1:B:1456:TYR:HD1	2.21	0.44
1:C:1216:ASN:HA	1:C:1219:ILE:HD12	1.99	0.44
1:C:1443:SER:CB	1:C:1477:ALA:HB2	2.46	0.44
1:C:1563:ARG:O	1:C:1566:ALA:HB3	2.17	0.44
1:D:1071:VAL:O	1:D:1074:ALA:HB3	2.18	0.44
1:D:1166:LEU:HD11	1:D:1213:ARG:HD3	2.00	0.44
1:B:1095:THR:HG23	1:B:1115:LEU:HD11	2.00	0.44
1:B:1119:ARG:HD2	1:B:1119:ARG:HA	1.86	0.44
1:B:1407:VAL:O	1:B:1555:GLN:HA	2.17	0.44
1:D:1114:THR:OG1	1:D:1116:GLU:HB2	2.17	0.44
1:D:1120:PRO:O	1:D:1121:TYR:C	2.56	0.44
1:A:1053:ASN:ND2	1:A:1451:ASN:O	2.51	0.44
1:A:1145:PHE:HA	1:A:1148:LYS:HB2	1.99	0.44
1:B:1355:SER:HA	1:B:1400:GLU:HG2	1.99	0.44
1:A:1111:ASN:N	1:A:1118:LEU:HD21	2.33	0.44
1:A:1159:LEU:O	1:A:1162:THR:HB	2.18	0.44
1:A:1358:ARG:NE	1:A:1404:PRO:HG2	2.33	0.44
1:B:1381:MET:CE	1:C:1578:TYR:HB3	2.48	0.44
1:B:1445:PHE:CE1	1:B:1457:LYS:HG3	2.53	0.44
1:C:1405:LEU:HD21	1:C:1420:TYR:CZ	2.53	0.44
1:D:1053:ASN:ND2	1:D:1451:ASN:O	2.48	0.44
1:B:1126:VAL:HG23	1:B:1350:TYR:CE2	2.53	0.44
1:B:1411:TYR:HB2	1:B:1414:THR:HG21	2.00	0.44
1:D:1331:ARG:HB3	1:D:1333:LEU:HB2	2.00	0.44
1:B:1381:MET:O	1:B:1391:LEU:HA	2.18	0.43
1:D:1040:ASN:HB2	1:D:1115:LEU:HD21	2.00	0.43
1:B:1552:ASN:O	1:B:1555:GLN:HB2	2.16	0.43
1:C:1050:ASP:HB2	1:C:1531:LYS:CB	2.47	0.43
1:C:1381:MET:O	1:C:1391:LEU:HA	2.18	0.43
1:A:1287:LYS:HD2	1:A:1287:LYS:HA	1.85	0.43
1:B:1051:PRO:HG2	1:B:1448:PHE:HE2	1.82	0.43
1:B:1536:HIS:O	1:B:1540:MET:HG3	2.18	0.43
1:C:1030:TYR:O	1:C:1034:PHE:HD2	2.01	0.43
1:C:1190:TRP:HZ2	1:C:1221:LEU:HD22	1.82	0.43
1:D:1050:ASP:HB3	1:D:1051:PRO:CD	2.45	0.43
1:D:1109:TRP:HB3	1:D:1118:LEU:HG	2.00	0.43
1:A:1021:ARG:O	1:A:1024:ALA:HB3	2.19	0.43
1:A:1044:PRO:HB2	1:A:1056:ALA:O	2.18	0.43
1:A:1169:LYS:N	1:A:1206:ASP:OD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:LYS:HG3	1:A:1297:LEU:HD21	1.99	0.43
1:B:1159:LEU:O	1:B:1162:THR:HB	2.19	0.43
1:B:1581:ILE:HD11	1:C:1382:LEU:CG	2.44	0.43
1:C:1071:VAL:O	1:C:1074:ALA:HB3	2.17	0.43
1:C:1243:ILE:HA	1:C:1246:ARG:CZ	2.48	0.43
1:C:1536:HIS:CD2	1:C:1537:HIS:N	2.85	0.43
1:A:1080:ILE:HD12	1:A:1085:MET:HA	2.01	0.43
1:A:1322:GLU:HG2	1:A:1324:ARG:HH21	1.83	0.43
1:D:1397:THR:HB	1:D:1441:SER:HG	1.82	0.43
1:C:1185:LEU:HD21	1:C:1190:TRP:CE3	2.53	0.43
1:D:1153:ILE:CG1	1:D:1184:THR:HA	2.49	0.43
1:D:1443:SER:CB	1:D:1477:ALA:HB2	2.48	0.43
1:A:1132:VAL:HG13	1:A:1318:VAL:HG13	2.01	0.43
1:D:1394:TRP:NE1	1:D:1467:LYS:HD3	2.34	0.43
1:D:1409:ARG:HG3	1:D:1559:HIS:CE1	2.53	0.43
1:C:1358:ARG:CZ	1:C:1404:PRO:HG2	2.49	0.43
1:C:1414:THR:CG2	1:C:1572:GLN:HA	2.49	0.43
1:D:1179:ILE:HG23	1:D:1185:LEU:HD13	2.01	0.43
1:D:1185:LEU:HD21	1:D:1190:TRP:CE3	2.54	0.43
1:B:1381:MET:HE3	1:C:1578:TYR:HB3	2.01	0.43
1:B:1536:HIS:CD2	1:B:1537:HIS:N	2.87	0.43
1:C:1050:ASP:HB2	1:C:1531:LYS:HG3	2.01	0.43
1:D:1190:TRP:HZ2	1:D:1221:LEU:HD22	1.84	0.43
1:D:1287:LYS:O	1:D:1291:ASP:OD1	2.37	0.43
1:B:1445:PHE:CZ	1:B:1455:GLN:HB3	2.54	0.42
1:D:1241:GLN:HG3	1:D:1289:GLN:HE22	1.84	0.42
1:A:1029:ARG:HD2	1:A:1165:MET:SD	2.59	0.42
1:A:1245:LYS:HA	1:A:1248:LYS:HD2	2.00	0.42
1:B:1397:THR:HB	1:B:1441:SER:OG	2.18	0.42
1:C:1264:TYR:HE2	1:C:1296:ALA:HB3	1.84	0.42
1:D:1021:ARG:O	1:D:1024:ALA:HB3	2.19	0.42
1:B:1208:LEU:O	1:B:1212:LYS:HG2	2.20	0.42
1:B:1403:MET:SD	1:B:1540:MET:CE	3.07	0.42
1:B:1443:SER:CB	1:B:1477:ALA:HB2	2.49	0.42
1:B:1500:LYS:NZ	1:B:1505:GLU:OE2	2.47	0.42
1:C:1175:ILE:HG22	1:C:1193:PHE:CE1	2.55	0.42
1:A:1155:LEU:HD22	1:A:1221:LEU:HD21	2.02	0.42
1:B:1151:ILE:HG13	1:B:1229:LEU:HD11	2.00	0.42
1:C:1053:ASN:ND2	1:C:1451:ASN:O	2.52	0.42
1:C:1333:LEU:HD23	1:C:1374:HIS:HE1	1.85	0.42
1:D:1067:TYR:OH	1:D:1088:ARG:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1198:ARG:O	1:C:1202:LEU:HG	2.20	0.42
1:C:1497:ARG:H	1:C:1497:ARG:HG2	1.56	0.42
1:A:1040:ASN:HB2	1:A:1115:LEU:HD21	2.02	0.42
1:A:1166:LEU:O	1:A:1210:ASN:ND2	2.53	0.42
1:A:1413:ASN:CB	1:A:1574:LYS:HE2	2.50	0.42
1:D:1291:ASP:O	1:D:1295:GLN:OE1	2.37	0.42
1:B:1273:GLU:HA	1:B:1273:GLU:OE1	2.20	0.42
1:B:1347:LYS:O	1:B:1349:TYR:CE1	2.72	0.42
1:C:1021:ARG:O	1:C:1024:ALA:HB3	2.19	0.42
1:C:1271:ILE:HB	1:C:1290:LYS:HE2	2.02	0.42
1:A:1443:SER:C	1:A:1456:TYR:HD1	2.23	0.42
1:B:1053:ASN:ND2	1:B:1451:ASN:O	2.52	0.42
1:C:1345:LEU:HD23	1:C:1345:LEU:HA	1.85	0.42
1:C:1389:LYS:HD2	1:C:1575:MET:CE	2.49	0.42
1:C:1398:MET:HG3	1:C:1427:GLN:NE2	2.35	0.42
1:D:1215:LYS:O	1:D:1219:ILE:N	2.50	0.42
1:B:1345:LEU:HD23	1:B:1345:LEU:HA	1.85	0.42
1:C:1119:ARG:HA	1:C:1119:ARG:HD2	1.88	0.42
1:C:1229:LEU:HD22	1:C:1231:TRP:CZ2	2.54	0.42
1:C:1382:LEU:CD2	1:C:1390:GLY:C	2.89	0.42
1:D:1504:ALA:HA	1:D:1529:ILE:HD13	2.01	0.42
1:A:1511:TYR:CD1	1:A:1531:LYS:HA	2.55	0.41
1:B:1389:LYS:HG3	1:B:1575:MET:CE	2.49	0.41
1:C:1179:ILE:H	1:C:1179:ILE:HD12	1.85	0.41
1:C:1407:VAL:O	1:C:1555:GLN:HA	2.20	0.41
1:C:1430:TYR:CG	1:C:1461:VAL:HG13	2.55	0.41
1:A:1483:LEU:HD11	1:A:1540:MET:SD	2.60	0.41
1:B:1012:VAL:HG13	1:B:1016:GLU:HB2	2.01	0.41
1:B:1355:SER:C	1:B:1357:ALA:N	2.74	0.41
1:C:1271:ILE:CG2	1:C:1290:LYS:HE3	2.50	0.41
1:A:1197:ILE:HG22	1:A:1218:ILE:CD1	2.50	0.41
1:D:1383:ALA:O	1:D:1389:LYS:HA	2.20	0.41
1:D:1405:LEU:HD21	1:D:1420:TYR:CZ	2.55	0.41
1:D:1089:ILE:HG22	1:D:1093:LEU:HD12	2.02	0.41
1:D:1159:LEU:O	1:D:1162:THR:HB	2.20	0.41
1:D:1193:PHE:O	1:D:1196:LYS:HB3	2.21	0.41
1:B:1359:GLN:O	1:B:1363:ILE:HD12	2.21	0.41
1:B:1456:TYR:C	1:B:1457:LYS:HG2	2.40	0.41
1:C:1231:TRP:HH2	1:C:1264:TYR:HE1	1.69	0.41
1:A:1071:VAL:O	1:A:1074:ALA:HB3	2.19	0.41
1:B:1050:ASP:HB2	1:B:1531:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1425:ARG:HG2	1:B:1425:ARG:H	1.76	0.41
1:C:1264:TYR:HB3	1:C:1297:LEU:HD22	2.03	0.41
1:D:1080:ILE:HD12	1:D:1085:MET:HA	2.03	0.41
1:B:1511:TYR:CD1	1:B:1531:LYS:HA	2.55	0.41
1:C:1395:SER:HB2	1:C:1468:ARG:HH22	1.86	0.41
1:D:1407:VAL:O	1:D:1555:GLN:HA	2.20	0.41
1:A:1190:TRP:HZ2	1:A:1221:LEU:HD22	1.86	0.41
1:B:1132:VAL:HG13	1:B:1318:VAL:HG13	2.01	0.41
1:B:1182:LYS:HE2	1:B:1186:VAL:HG13	2.02	0.41
1:C:1082:THR:CG2	1:C:1145:PHE:HB3	2.49	0.41
1:A:1357:ALA:O	1:A:1360:ALA:HB3	2.21	0.41
1:B:1030:TYR:O	1:B:1034:PHE:HD2	2.04	0.41
1:B:1118:LEU:HA	1:B:1118:LEU:HD22	1.89	0.41
1:B:1231:TRP:CD1	1:B:1231:TRP:C	2.93	0.41
1:B:1357:ALA:O	1:B:1360:ALA:HB3	2.21	0.41
1:B:1386:ASN:HB2	1:B:1387:ARG:H	1.69	0.41
1:C:1040:ASN:HB2	1:C:1115:LEU:HD21	2.02	0.41
1:C:1391:LEU:HB2	1:C:1419:THR:HG21	2.03	0.41
1:C:1397:THR:HB	1:C:1441:SER:OG	2.21	0.41
1:D:1029:ARG:O	1:D:1030:TYR:C	2.59	0.41
1:B:1071:VAL:HG11	1:B:1089:ILE:HG13	2.02	0.41
1:B:1446:TYR:CG	1:B:1528:ALA:HB1	2.56	0.41
1:C:1159:LEU:O	1:C:1162:THR:HB	2.21	0.41
1:D:1344:LYS:HB2	1:D:1344:LYS:HE2	1.81	0.41
1:A:1199:GLU:HA	1:A:1202:LEU:HD12	2.03	0.40
1:A:1355:SER:H	1:A:1358:ARG:HD3	1.86	0.40
1:B:1021:ARG:O	1:B:1024:ALA:HB3	2.21	0.40
1:B:1177:THR:O	1:B:1181:SER:OG	2.36	0.40
1:D:1160:LYS:HA	1:D:1176:PHE:CZ	2.56	0.40
1:D:1324:ARG:HG3	1:D:1369:GLU:OE2	2.20	0.40
1:A:1135:LEU:HB3	1:A:1314:ILE:HG23	2.02	0.40
1:B:1176:PHE:HB3	1:B:1180:LEU:HG	2.03	0.40
1:B:1384:ILE:CD1	1:C:1579:LEU:HD21	2.51	0.40
1:C:1126:VAL:HG23	1:C:1350:TYR:CE2	2.56	0.40
1:C:1193:PHE:CE2	1:C:1197:ILE:HD11	2.56	0.40
1:A:1130:ASN:HB3	1:A:1134:TYR:CE2	2.57	0.40
1:A:1169:LYS:HB3	1:A:1204:SER:HB2	2.03	0.40
1:A:1398:MET:HG2	1:A:1427:GLN:NE2	2.35	0.40
1:B:1485:ILE:HG12	1:B:1548:PHE:CD1	2.57	0.40
1:C:1273:GLU:HA	1:C:1276:LYS:HE2	2.03	0.40
1:D:1422:PHE:O	1:D:1426:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:ARG:O	1:A:1030:TYR:C	2.59	0.40
1:B:1011:THR:HG22	1:B:1012:VAL:N	2.36	0.40
1:B:1029:ARG:O	1:B:1030:TYR:C	2.60	0.40
1:C:1029:ARG:HD2	1:C:1165:MET:SD	2.62	0.40
1:C:1392:VAL:HG21	1:C:1466:LEU:HG	2.02	0.40
1:D:1321:THR:O	1:D:1367:LYS:NZ	2.48	0.40
1:A:1397:THR:HB	1:A:1441:SER:OG	2.22	0.40
1:B:1416:LEU:HB3	1:B:1420:TYR:CE2	2.55	0.40
1:C:1230:VAL:O	1:C:1233:GLU:HB2	2.20	0.40
1:D:1485:ILE:HG23	1:D:1486:GLY:N	2.36	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	572/596 (96%)	478 (84%)	79 (14%)	15 (3%)	5	35
1	B	571/596 (96%)	483 (85%)	74 (13%)	14 (2%)	5	36
1	C	571/596 (96%)	468 (82%)	88 (15%)	15 (3%)	5	35
1	D	572/596 (96%)	463 (81%)	91 (16%)	18 (3%)	4	32
All	All	2286/2384 (96%)	1892 (83%)	332 (14%)	62 (3%)	5	35

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1356	GLU
1	A	1473	ASP
1	B	1356	GLU
1	B	1471	SER
1	C	1356	GLU

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Mol	Chain	Res	Type
1	C	1582	THR
1	D	1356	GLU
1	A	1167	ASN
1	A	1170	GLY
1	A	1177	THR
1	A	1551	ASN
1	B	1177	THR
1	B	1207	ASP
1	B	1551	ASN
1	B	1552	ASN
1	C	1471	SER
1	C	1551	ASN
1	C	1552	ASN
1	C	1581	ILE
1	D	1121	TYR
1	D	1177	THR
1	D	1386	ASN
1	D	1471	SER
1	D	1551	ASN
1	D	1578	TYR
1	A	1121	TYR
1	A	1552	ASN
1	B	1121	TYR
1	B	1206	ASP
1	B	1467	LYS
1	C	1121	TYR
1	C	1177	THR
1	D	1343	GLU
1	D	1468	ARG
1	D	1469	GLY
1	D	1552	ASN
1	D	1583	ARG
1	A	1178	THR
1	A	1207	ASP
1	C	1167	ASN
1	C	1207	ASP
1	C	1487	VAL
1	D	1207	ASP
1	A	1085	MET
1	A	1176	PHE
1	A	1467	LYS
1	A	1487	VAL

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Mol	Chain	Res	Type
1	A	1527	SER
1	B	1085	MET
1	B	1178	THR
1	B	1468	ARG
1	C	1179	ILE
1	C	1241	GLN
1	C	1467	LYS
1	D	1085	MET
1	D	1178	THR
1	D	1487	VAL
1	B	1487	VAL
1	C	1085	MET
1	D	1287	LYS
1	B	1170	GLY
1	D	1384	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	512/532 (96%)	460 (90%)	52 (10%)	7 30
1	B	511/532 (96%)	460 (90%)	51 (10%)	7 30
1	C	511/532 (96%)	449 (88%)	62 (12%)	5 24
1	D	512/532 (96%)	445 (87%)	67 (13%)	4 22
All	All	2046/2128 (96%)	1814 (89%)	232 (11%)	6 27

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1013	SER
1	A	1017	MET
1	A	1087	GLU
1	A	1116	GLU
1	A	1123	VAL
1	A	1128	SER

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Mol	Chain	Res	Type
1	A	1163	ILE
1	A	1168	VAL
1	A	1169	LYS
1	A	1174	ASP
1	A	1182	LYS
1	A	1183	THR
1	A	1186	VAL
1	A	1200	LYS
1	A	1204	SER
1	A	1205	GLN
1	A	1208	LEU
1	A	1239	LYS
1	A	1249	GLU
1	A	1256	SER
1	A	1277	LYS
1	A	1297	LEU
1	A	1332	GLN
1	A	1333	LEU
1	A	1334	PHE
1	A	1342	GLU
1	A	1343	GLU
1	A	1345	LEU
1	A	1347	LYS
1	A	1358	ARG
1	A	1372	LYS
1	A	1385	GLU
1	A	1387	ARG
1	A	1389	LYS
1	A	1399	PHE
1	A	1408	MET
1	A	1409	ARG
1	A	1425	ARG
1	A	1436	ILE
1	A	1462	PRO
1	A	1463	SER
1	A	1464	LEU
1	A	1466	LEU
1	A	1474	LYS
1	A	1485	ILE
1	A	1526	LYS
1	A	1565	LYS
1	A	1568	GLN

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Mol	Chain	Res	Type
1	A	1569	ILE
1	A	1582	THR
1	A	1583	ARG
1	A	1584	GLU
1	B	1013	SER
1	B	1036	THR
1	B	1037	GLU
1	B	1055	VAL
1	B	1057	GLU
1	B	1116	GLU
1	B	1118	LEU
1	B	1119	ARG
1	B	1128	SER
1	B	1157	LYS
1	B	1168	VAL
1	B	1169	LYS
1	B	1174	ASP
1	B	1182	LYS
1	B	1183	THR
1	B	1186	VAL
1	B	1198	ARG
1	B	1209	GLU
1	B	1239	LYS
1	B	1243	ILE
1	B	1248	LYS
1	B	1249	GLU
1	B	1253	GLU
1	B	1256	SER
1	B	1262	LYS
1	B	1274	VAL
1	B	1277	LYS
1	B	1290	LYS
1	B	1302	LYS
1	B	1316	ASN
1	B	1320	LYS
1	B	1333	LEU
1	B	1342	GLU
1	B	1359	GLN
1	B	1368	LYS
1	B	1386	ASN
1	B	1389	LYS
1	B	1399	PHE

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Mol	Chain	Res	Type
1	B	1403	MET
1	B	1425	ARG
1	B	1450	MET
1	B	1455	GLN
1	B	1464	LEU
1	B	1467	LYS
1	B	1468	ARG
1	B	1474	LYS
1	B	1489	VAL
1	B	1498	PHE
1	B	1523	PHE
1	B	1574	LYS
1	B	1579	LEU
1	C	1013	SER
1	C	1037	GLU
1	C	1085	MET
1	C	1099	MET
1	C	1113	LYS
1	C	1116	GLU
1	C	1118	LEU
1	C	1119	ARG
1	C	1157	LYS
1	C	1169	LYS
1	C	1174	ASP
1	C	1182	LYS
1	C	1184	THR
1	C	1186	VAL
1	C	1196	LYS
1	C	1198	ARG
1	C	1200	LYS
1	C	1205	GLN
1	C	1206	ASP
1	C	1211	ILE
1	C	1231	TRP
1	C	1239	LYS
1	C	1253	GLU
1	C	1262	LYS
1	C	1265	LYS
1	C	1272	GLU
1	C	1276	LYS
1	C	1277	LYS
1	C	1283	LYS

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Mol	Chain	Res	Type
1	C	1287	LYS
1	C	1288	SER
1	C	1307	ILE
1	C	1329	GLU
1	C	1333	LEU
1	C	1347	LYS
1	C	1373	LYS
1	C	1386	ASN
1	C	1389	LYS
1	C	1399	PHE
1	C	1403	MET
1	C	1405	LEU
1	C	1418	GLU
1	C	1425	ARG
1	C	1452	LEU
1	C	1455	GLN
1	C	1463	SER
1	C	1466	LEU
1	C	1467	LYS
1	C	1468	ARG
1	C	1471	SER
1	C	1473	ASP
1	C	1474	LYS
1	C	1483	LEU
1	C	1490	GLU
1	C	1497	ARG
1	C	1498	PHE
1	C	1501	LYS
1	C	1568	GLN
1	C	1574	LYS
1	C	1575	MET
1	C	1577	MET
1	C	1579	LEU
1	D	1013	SER
1	D	1015	GLU
1	D	1020	LEU
1	D	1037	GLU
1	D	1057	GLU
1	D	1083	THR
1	D	1099	MET
1	D	1113	LYS
1	D	1116	GLU

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Mol	Chain	Res	Type
1	D	1118	LEU
1	D	1119	ARG
1	D	1128	SER
1	D	1151	ILE
1	D	1169	LYS
1	D	1172	THR
1	D	1174	ASP
1	D	1175	ILE
1	D	1181	SER
1	D	1186	VAL
1	D	1205	GLN
1	D	1206	ASP
1	D	1212	LYS
1	D	1213	ARG
1	D	1219	ILE
1	D	1236	GLU
1	D	1265	LYS
1	D	1272	GLU
1	D	1281	GLU
1	D	1287	LYS
1	D	1290	LYS
1	D	1291	ASP
1	D	1298	GLU
1	D	1307	ILE
1	D	1312	SER
1	D	1331	ARG
1	D	1332	GLN
1	D	1333	LEU
1	D	1345	LEU
1	D	1347	LYS
1	D	1355	SER
1	D	1368	LYS
1	D	1373	LYS
1	D	1387	ARG
1	D	1388	TYR
1	D	1395	SER
1	D	1399	PHE
1	D	1403	MET
1	D	1407	VAL
1	D	1408	MET
1	D	1418	GLU
1	D	1436	ILE

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Mol	Chain	Res	Type
1	D	1441	SER
1	D	1455	GLN
1	D	1457	LYS
1	D	1461	VAL
1	D	1463	SER
1	D	1466	LEU
1	D	1468	ARG
1	D	1474	LYS
1	D	1483	LEU
1	D	1485	ILE
1	D	1498	PHE
1	D	1501	LYS
1	D	1577	MET
1	D	1579	LEU
1	D	1582	THR
1	D	1583	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1039	GLN
1	B	1332	GLN
1	B	1453	ASN
1	C	1552	ASN
1	D	1039	GLN

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

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	574/596 (96%)	0.42	8 (1%) 75 66	60, 104, 157, 203	0
1	B	573/596 (96%)	0.44	17 (2%) 50 38	65, 105, 187, 230	0
1	C	573/596 (96%)	0.55	31 (5%) 25 21	60, 113, 212, 269	0
1	D	574/596 (96%)	0.66	52 (9%) 9 7	68, 119, 215, 279	0
All	All	2294/2384 (96%)	0.52	108 (4%) 31 25	60, 109, 199, 279	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1264	TYR	4.9
1	C	1286	LEU	4.8
1	B	1271	ILE	4.3
1	D	1201	LEU	4.1
1	B	1275	PHE	4.1
1	D	1267	TYR	4.0
1	C	1271	ILE	3.9
1	D	1228	PHE	3.8
1	D	1171	ILE	3.7
1	C	1228	PHE	3.7
1	B	1228	PHE	3.7
1	D	1234	PHE	3.6
1	D	1243	ILE	3.6
1	D	1286	LEU	3.5
1	D	1190	TRP	3.4
1	C	1244	PHE	3.4
1	C	1296	ALA	3.4
1	D	1264	TYR	3.3
1	D	1274	VAL	3.3
1	D	1260	LEU	3.2
1	C	1254	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	1250	VAL	3.2
1	D	1271	ILE	3.2
1	D	1263	VAL	3.1
1	A	1171	ILE	3.1
1	D	1217	ILE	3.1
1	B	1267	TYR	3.0
1	D	1248	LYS	3.0
1	B	1281	GLU	3.0
1	D	1155	LEU	3.0
1	D	1185	LEU	2.9
1	D	1254	HIS	2.9
1	C	1293	VAL	2.9
1	D	1145	PHE	2.8
1	D	1229	LEU	2.8
1	B	1268	LEU	2.8
1	C	1190	TRP	2.8
1	D	1193	PHE	2.8
1	C	1274	VAL	2.8
1	D	1293	VAL	2.7
1	D	1194	LEU	2.7
1	C	1297	LEU	2.7
1	C	1275	PHE	2.7
1	D	1182	LYS	2.7
1	D	1296	ALA	2.6
1	B	1274	VAL	2.6
1	C	1250	VAL	2.6
1	B	1286	LEU	2.6
1	A	1472	HIS	2.6
1	C	1234	PHE	2.5
1	C	1231	TRP	2.5
1	C	1107	TYR	2.5
1	C	1292	LYS	2.5
1	D	1175	ILE	2.5
1	A	1170	GLY	2.5
1	C	1246	ARG	2.5
1	C	1304	GLU	2.5
1	C	1105	HIS	2.5
1	D	1198	ARG	2.5
1	D	1292	LYS	2.5
1	C	1229	LEU	2.5
1	D	1285	LEU	2.4
1	D	1289	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	1244	PHE	2.4
1	D	1257	PRO	2.4
1	A	1264	TYR	2.4
1	C	1260	LEU	2.4
1	D	1150	LEU	2.4
1	D	1197	ILE	2.4
1	D	1187	PRO	2.3
1	C	1267	TYR	2.3
1	D	1326	LEU	2.3
1	C	1289	GLN	2.3
1	D	1042	LEU	2.3
1	A	1153	ILE	2.3
1	D	1107	TYR	2.3
1	D	1232	THR	2.2
1	B	1293	VAL	2.2
1	A	1190	TRP	2.2
1	C	1150	LEU	2.2
1	B	1150	LEU	2.2
1	D	1080	ILE	2.2
1	D	1297	LEU	2.2
1	B	1283	LYS	2.2
1	D	1176	PHE	2.2
1	C	1106	LEU	2.2
1	D	1290	LYS	2.2
1	D	1188	SER	2.2
1	B	1264	TYR	2.1
1	B	1251	PHE	2.1
1	B	1289	GLN	2.1
1	C	1285	LEU	2.1
1	C	1145	PHE	2.1
1	D	1269	LEU	2.1
1	B	1234	PHE	2.1
1	C	1110	TYR	2.1
1	D	1221	LEU	2.1
1	B	1241	GLN	2.1
1	D	1170	GLY	2.1
1	D	1222	LYS	2.1
1	D	1299	LYS	2.1
1	C	1257	PRO	2.0
1	B	1375	TRP	2.0
1	C	1268	LEU	2.0
1	D	1246	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1286	LEU	2.0
1	A	1204	SER	2.0
1	D	1034	PHE	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.