Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 12:45 PM EST

PDB ID	:	4EZ4
Title	:	free KDM6B structure
Authors	:	Cheng, Z.J.; Patel, D.J.
Deposited on	:	2012-05-02
Resolution	:	2.99 Å(reported)

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

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

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

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

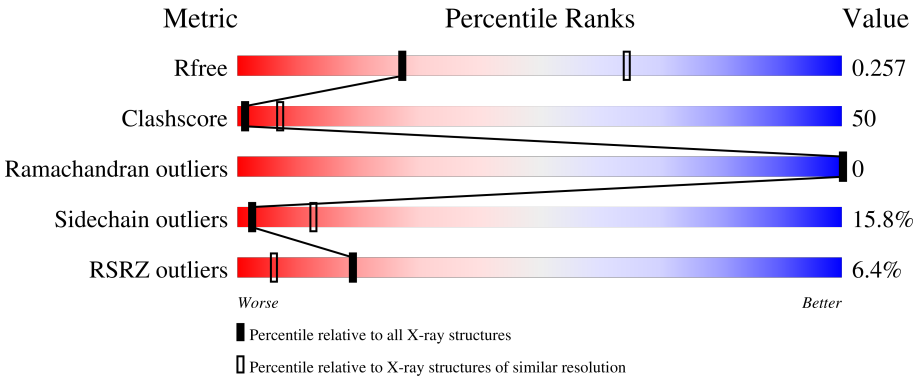
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	486	7% 39% 45% 9% 8%
1	B	486	5% 40% 43% 8% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7268 atoms, of which 32 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 Lysine-specific demethylase 6B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	448	Total	C	H	N	O	S	0	1	0
			3620	2293	16	625	667	19			
1	B	447	Total	C	H	N	O	S	0	1	0
			3612	2290	16	627	660	19			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1297	LEU	-	SEE REMARK 999	UNP Q5NCY0
A	1298	GLU	-	SEE REMARK 999	UNP Q5NCY0
A	1299	VAL	-	SEE REMARK 999	UNP Q5NCY0
A	1300	LEU	-	SEE REMARK 999	UNP Q5NCY0
A	1301	PHE	-	SEE REMARK 999	UNP Q5NCY0
A	1302	GLN	-	SEE REMARK 999	UNP Q5NCY0
A	1303	GLY	-	SEE REMARK 999	UNP Q5NCY0
A	1304	PRO	-	SEE REMARK 999	UNP Q5NCY0
A	1305	THR	-	SEE REMARK 999	UNP Q5NCY0
A	1306	LYS	-	SEE REMARK 999	UNP Q5NCY0
A	1307	ALA	-	SEE REMARK 999	UNP Q5NCY0
A	1308	ALA	-	SEE REMARK 999	UNP Q5NCY0
A	1309	ARG	-	SEE REMARK 999	UNP Q5NCY0
A	1310	LYS	-	SEE REMARK 999	UNP Q5NCY0
A	1311	SER	-	SEE REMARK 999	UNP Q5NCY0
A	1312	ALA	-	SEE REMARK 999	UNP Q5NCY0
A	1313	PRO	-	SEE REMARK 999	UNP Q5NCY0
A	1314	ALA	-	SEE REMARK 999	UNP Q5NCY0
A	1315	THR	-	SEE REMARK 999	UNP Q5NCY0
A	1316	GLY	-	SEE REMARK 999	UNP Q5NCY0
A	1317	GLY	-	SEE REMARK 999	UNP Q5NCY0
A	1318	GLY	-	SEE REMARK 999	UNP Q5NCY0
A	1319	SER	-	SEE REMARK 999	UNP Q5NCY0
A	1320	SER	-	SEE REMARK 999	UNP Q5NCY0
A	1321	GLY	-	SEE REMARK 999	UNP Q5NCY0

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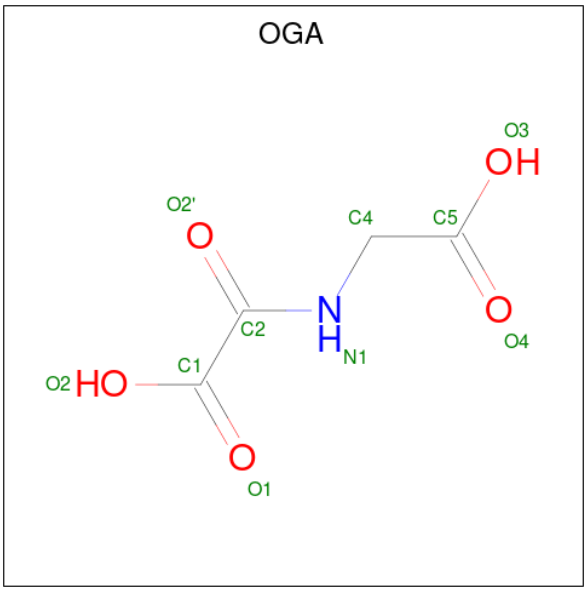
Chain	Residue	Modelled	Actual	Comment	Reference
A	1322	SER	-	SEE REMARK 999	UNP Q5NCY0
B	1297	LEU	-	SEE REMARK 999	UNP Q5NCY0
B	1298	GLU	-	SEE REMARK 999	UNP Q5NCY0
B	1299	VAL	-	SEE REMARK 999	UNP Q5NCY0
B	1300	LEU	-	SEE REMARK 999	UNP Q5NCY0
B	1301	PHE	-	SEE REMARK 999	UNP Q5NCY0
B	1302	GLN	-	SEE REMARK 999	UNP Q5NCY0
B	1303	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1304	PRO	-	SEE REMARK 999	UNP Q5NCY0
B	1305	THR	-	SEE REMARK 999	UNP Q5NCY0
B	1306	LYS	-	SEE REMARK 999	UNP Q5NCY0
B	1307	ALA	-	SEE REMARK 999	UNP Q5NCY0
B	1308	ALA	-	SEE REMARK 999	UNP Q5NCY0
B	1309	ARG	-	SEE REMARK 999	UNP Q5NCY0
B	1310	LYS	-	SEE REMARK 999	UNP Q5NCY0
B	1311	SER	-	SEE REMARK 999	UNP Q5NCY0
B	1312	ALA	-	SEE REMARK 999	UNP Q5NCY0
B	1313	PRO	-	SEE REMARK 999	UNP Q5NCY0
B	1314	ALA	-	SEE REMARK 999	UNP Q5NCY0
B	1315	THR	-	SEE REMARK 999	UNP Q5NCY0
B	1316	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1317	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1318	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1319	SER	-	SEE REMARK 999	UNP Q5NCY0
B	1320	SER	-	SEE REMARK 999	UNP Q5NCY0
B	1321	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1322	SER	-	SEE REMARK 999	UNP Q5NCY0

- Molecule 2 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: $C_4H_5NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 10 4 1 5	0	0
2	B	1	Total C N O 10 4 1 5	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0
3	B	1	Total Ni 1 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0

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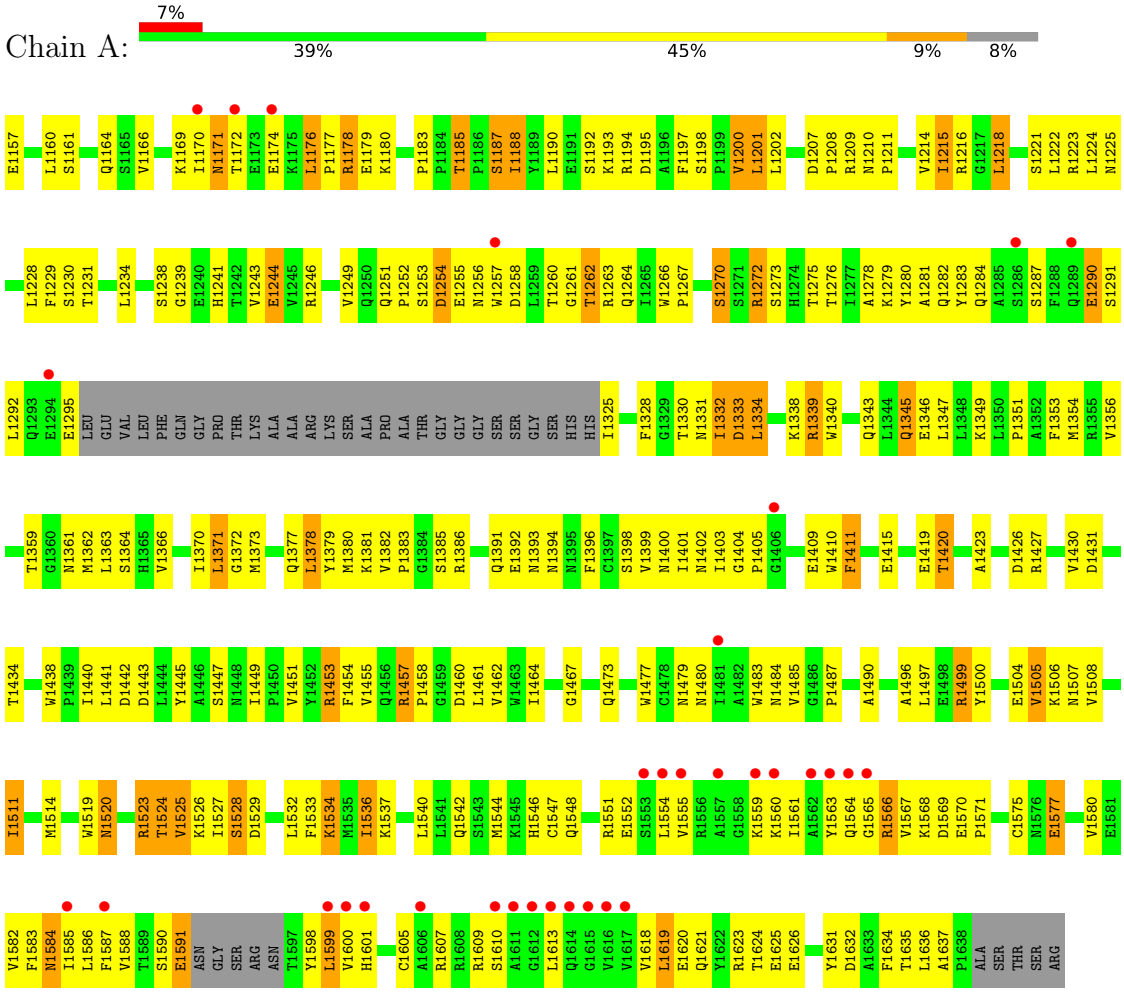
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	7	Total O 7 7	0	0

3 Residue-property plots (i)

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

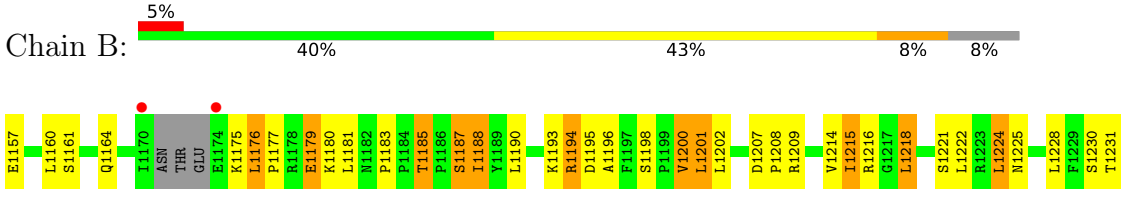
• Molecule 1: Lysine-specific demethylase 6B

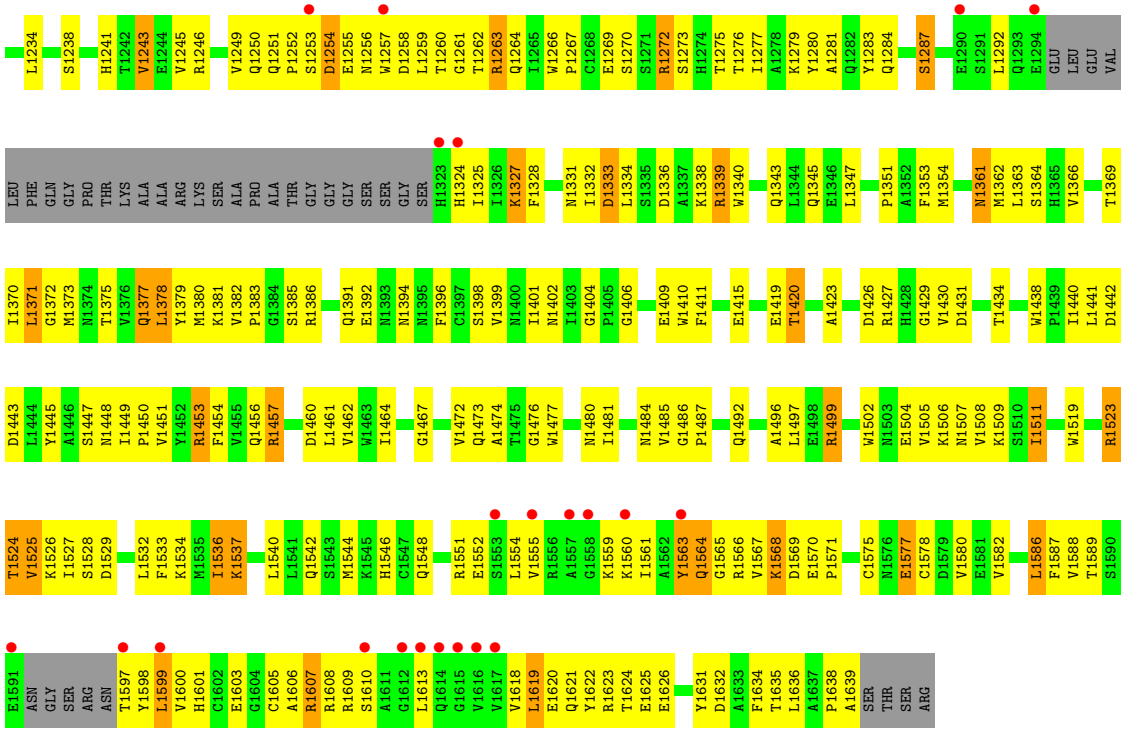
Chain A:



• Molecule 1: Lysine-specific demethylase 6B

Chain B:




L1234 S1238 H1241 T1242 V1243 E1244 V1245 R1246 V1249 Q1250 Q1251 P1252 S1253 D1254 E1255 N1256 W1257 D1258 L1259 T1260 G1261 T1262 R1263 Q1264 I1265 W1266 P1267 C1268 E1269 S1270 S1271 R1272 S1273 H1274 T1275 T1276 I1277 A1278 K1279 Y1280 A1281 Q1282 Y1283 Q1284 S1287 E1290 S1291 L1292 Q1293 E1294 GLU LEU GLU VAL
LEU PHE GLN GLY PRO THR LYS ALA ALA ARG LYS SER ALA PRO ALA THR GLY GLY GLY SER SER GLY SER H1323 H1324 I1325 I1326 K1327 F1328 N1331 I1332 D1333 L1334 S1335 D1336 A1337 K1338 R1339 W1340 Q1343 L1344 Q1345 E1346 L1347 P1351 A1352 F1353 M1354 N1361 M1362 L1363 S1364 H1365 V1366 T1369
I1370 L1371 G1372 M1373 N1374 T1375 V1376 Q1377 L1378 Y1379 M1380 K1381 V1382 P1383 G1384 S1385 R1386 Q1391 E1392 N1393 N1394 N1395 F1396 C1397 S1398 V1399 N1400 I1401 N1402 I1403 G1404 P1405 G1406 E1409 W1410 F1411 E1415 E1419 T1420 A1423 D1426 R1427 H1428 G1429 V1430 D1431 T1434 W1438 P1439 I1440 L1441 D1442
D1443 L1444 Y1445 A1446 S1447 N1448 I1449 P1450 V1451 Y1452 R1453 F1454 V1455 Q1456 R1457 D1460 L1461 V1462 W1463 I1464 G1467 V1472 Q1473 A1474 T1475 G1476 W1477 N1480 I1481 N1484 V1485 G1486 P1487 Q1492 A1496 L1497 E1498 R1499 W1502 N1503 E1504 V1505 K1506 N1507 V1508 K1509 S1510 I1511 W1519 R1523
T1524 V1525 K1526 I1527 S1528 D1529 L1532 F1533 K1534 M1535 I1536 K1537 L1540 L1541 Q1542 S1543 M1544 K1545 H1546 C1547 Q1548 R1551 E1552 S1553 L1554 V1555 R1556 A1557 G1558 K1559 K1560 I1561 A1562 Y1563 Q1564 G1565 R1566 V1567 K1568 D1569 E1570 P1571 C1575 N1576 E1577 C1578 D1579 V1580 E1581 V1582 L1586 F1587 V1588 T1589 S1590
E1591 ASN GLY SER ARG ASN T1597 Y1598 L1599 V1600 H1601 C1602 E1603 G1604 C1605 A1606 R1607 R1608 R1609 S1610 A1611 G1612 L1613 Q1614 G1615 V1616 V1617 V1618 L1619 E1620 Q1621 Y1622 R1623 T1624 E1625 E1626 Y1631 D1632 A1633 F1634 T1635 L1636 A1637 P1638 A1639 SER THR SER ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.66Å 123.71Å 82.04Å 90.00° 109.62° 90.00°	Depositor
Resolution (Å)	49.73 – 2.99 49.73 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.6 (49.73-2.99) 95.7 (49.73-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.190 , 0.250 0.213 , 0.257	Depositor DCC
R_{free} test set	1079 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7268	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9848e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: ZN, NI, OGA

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	0.51	0/3700	0.69	1/5035 (0.0%)
1	B	0.52	1/3693 (0.0%)	0.70	1/5024 (0.0%)
All	All	0.52	1/7393 (0.0%)	0.69	2/10059 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1361	ASN	CG-OD1	-5.02	1.12	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1333	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	1334	LEU	CA-CB-CG	-5.17	103.40	115.30

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	3604	16	3524	364	0
1	B	3596	16	3517	374	0
2	A	10	0	3	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	3	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	5	0	0	0	0
5	B	7	0	0	0	0
All	All	7236	32	7047	713	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 50.

All (713) 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:1193:LYS:CE	1:B:1578:CYS:HA	1.53	1.38
1:B:1568:LYS:HE3	1:B:1568:LYS:CA	1.41	1.37
1:A:1215:ILE:HD12	1:A:1215:ILE:O	1.17	1.32
1:B:1215:ILE:O	1:B:1215:ILE:HD12	1.21	1.27
1:A:1339:ARG:HH11	1:A:1339:ARG:CB	1.46	1.26
1:B:1568:LYS:HA	1:B:1568:LYS:CE	1.58	1.25
1:A:1339:ARG:HB2	1:A:1339:ARG:NH1	1.49	1.24
1:B:1563:TYR:CE1	1:B:1623:ARG:HG2	1.75	1.21
1:B:1568:LYS:CE	1:B:1569:ASP:H	1.57	1.16
1:B:1566:ARG:NH1	1:B:1570:GLU:HG2	1.60	1.15
1:B:1339:ARG:HG2	1:B:1339:ARG:HH21	1.08	1.13
1:A:1332:ILE:HD12	1:A:1378:LEU:HD23	1.19	1.12
1:A:1371:LEU:H	1:A:1371:LEU:HD12	1.09	1.12
1:B:1371:LEU:HD12	1:B:1371:LEU:H	1.14	1.11
1:A:1177:PRO:HD2	1:A:1180:LYS:HG2	1.33	1.08
1:B:1568:LYS:HE2	1:B:1569:ASP:H	1.00	1.07
1:B:1332:ILE:HD12	1:B:1378:LEU:HD23	1.37	1.06
1:A:1193:LYS:HE3	1:B:1578:CYS:HA	1.12	1.06
1:B:1215:ILE:CD1	1:B:1218:LEU:HB3	1.86	1.05
1:A:1582:VAL:HG12	1:A:1586:LEU:CD2	1.87	1.04
1:A:1371:LEU:HD12	1:A:1371:LEU:N	1.67	1.03
1:B:1563:TYR:HE1	1:B:1623:ARG:HG2	1.04	1.03
1:B:1564:GLN:HE21	1:B:1565:GLY:H	1.04	1.03
1:A:1215:ILE:O	1:A:1215:ILE:CD1	2.08	1.02
1:A:1215:ILE:CD1	1:A:1218:LEU:HB3	1.89	1.02
1:B:1339:ARG:HH21	1:B:1339:ARG:CG	1.73	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1527:ILE:HD13	1:B:1533:PHE:HB2	1.43	1.01
1:B:1399:VAL:HG13	1:B:1461:LEU:HD11	1.42	1.01
1:B:1371:LEU:HD12	1:B:1371:LEU:N	1.71	1.00
1:A:1272:ARG:CZ	1:A:1272:ARG:HB3	1.88	1.00
1:B:1536:ILE:HD12	1:B:1536:ILE:C	1.82	1.00
1:A:1399:VAL:HG13	1:A:1461:LEU:HD11	1.42	0.99
1:B:1568:LYS:CE	1:B:1569:ASP:N	2.25	0.99
1:A:1566:ARG:HH11	1:A:1566:ARG:HG2	1.25	0.98
1:B:1215:ILE:O	1:B:1215:ILE:CD1	2.12	0.98
1:B:1272:ARG:CZ	1:B:1272:ARG:HB3	1.90	0.97
1:B:1568:LYS:CA	1:B:1568:LYS:CE	2.30	0.97
1:A:1536:ILE:C	1:A:1536:ILE:HD12	1.85	0.96
1:B:1164:GLN:NE2	1:B:1534:LYS:HG3	1.80	0.96
1:B:1272:ARG:HB3	1:B:1272:ARG:NH1	1.80	0.96
1:B:1215:ILE:HD11	1:B:1218:LEU:HB3	1.47	0.96
1:B:1568:LYS:HE2	1:B:1569:ASP:N	1.80	0.95
1:A:1272:ARG:HB3	1:A:1272:ARG:NH1	1.81	0.95
1:A:1527:ILE:HD13	1:A:1533:PHE:HB2	1.45	0.94
1:A:1193:LYS:NZ	1:B:1578:CYS:HA	1.82	0.93
1:A:1332:ILE:CD1	1:A:1378:LEU:HD23	1.99	0.93
1:B:1177:PRO:HD2	1:B:1180:LYS:HG2	1.51	0.93
1:A:1160:LEU:HG	1:A:1497:LEU:HD23	1.51	0.93
1:A:1371:LEU:H	1:A:1371:LEU:CD1	1.82	0.92
1:B:1568:LYS:HE3	1:B:1568:LYS:C	1.90	0.92
1:A:1215:ILE:HD12	1:A:1215:ILE:C	1.90	0.92
1:A:1339:ARG:HH11	1:A:1339:ARG:HB2	0.76	0.92
1:A:1527:ILE:HD12	1:A:1636:LEU:HD12	1.51	0.91
1:B:1566:ARG:HH12	1:B:1570:GLU:HG2	1.29	0.89
1:B:1371:LEU:H	1:B:1371:LEU:CD1	1.85	0.89
1:B:1164:GLN:HE22	1:B:1534:LYS:HG3	1.37	0.87
1:B:1215:ILE:HD12	1:B:1215:ILE:C	1.94	0.87
1:B:1160:LEU:HG	1:B:1497:LEU:HD23	1.53	0.87
1:A:1177:PRO:CD	1:A:1180:LYS:HG2	2.05	0.87
1:A:1171:ASN:H	1:A:1171:ASN:ND2	1.71	0.87
1:A:1276:THR:OG1	1:A:1278:ALA:HB3	1.75	0.87
1:B:1177:PRO:CD	1:B:1180:LYS:HG2	2.05	0.87
1:A:1215:ILE:HD13	1:A:1218:LEU:HB3	1.56	0.87
1:A:1536:ILE:HD11	1:A:1634:PHE:CE2	2.10	0.86
1:A:1566:ARG:HH11	1:A:1566:ARG:CG	1.89	0.86
1:B:1563:TYR:CE1	1:B:1623:ARG:CG	2.59	0.86
1:B:1177:PRO:CG	1:B:1180:LYS:HG2	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1339:ARG:HG2	1:B:1339:ARG:NH2	1.71	0.85
1:A:1582:VAL:HG12	1:A:1586:LEU:HD23	1.58	0.85
1:A:1528:SER:HA	1:A:1637:ALA:O	1.77	0.85
1:B:1506:LYS:O	1:B:1507:ASN:HB2	1.75	0.85
1:B:1276:THR:OG1	1:B:1279:LYS:HG3	1.77	0.84
1:B:1566:ARG:NH1	1:B:1570:GLU:CG	2.40	0.84
1:A:1266:TRP:CD1	1:A:1440:ILE:HD12	2.12	0.84
1:A:1170:ILE:HG22	1:A:1170:ILE:O	1.75	0.84
1:B:1597:THR:O	1:B:1598:TYR:CD2	2.30	0.84
1:A:1193:LYS:HE3	1:B:1578:CYS:CA	2.02	0.84
1:A:1160:LEU:CG	1:A:1497:LEU:HD23	2.07	0.83
1:A:1215:ILE:HD11	1:A:1218:LEU:HB3	1.58	0.83
1:A:1447:SER:HB2	1:A:1449:ILE:HG13	1.58	0.83
1:A:1555:VAL:HG23	1:A:1561:ILE:HD11	1.61	0.83
1:B:1563:TYR:CD1	1:B:1623:ARG:NE	2.46	0.83
1:B:1607:ARG:NH2	1:B:1613:LEU:CD1	2.42	0.83
1:A:1160:LEU:CD2	1:A:1497:LEU:HD23	2.09	0.82
1:A:1506:LYS:O	1:A:1507:ASN:HB2	1.78	0.82
1:B:1160:LEU:CD2	1:B:1497:LEU:HD23	2.09	0.82
1:B:1536:ILE:HD11	1:B:1634:PHE:CE2	2.15	0.82
1:B:1272:ARG:NH1	1:B:1272:ARG:CB	2.42	0.82
1:B:1536:ILE:HD12	1:B:1536:ILE:O	1.79	0.82
1:B:1160:LEU:CG	1:B:1497:LEU:HD23	2.09	0.82
1:B:1215:ILE:HD13	1:B:1218:LEU:HB3	1.62	0.81
1:B:1215:ILE:CD1	1:B:1218:LEU:CB	2.58	0.81
1:B:1568:LYS:HE3	1:B:1569:ASP:N	1.89	0.81
1:B:1607:ARG:NH2	1:B:1613:LEU:HD11	1.96	0.81
1:B:1555:VAL:HG23	1:B:1561:ILE:HD11	1.62	0.80
1:A:1193:LYS:CE	1:B:1578:CYS:CA	2.49	0.80
1:A:1527:ILE:HD11	1:A:1533:PHE:CD1	2.17	0.80
1:A:1582:VAL:CG1	1:A:1586:LEU:CD2	2.60	0.80
1:B:1201:LEU:HD12	1:B:1201:LEU:C	2.01	0.80
1:A:1177:PRO:HD2	1:A:1180:LYS:CG	2.11	0.80
1:A:1193:LYS:NZ	1:B:1578:CYS:CA	2.45	0.80
1:A:1215:ILE:HD13	1:A:1218:LEU:CB	2.12	0.80
1:B:1563:TYR:CE2	1:B:1564:GLN:O	2.34	0.80
1:A:1164:GLN:NE2	1:A:1534:LYS:HD2	1.97	0.79
1:A:1398:SER:HB3	1:A:1464:ILE:HD13	1.63	0.79
1:B:1527:ILE:O	1:B:1527:ILE:HD12	1.82	0.79
1:B:1527:ILE:HD11	1:B:1533:PHE:CD1	2.18	0.79
1:B:1177:PRO:HG2	1:B:1180:LYS:HG2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1398:SER:HB3	1:B:1464:ILE:HD13	1.65	0.78
1:B:1215:ILE:HD13	1:B:1218:LEU:CB	2.14	0.78
1:B:1638:PRO:O	1:B:1639:ALA:CB	2.31	0.78
1:B:1333:ASP:C	1:B:1334:LEU:HD23	2.04	0.78
1:B:1381:LYS:HE3	1:B:1480:ASN:OD1	1.84	0.78
1:B:1215:ILE:CD1	1:B:1215:ILE:C	2.53	0.77
1:B:1266:TRP:CD1	1:B:1440:ILE:HD12	2.20	0.77
1:A:1215:ILE:HG13	1:A:1461:LEU:HB3	1.66	0.77
1:A:1536:ILE:HD12	1:A:1536:ILE:O	1.83	0.77
1:A:1272:ARG:NH1	1:A:1272:ARG:CB	2.48	0.76
1:B:1215:ILE:HG13	1:B:1461:LEU:HB3	1.66	0.76
1:B:1564:GLN:HE21	1:B:1565:GLY:N	1.82	0.76
1:B:1568:LYS:HE3	1:B:1568:LYS:HA	0.77	0.76
1:A:1582:VAL:HG12	1:A:1586:LEU:HD22	1.68	0.76
1:A:1164:GLN:NE2	1:A:1534:LYS:HG3	2.00	0.76
1:A:1215:ILE:CD1	1:A:1218:LEU:CB	2.63	0.76
1:A:1334:LEU:N	1:A:1334:LEU:HD23	2.01	0.76
1:A:1215:ILE:CD1	1:A:1215:ILE:C	2.50	0.76
1:A:1333:ASP:C	1:A:1334:LEU:HD23	2.06	0.76
1:B:1187:SER:O	1:B:1188:ILE:HD13	1.86	0.75
1:A:1174:GLU:O	1:A:1176:LEU:HD12	1.86	0.75
1:B:1447:SER:HB2	1:B:1449:ILE:HG13	1.66	0.75
1:A:1582:VAL:CG1	1:A:1586:LEU:HD22	2.16	0.75
1:A:1176:LEU:HD12	1:A:1176:LEU:N	2.00	0.75
1:B:1243:VAL:HG11	1:B:1277:ILE:HG12	1.67	0.75
1:A:1201:LEU:C	1:A:1201:LEU:HD12	2.07	0.75
1:B:1334:LEU:HD23	1:B:1334:LEU:N	2.00	0.75
1:B:1370:ILE:HG21	1:B:1511:ILE:HG23	1.68	0.75
1:A:1381:LYS:HE3	1:A:1480:ASN:OD1	1.87	0.74
1:A:1519:TRP:CE2	1:A:1540:LEU:HD22	2.23	0.73
1:A:1332:ILE:HD12	1:A:1378:LEU:CD2	2.10	0.73
1:B:1243:VAL:CG1	1:B:1277:ILE:HG12	2.18	0.73
1:A:1370:ILE:HG21	1:A:1511:ILE:HG23	1.71	0.73
1:B:1331:ASN:HA	1:B:1377:GLN:NE2	2.04	0.73
1:B:1267:PRO:HG3	1:B:1430:VAL:CG2	2.19	0.72
1:A:1527:ILE:CD1	1:A:1533:PHE:CD1	2.72	0.72
1:B:1336:ASP:OD2	1:B:1339:ARG:HG3	1.89	0.72
1:B:1533:PHE:CE2	1:B:1636:LEU:CD2	2.72	0.72
1:B:1582:VAL:HG11	1:B:1586:LEU:HB3	1.70	0.72
1:B:1394:ASN:HA	1:B:1499:ARG:HG2	1.70	0.72
1:A:1255:GLU:HB2	1:A:1257:TRP:NE1	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1638:PRO:O	1:B:1639:ALA:HB2	1.89	0.71
1:A:1399:VAL:CG1	1:A:1461:LEU:HD11	2.20	0.71
1:B:1398:SER:HB3	1:B:1464:ILE:CD1	2.20	0.71
1:A:1171:ASN:ND2	1:A:1171:ASN:N	2.34	0.71
1:A:1623:ARG:HB2	1:A:1626:GLU:HG3	1.73	0.71
1:B:1607:ARG:CZ	1:B:1613:LEU:HD11	2.21	0.71
1:B:1527:ILE:CD1	1:B:1533:PHE:CD1	2.74	0.71
1:A:1194:ARG:HG3	1:A:1195:ASP:H	1.56	0.71
1:B:1399:VAL:CG1	1:B:1461:LEU:HD11	2.19	0.71
1:B:1164:GLN:NE2	1:B:1534:LYS:CG	2.53	0.71
1:B:1214:VAL:HG22	1:B:1454:PHE:CE1	2.26	0.71
1:B:1328:PHE:HE1	1:B:1381:LYS:HG2	1.55	0.71
1:B:1563:TYR:CD2	1:B:1564:GLN:O	2.44	0.70
1:B:1176:LEU:HD12	1:B:1176:LEU:N	2.05	0.70
1:A:1284:GLN:HE22	1:A:1380:MET:HB3	1.56	0.70
1:B:1332:ILE:CD1	1:B:1378:LEU:HD23	2.18	0.70
1:A:1257:TRP:CD2	1:A:1264:GLN:HG3	2.26	0.70
1:A:1187:SER:O	1:A:1188:ILE:HD13	1.91	0.69
1:A:1239:GLY:O	1:A:1278:ALA:HB2	1.92	0.69
1:A:1257:TRP:CE3	1:A:1264:GLN:HG3	2.27	0.69
1:B:1527:ILE:HD13	1:B:1533:PHE:CB	2.21	0.69
1:A:1328:PHE:HE1	1:A:1381:LYS:HG2	1.58	0.69
1:A:1398:SER:HB3	1:A:1464:ILE:CD1	2.22	0.69
1:B:1177:PRO:HD2	1:B:1180:LYS:CG	2.22	0.69
1:A:1193:LYS:HZ3	1:B:1578:CYS:HB2	1.57	0.69
1:A:1276:THR:HG23	1:A:1279:LYS:HE3	1.75	0.69
1:A:1525:VAL:HG13	1:A:1526:LYS:O	1.92	0.69
1:B:1284:GLN:HE22	1:B:1380:MET:HB3	1.57	0.69
1:B:1597:THR:HG22	1:B:1598:TYR:HD2	1.57	0.69
1:A:1214:VAL:HG22	1:A:1454:PHE:CE1	2.28	0.69
1:B:1564:GLN:NE2	1:B:1565:GLY:H	1.85	0.69
1:B:1372:GLY:HA2	1:B:1377:GLN:HG2	1.75	0.68
1:A:1192:SER:HB3	1:B:1577:GLU:HB3	1.74	0.68
1:B:1623:ARG:HB2	1:B:1626:GLU:HG3	1.74	0.68
1:B:1272:ARG:CG	1:B:1272:ARG:HH11	2.06	0.68
1:B:1563:TYR:CD2	1:B:1563:TYR:C	2.67	0.68
1:A:1267:PRO:HG3	1:A:1430:VAL:CG2	2.24	0.68
1:A:1423:ALA:HB1	1:A:1427:ARG:HH21	1.57	0.68
1:A:1185:THR:HG21	1:A:1454:PHE:CD2	2.29	0.68
1:B:1423:ALA:HB1	1:B:1427:ARG:HH21	1.59	0.68
1:B:1525:VAL:HG13	1:B:1526:LYS:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1372:GLY:HA2	1:A:1377:GLN:HG2	1.76	0.67
1:B:1175:LYS:HG3	1:B:1176:LEU:N	2.08	0.67
1:B:1272:ARG:NH1	1:B:1272:ARG:N	2.41	0.67
1:A:1394:ASN:HA	1:A:1499:ARG:HG2	1.77	0.67
1:A:1537:LYS:HE3	1:A:1634:PHE:O	1.94	0.67
1:A:1238:SER:OG	1:A:1241:HIS:HB2	1.95	0.67
1:B:1406:GLY:HA3	1:B:1476:GLY:HA3	1.76	0.67
1:B:1272:ARG:NH1	1:B:1272:ARG:H	1.91	0.67
1:B:1194:ARG:CB	1:B:1194:ARG:HH21	2.07	0.67
1:A:1339:ARG:CB	1:A:1339:ARG:NH1	2.30	0.66
1:A:1346:GLU:OE1	1:A:1349:LYS:NZ	2.26	0.66
1:B:1386:ARG:HD3	1:B:1438:TRP:CE3	2.30	0.66
1:A:1164:GLN:NE2	1:A:1534:LYS:CG	2.57	0.66
1:B:1253:SER:HA	1:B:1473:GLN:NE2	2.11	0.66
1:A:1188:ILE:O	1:A:1216:ARG:N	2.22	0.66
1:A:1171:ASN:N	1:A:1171:ASN:HD22	1.93	0.66
1:B:1188:ILE:O	1:B:1216:ARG:N	2.22	0.66
1:A:1349:LYS:HE2	1:B:1505:VAL:O	1.96	0.65
1:B:1563:TYR:HD2	1:B:1563:TYR:O	1.78	0.65
1:B:1519:TRP:CD2	1:B:1540:LEU:HD22	2.31	0.65
1:A:1176:LEU:N	1:A:1176:LEU:CD1	2.59	0.65
1:B:1272:ARG:CB	1:B:1272:ARG:HH11	2.09	0.65
1:A:1363:LEU:HD21	1:A:1396:PHE:CD1	2.31	0.65
1:A:1527:ILE:HD12	1:A:1527:ILE:O	1.96	0.65
1:A:1519:TRP:CD2	1:A:1540:LEU:HD22	2.31	0.65
1:A:1253:SER:HA	1:A:1473:GLN:NE2	2.11	0.65
1:B:1607:ARG:NH2	1:B:1613:LEU:HD12	2.11	0.65
1:A:1255:GLU:HB2	1:A:1257:TRP:HE1	1.61	0.65
1:A:1577:GLU:HG3	1:A:1605:CYS:HB3	1.79	0.64
1:A:1585:ILE:HA	1:A:1619:LEU:O	1.96	0.64
1:A:1386:ARG:CG	1:A:1438:TRP:CZ3	2.80	0.64
1:A:1527:ILE:HD13	1:A:1533:PHE:CB	2.24	0.64
1:A:1527:ILE:CD1	1:A:1636:LEU:HD12	2.27	0.64
1:A:1536:ILE:CD1	1:A:1634:PHE:CE2	2.80	0.64
1:B:1536:ILE:CD1	1:B:1540:LEU:HD12	2.26	0.64
1:A:1536:ILE:C	1:A:1536:ILE:CD1	2.58	0.64
1:A:1164:GLN:HE22	1:A:1534:LYS:HD2	1.62	0.64
1:A:1386:ARG:HD3	1:A:1438:TRP:CE3	2.33	0.64
1:B:1563:TYR:HE1	1:B:1623:ARG:CG	1.94	0.64
1:A:1194:ARG:HG3	1:A:1195:ASP:N	2.13	0.64
1:B:1533:PHE:CE2	1:B:1636:LEU:HD21	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:ASP:OD1	1:A:1261:GLY:N	2.32	0.63
1:A:1536:ILE:HG12	1:A:1634:PHE:CZ	2.33	0.63
1:A:1607:ARG:CZ	1:A:1613:LEU:HD11	2.27	0.63
1:A:1359:THR:HG23	1:B:1429:GLY:O	1.98	0.63
1:A:1536:ILE:CG1	1:A:1634:PHE:CE2	2.80	0.63
1:A:1215:ILE:CG1	1:A:1461:LEU:HB3	2.28	0.63
1:B:1185:THR:HG21	1:B:1454:PHE:CD2	2.33	0.63
1:B:1536:ILE:HD11	1:B:1540:LEU:HD12	1.81	0.63
1:A:1200:VAL:CG1	1:A:1201:LEU:N	2.62	0.63
1:B:1598:TYR:O	1:B:1599:LEU:HD13	1.98	0.63
1:B:1194:ARG:HH21	1:B:1194:ARG:HB2	1.64	0.63
1:B:1331:ASN:HB3	1:B:1377:GLN:HE22	1.64	0.63
1:A:1582:VAL:CG1	1:A:1586:LEU:HD23	2.28	0.63
1:B:1195:ASP:O	1:B:1198:SER:HB3	1.98	0.62
1:B:1272:ARG:HH11	1:B:1272:ARG:H	1.45	0.62
1:B:1252:PRO:HD2	1:B:1255:GLU:HG3	1.81	0.62
1:B:1536:ILE:CG1	1:B:1634:PHE:CE2	2.81	0.62
1:B:1519:TRP:CE2	1:B:1540:LEU:HD22	2.34	0.62
1:A:1590:SER:O	1:A:1591:GLU:O	2.17	0.62
1:B:1563:TYR:CD1	1:B:1623:ARG:HG2	2.32	0.62
1:A:1164:GLN:HE22	1:A:1534:LYS:HG3	1.63	0.62
1:B:1331:ASN:HD22	1:B:1377:GLN:HE21	1.47	0.62
1:B:1176:LEU:HB3	1:B:1177:PRO:HD2	1.80	0.62
1:A:1276:THR:OG1	1:A:1279:LYS:HG3	1.99	0.62
1:A:1527:ILE:HD12	1:A:1636:LEU:CD1	2.26	0.62
1:A:1164:GLN:NE2	1:A:1534:LYS:CD	2.63	0.62
1:B:1533:PHE:CD2	1:B:1636:LEU:HD21	2.35	0.61
1:B:1328:PHE:CE1	1:B:1381:LYS:HG2	2.35	0.61
1:A:1363:LEU:HD21	1:A:1396:PHE:CE1	2.34	0.61
1:A:1536:ILE:CD1	1:A:1540:LEU:HD12	2.30	0.61
1:A:1176:LEU:CD1	1:A:1176:LEU:H	2.14	0.61
1:A:1254:ASP:OD1	1:A:1254:ASP:N	2.23	0.61
1:A:1568:LYS:HG2	1:A:1569:ASP:OD2	2.00	0.61
1:B:1386:ARG:CG	1:B:1438:TRP:CZ3	2.83	0.61
1:B:1536:ILE:C	1:B:1536:ILE:CD1	2.55	0.61
1:A:1588:VAL:HG21	1:A:1619:LEU:HD11	1.82	0.61
1:A:1280:TYR:HE2	1:A:1284:GLN:HE21	1.48	0.61
1:B:1253:SER:HB2	1:B:1411:PHE:HZ	1.66	0.61
1:B:1238:SER:OG	1:B:1241:HIS:HB2	2.00	0.60
1:A:1214:VAL:HG21	1:A:1454:PHE:CD1	2.36	0.60
1:A:1272:ARG:NH1	1:A:1272:ARG:N	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1243:VAL:CG1	1:B:1277:ILE:CG1	2.79	0.60
1:B:1506:LYS:O	1:B:1507:ASN:CB	2.49	0.60
1:A:1252:PRO:HD2	1:A:1255:GLU:HG3	1.81	0.60
1:A:1272:ARG:H	1:A:1272:ARG:HH11	1.50	0.60
1:B:1386:ARG:HG3	1:B:1438:TRP:CZ3	2.36	0.60
1:B:1588:VAL:HG21	1:B:1619:LEU:HD11	1.84	0.60
1:B:1202:LEU:HD13	1:B:1353:PHE:CG	2.37	0.60
1:B:1336:ASP:OD2	1:B:1339:ARG:CG	2.50	0.60
1:B:1409:GLU:OE2	1:B:1453:ARG:NH2	2.29	0.60
1:B:1536:ILE:HG12	1:B:1634:PHE:CZ	2.36	0.60
1:B:1588:VAL:HA	1:B:1599:LEU:O	2.02	0.60
1:B:1175:LYS:HG3	1:B:1176:LEU:H	1.66	0.60
1:B:1201:LEU:HD11	1:B:1353:PHE:CZ	2.36	0.60
1:A:1201:LEU:HD11	1:A:1353:PHE:CZ	2.36	0.59
1:A:1588:VAL:HA	1:A:1599:LEU:O	2.02	0.59
1:B:1254:ASP:OD1	1:B:1254:ASP:N	2.29	0.59
1:B:1258:ASP:OD1	1:B:1261:GLY:N	2.35	0.59
1:A:1381:LYS:NZ	2:A:1701:OGA:O3	2.32	0.59
1:A:1555:VAL:CG2	1:A:1561:ILE:HD11	2.31	0.59
1:B:1200:VAL:CG1	1:B:1201:LEU:N	2.64	0.59
1:B:1251:GLN:OE1	1:B:1256:ASN:HA	2.02	0.59
1:B:1160:LEU:HD21	1:B:1497:LEU:HD23	1.85	0.59
1:B:1218:LEU:O	1:B:1221:SER:HB3	2.02	0.59
1:A:1253:SER:HB2	1:A:1411:PHE:HZ	1.67	0.59
1:B:1215:ILE:CG1	1:B:1461:LEU:HB3	2.32	0.59
1:B:1536:ILE:CD1	1:B:1540:LEU:CD1	2.81	0.59
1:B:1255:GLU:HB2	1:B:1257:TRP:NE1	2.18	0.59
1:B:1536:ILE:CD1	1:B:1634:PHE:CE2	2.84	0.59
1:A:1195:ASP:O	1:A:1198:SER:HB3	2.03	0.59
1:A:1527:ILE:CD1	1:A:1636:LEU:CD1	2.81	0.59
1:B:1363:LEU:HD21	1:B:1396:PHE:CD1	2.38	0.59
1:A:1386:ARG:HG3	1:A:1438:TRP:CZ3	2.37	0.58
1:A:1177:PRO:CG	1:A:1180:LYS:HG2	2.32	0.58
1:B:1597:THR:HG22	1:B:1598:TYR:CD2	2.36	0.58
1:A:1536:ILE:HD11	1:A:1540:LEU:HD12	1.86	0.58
1:B:1214:VAL:HG21	1:B:1454:PHE:CD1	2.38	0.58
1:B:1334:LEU:HA	1:B:1340:TRP:CD1	2.39	0.58
1:B:1201:LEU:HD11	1:B:1353:PHE:HZ	1.67	0.58
1:B:1230:SER:O	1:B:1234:LEU:HG	2.04	0.58
1:B:1331:ASN:HD22	1:B:1377:GLN:NE2	2.01	0.58
1:A:1334:LEU:HA	1:A:1340:TRP:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1555:VAL:CG2	1:B:1561:ILE:HD11	2.32	0.58
1:A:1485:VAL:O	1:A:1487:PRO:HD3	2.04	0.58
1:A:1160:LEU:HD21	1:A:1497:LEU:HD23	1.83	0.58
1:B:1280:TYR:HE2	1:B:1284:GLN:HE21	1.52	0.57
1:B:1267:PRO:HG3	1:B:1430:VAL:HG21	1.85	0.57
1:A:1201:LEU:HD11	1:A:1353:PHE:HZ	1.69	0.57
1:A:1565:GLY:O	1:A:1566:ARG:CG	2.52	0.57
1:B:1588:VAL:CG1	1:B:1598:TYR:HD1	2.18	0.57
1:A:1193:LYS:HZ1	1:B:1578:CYS:C	2.06	0.57
1:A:1536:ILE:CG1	1:A:1634:PHE:CZ	2.88	0.57
1:A:1272:ARG:CB	1:A:1272:ARG:HH11	2.16	0.57
1:B:1331:ASN:CB	1:B:1377:GLN:HE22	2.18	0.57
1:B:1394:ASN:O	1:B:1496:ALA:HA	2.04	0.57
1:A:1566:ARG:CG	1:A:1566:ARG:NH1	2.57	0.57
1:B:1536:ILE:CG1	1:B:1634:PHE:CZ	2.87	0.57
1:A:1566:ARG:HG2	1:A:1566:ARG:NH1	2.06	0.57
1:A:1455:VAL:HG12	1:A:1457:ARG:HD2	1.87	0.57
1:A:1394:ASN:O	1:A:1496:ALA:HA	2.05	0.56
1:B:1339:ARG:HH21	1:B:1339:ARG:CB	2.17	0.56
1:B:1363:LEU:HD21	1:B:1396:PHE:CE1	2.38	0.56
1:A:1176:LEU:HB3	1:A:1180:LYS:CB	2.36	0.56
1:A:1328:PHE:CE1	1:A:1381:LYS:HG2	2.40	0.56
1:A:1231:THR:OG1	1:A:1380:MET:CE	2.53	0.56
1:A:1340:TRP:O	1:A:1343:GLN:HB2	2.06	0.56
1:B:1597:THR:O	1:B:1598:TYR:CG	2.58	0.56
1:A:1215:ILE:CD1	1:A:1461:LEU:H	2.18	0.56
1:B:1373:MET:SD	1:B:1511:ILE:CG2	2.94	0.56
1:B:1577:GLU:HG3	1:B:1605:CYS:HB3	1.86	0.56
1:B:1588:VAL:HG12	1:B:1598:TYR:HD1	1.69	0.56
1:A:1231:THR:CG2	1:A:1281:ALA:HB1	2.35	0.56
1:A:1193:LYS:HZ1	1:B:1578:CYS:CA	2.18	0.56
1:A:1346:GLU:OE1	1:A:1349:LYS:HE3	2.05	0.56
1:B:1527:ILE:CD1	1:B:1533:PHE:HD1	2.19	0.56
1:B:1598:TYR:O	1:B:1599:LEU:CD1	2.53	0.56
1:A:1253:SER:CA	1:A:1473:GLN:NE2	2.69	0.56
1:A:1366:VAL:HG21	1:A:1370:ILE:HD11	1.87	0.56
1:A:1559:LYS:HE3	1:A:1613:LEU:HB2	1.88	0.56
1:A:1214:VAL:CG2	1:A:1454:PHE:CD1	2.89	0.56
1:A:1246:ARG:HD2	1:A:1270:SER:OG	2.06	0.56
1:B:1533:PHE:CE2	1:B:1636:LEU:HD22	2.41	0.56
1:B:1533:PHE:CZ	1:B:1636:LEU:HD22	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1567:VAL:HG23	1:B:1568:LYS:N	2.21	0.56
1:A:1536:ILE:CD1	1:A:1540:LEU:CD1	2.84	0.55
1:B:1253:SER:CA	1:B:1473:GLN:NE2	2.68	0.55
1:B:1340:TRP:O	1:B:1343:GLN:HB2	2.06	0.55
1:B:1392:GLU:HG3	1:B:1398:SER:HB2	1.88	0.55
1:A:1193:LYS:HZ3	1:B:1578:CYS:CB	2.19	0.55
1:A:1200:VAL:HG12	1:A:1201:LEU:N	2.21	0.55
1:A:1251:GLN:OE1	1:A:1256:ASN:HA	2.05	0.55
1:B:1603:GLU:O	1:B:1607:ARG:HG3	2.06	0.55
1:A:1290:GLU:HG2	1:A:1291:SER:N	2.20	0.55
1:B:1533:PHE:CD2	1:B:1636:LEU:CD2	2.89	0.55
1:A:1339:ARG:HH11	1:A:1339:ARG:CG	2.16	0.55
1:B:1258:ASP:OD2	1:B:1262:THR:OG1	2.20	0.55
1:A:1202:LEU:HD13	1:A:1353:PHE:CG	2.42	0.55
1:A:1272:ARG:NH1	1:A:1272:ARG:H	2.05	0.55
1:A:1276:THR:HG23	1:A:1279:LYS:CE	2.36	0.55
1:B:1577:GLU:OE1	1:B:1601:HIS:ND1	2.38	0.55
1:A:1207:ASP:OD2	1:A:1209:ARG:NH1	2.39	0.55
1:A:1332:ILE:HG13	1:A:1378:LEU:O	2.06	0.55
1:A:1547:CYS:SG	1:A:1584:ASN:OD1	2.65	0.55
1:B:1485:VAL:O	1:B:1487:PRO:HD3	2.06	0.55
1:A:1392:GLU:HG3	1:A:1398:SER:HB2	1.89	0.55
1:A:1346:GLU:OE1	1:A:1349:LYS:CE	2.55	0.54
1:A:1398:SER:CB	1:A:1464:ILE:HD13	2.33	0.54
1:B:1582:VAL:HG12	1:B:1582:VAL:O	2.06	0.54
1:B:1372:GLY:HA2	1:B:1377:GLN:CG	2.37	0.54
1:A:1223:ARG:NH1	1:B:1578:CYS:SG	2.77	0.54
1:A:1331:ASN:HA	1:A:1377:GLN:NE2	2.22	0.54
1:A:1363:LEU:CD2	1:A:1396:PHE:CE1	2.91	0.54
1:B:1272:ARG:HH11	1:B:1272:ARG:HG2	1.71	0.54
1:B:1561:ILE:HA	1:B:1618:VAL:HG13	1.88	0.54
1:A:1577:GLU:OE1	1:A:1601:HIS:ND1	2.40	0.54
1:B:1214:VAL:CG2	1:B:1454:PHE:CD1	2.90	0.54
1:B:1559:LYS:HE3	1:B:1613:LEU:HB2	1.89	0.54
1:A:1409:GLU:OE2	1:A:1453:ARG:NH2	2.32	0.54
1:B:1502:TRP:CZ2	1:B:1506:LYS:HE2	2.43	0.54
1:A:1527:ILE:CD1	1:A:1533:PHE:HD1	2.18	0.53
1:B:1551:ARG:NH1	1:B:1620:GLU:OE1	2.42	0.53
1:B:1586:LEU:HD12	1:B:1619:LEU:HD12	1.90	0.53
1:A:1215:ILE:HD11	1:A:1461:LEU:H	1.73	0.53
1:A:1225:ASN:HB3	1:A:1228:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1230:SER:O	1:A:1234:LEU:HG	2.09	0.53
1:A:1415:GLU:HB2	1:A:1467:GLY:HA3	1.90	0.53
1:B:1536:ILE:HG13	1:B:1634:PHE:CE2	2.44	0.53
1:A:1566:ARG:NH1	1:A:1566:ARG:HB3	2.24	0.53
1:B:1333:ASP:O	1:B:1334:LEU:HD23	2.08	0.53
1:B:1582:VAL:CG1	1:B:1586:LEU:HB3	2.36	0.53
1:A:1555:VAL:HG23	1:A:1561:ILE:CD1	2.37	0.53
1:A:1218:LEU:O	1:A:1221:SER:HB3	2.09	0.52
1:A:1577:GLU:CG	1:A:1605:CYS:HB3	2.38	0.52
1:A:1333:ASP:O	1:A:1334:LEU:HD23	2.09	0.52
1:B:1609:ARG:HG3	1:B:1610:SER:N	2.25	0.52
1:A:1400:ASN:ND2	2:A:1701:OGA:O4	2.42	0.52
1:A:1533:PHE:CZ	1:A:1537:LYS:HD2	2.45	0.52
1:B:1373:MET:SD	1:B:1511:ILE:HG21	2.50	0.52
1:B:1523:ARG:HD3	1:B:1524:THR:HG23	1.92	0.52
1:A:1373:MET:SD	1:A:1511:ILE:CG2	2.97	0.52
1:A:1585:ILE:O	1:A:1586:LEU:HD23	2.09	0.52
1:A:1169:LYS:HB3	1:A:1171:ASN:HD21	1.75	0.52
1:B:1398:SER:CB	1:B:1464:ILE:HD13	2.37	0.52
1:A:1177:PRO:HG2	1:A:1180:LYS:HG2	1.92	0.52
1:A:1258:ASP:OD1	1:A:1261:GLY:CA	2.57	0.52
1:B:1215:ILE:CD1	1:B:1461:LEU:H	2.22	0.52
1:B:1492:GLN:HE21	1:B:1492:GLN:C	2.11	0.52
1:B:1231:THR:OG1	1:B:1380:MET:CE	2.58	0.52
1:B:1366:VAL:HG21	1:B:1370:ILE:HD11	1.91	0.52
1:A:1372:GLY:HA2	1:A:1377:GLN:CG	2.39	0.52
1:A:1544:MET:HE1	1:A:1631:TYR:CG	2.44	0.52
1:A:1561:ILE:HA	1:A:1618:VAL:HG13	1.92	0.51
1:B:1177:PRO:HB2	1:B:1179:GLU:OE2	2.10	0.51
1:B:1563:TYR:CD2	1:B:1563:TYR:O	2.61	0.51
1:B:1420:THR:O	1:B:1423:ALA:HB3	2.10	0.51
1:A:1257:TRP:CZ2	1:A:1264:GLN:CD	2.84	0.51
1:A:1280:TYR:C	1:A:1280:TYR:CD2	2.84	0.51
1:B:1214:VAL:CG2	1:B:1454:PHE:CE1	2.92	0.51
1:A:1164:GLN:HE22	1:A:1534:LYS:CD	2.24	0.51
1:A:1361:ASN:O	1:A:1364:SER:HB2	2.11	0.51
1:B:1391:GLN:OE1	1:B:1499:ARG:NH1	2.43	0.51
1:B:1431:ASP:OD2	1:B:1434:THR:HG23	2.11	0.51
1:A:1218:LEU:HD22	1:A:1461:LEU:HB2	1.93	0.51
1:A:1328:PHE:CD1	1:A:1385:SER:HB3	2.46	0.51
1:B:1257:TRP:CE3	1:B:1264:GLN:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:ARG:HH11	1:A:1272:ARG:CG	2.23	0.51
1:A:1609:ARG:HG3	1:A:1610:SER:N	2.25	0.51
1:B:1225:ASN:HB3	1:B:1228:LEU:HD12	1.93	0.51
1:B:1401:ILE:HG12	1:B:1461:LEU:HD12	1.93	0.51
1:A:1266:TRP:NE1	1:A:1440:ILE:HD12	2.26	0.50
1:B:1401:ILE:CG1	1:B:1461:LEU:HD12	2.42	0.50
1:B:1402:ASN:OD1	1:B:1404:GLY:N	2.44	0.50
1:B:1194:ARG:HB2	1:B:1194:ARG:NH2	2.26	0.50
1:B:1272:ARG:NH1	1:B:1272:ARG:CG	2.69	0.50
1:B:1527:ILE:HD11	1:B:1636:LEU:HA	1.92	0.50
1:B:1544:MET:HE1	1:B:1631:TYR:CG	2.45	0.50
1:A:1214:VAL:CG2	1:A:1454:PHE:CE1	2.92	0.50
1:A:1391:GLN:OE1	1:A:1499:ARG:NH1	2.45	0.50
1:B:1241:HIS:HB3	1:B:1277:ILE:CD1	2.41	0.50
1:A:1536:ILE:HG13	1:A:1634:PHE:CE2	2.46	0.50
1:A:1563:TYR:CZ	1:A:1565:GLY:HA2	2.47	0.50
1:B:1175:LYS:HA	1:B:1448:ASN:HD21	1.76	0.50
1:B:1577:GLU:CG	1:B:1605:CYS:HB3	2.41	0.50
1:A:1345:GLN:NE2	1:B:1506:LYS:NZ	2.59	0.50
1:B:1587:PHE:O	1:B:1600:VAL:HA	2.12	0.50
1:A:1252:PRO:HG2	1:A:1255:GLU:OE1	2.12	0.50
1:B:1563:TYR:CD1	1:B:1623:ARG:CD	2.95	0.50
1:B:1176:LEU:HD23	1:B:1180:LYS:HB3	1.93	0.49
1:B:1200:VAL:HG12	1:B:1201:LEU:N	2.27	0.49
1:B:1363:LEU:CD2	1:B:1396:PHE:CE1	2.95	0.49
1:B:1258:ASP:OD1	1:B:1261:GLY:CA	2.59	0.49
1:A:1229:PHE:HB2	1:A:1403:ILE:HD12	1.95	0.49
1:A:1440:ILE:HG22	1:A:1443:ASP:H	1.77	0.49
1:A:1164:GLN:HE22	1:A:1534:LYS:CG	2.23	0.49
1:B:1218:LEU:HD22	1:B:1461:LEU:HB2	1.93	0.49
1:B:1252:PRO:HB2	1:B:1255:GLU:HG2	1.94	0.49
1:B:1256:ASN:O	1:B:1264:GLN:HG2	2.12	0.49
1:A:1188:ILE:O	1:A:1188:ILE:HG22	2.09	0.49
1:B:1328:PHE:CD1	1:B:1385:SER:HB3	2.47	0.49
1:A:1255:GLU:CB	1:A:1257:TRP:HE1	2.24	0.49
1:B:1506:LYS:HB3	1:B:1508:VAL:HG23	1.94	0.49
1:A:1565:GLY:O	1:A:1566:ARG:HG3	2.12	0.49
1:B:1250:GLN:OE1	1:B:1324:HIS:ND1	2.46	0.49
1:B:1566:ARG:HH11	1:B:1570:GLU:HG2	1.67	0.49
1:A:1193:LYS:HE3	1:B:1577:GLU:O	2.13	0.48
1:B:1529:ASP:OD2	1:B:1532:LEU:N	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1267:PRO:HG3	1:A:1430:VAL:HG21	1.94	0.48
1:B:1566:ARG:HA	1:B:1570:GLU:OE1	2.13	0.48
1:B:1588:VAL:CG1	1:B:1598:TYR:CD1	2.95	0.48
1:B:1231:THR:CG2	1:B:1281:ALA:HB1	2.42	0.48
1:A:1520:ASN:O	1:A:1524:THR:OG1	2.31	0.48
1:A:1378:LEU:HG	1:A:1379:TYR:N	2.28	0.48
1:A:1190:LEU:O	1:B:1608:ARG:NH2	2.47	0.48
1:A:1222:LEU:CB	1:A:1224:LEU:HD12	2.43	0.48
1:A:1351:PRO:HG2	1:A:1354:MET:CE	2.43	0.48
1:A:1551:ARG:NH1	1:A:1620:GLU:OE1	2.46	0.48
1:A:1260:THR:OG1	1:A:1262:THR:OG1	2.30	0.48
1:A:1411:PHE:N	1:A:1411:PHE:CD1	2.82	0.48
1:B:1283:TYR:CE2	1:B:1382:VAL:HG11	2.48	0.48
1:A:1280:TYR:CD2	1:A:1280:TYR:O	2.67	0.48
1:A:1403:ILE:HB	1:A:1479:ASN:O	2.14	0.48
1:A:1526:LYS:HB3	1:A:1637:ALA:CB	2.44	0.48
1:B:1176:LEU:HD22	1:B:1181:LEU:HD23	1.96	0.48
1:A:1193:LYS:NZ	1:B:1578:CYS:CB	2.76	0.48
1:A:1207:ASP:OD1	1:A:1208:PRO:HD2	2.13	0.48
1:A:1362:MET:HE3	1:A:1487:PRO:O	2.14	0.48
1:A:1584:ASN:O	1:A:1586:LEU:HG	2.13	0.48
1:B:1415:GLU:HB2	1:B:1467:GLY:HA3	1.96	0.48
1:B:1222:LEU:CB	1:B:1224:LEU:HD12	2.44	0.47
1:A:1567:VAL:HG23	1:A:1570:GLU:HB2	1.95	0.47
1:B:1241:HIS:HB3	1:B:1277:ILE:HD12	1.95	0.47
1:B:1258:ASP:OD1	1:B:1262:THR:N	2.44	0.47
1:A:1272:ARG:N	1:A:1272:ARG:HH11	2.09	0.47
1:B:1472:VAL:HG12	1:B:1473:GLN:N	2.29	0.47
1:A:1253:SER:O	1:A:1438:TRP:HZ2	1.98	0.47
1:A:1523:ARG:HB2	1:B:1260:THR:HG23	1.95	0.47
1:A:1526:LYS:HE3	1:B:1269:GLU:CD	2.34	0.47
1:A:1178:ARG:HD3	1:A:1178:ARG:O	2.13	0.47
1:A:1257:TRP:CE2	1:A:1264:GLN:HG3	2.50	0.47
1:A:1372:GLY:CA	1:A:1377:GLN:CG	2.92	0.47
1:B:1351:PRO:HG2	1:B:1354:MET:CE	2.45	0.47
1:B:1363:LEU:HD12	1:B:1484:ASN:O	2.14	0.47
1:B:1472:VAL:HG21	2:B:1701:OGA:H4C2	1.95	0.47
1:A:1215:ILE:HG12	1:A:1218:LEU:HD13	1.97	0.47
1:A:1361:ASN:HD21	1:A:1485:VAL:HA	1.78	0.47
1:B:1411:PHE:CD1	1:B:1411:PHE:N	2.83	0.47
1:A:1190:LEU:HD23	1:A:1190:LEU:HA	1.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1363:LEU:HD12	1:A:1484:ASN:O	2.15	0.47
1:A:1566:ARG:NH1	1:A:1566:ARG:CB	2.78	0.47
1:B:1255:GLU:HB3	1:B:1264:GLN:OE1	2.15	0.47
1:B:1351:PRO:HG2	1:B:1354:MET:HE3	1.96	0.47
1:A:1253:SER:O	1:A:1438:TRP:CZ2	2.68	0.47
1:A:1420:THR:O	1:A:1423:ALA:HB3	2.15	0.47
1:A:1587:PHE:O	1:A:1600:VAL:HA	2.15	0.47
1:A:1252:PRO:HB2	1:A:1255:GLU:HG2	1.96	0.47
1:A:1275:THR:OG1	1:A:1279:LYS:HD2	2.15	0.47
1:A:1431:ASP:OD2	1:A:1434:THR:HG23	2.15	0.47
1:A:1570:GLU:HA	1:A:1571:PRO:HD2	1.80	0.47
1:B:1266:TRP:NE1	1:B:1440:ILE:HD12	2.30	0.47
1:A:1253:SER:HB2	1:A:1411:PHE:CZ	2.49	0.46
1:A:1276:THR:HG1	1:A:1279:LYS:HG3	1.80	0.46
1:A:1527:ILE:HD13	1:A:1533:PHE:CD1	2.49	0.46
1:B:1536:ILE:HD12	1:B:1537:LYS:N	2.30	0.46
1:B:1563:TYR:CE1	1:B:1623:ARG:NE	2.82	0.46
1:B:1555:VAL:HG23	1:B:1561:ILE:CD1	2.38	0.46
1:A:1529:ASP:OD2	1:A:1532:LEU:HB2	2.14	0.46
1:A:1523:ARG:O	1:B:1259:LEU:HG	2.16	0.46
1:B:1222:LEU:HB2	1:B:1224:LEU:CD1	2.45	0.46
1:B:1272:ARG:HH11	1:B:1272:ARG:N	2.07	0.46
1:A:1252:PRO:HG2	1:A:1255:GLU:CD	2.35	0.46
1:B:1188:ILE:O	1:B:1188:ILE:HG22	2.15	0.46
1:B:1225:ASN:O	1:B:1228:LEU:HD12	2.15	0.46
1:A:1373:MET:SD	1:A:1511:ILE:HG21	2.55	0.46
1:B:1201:LEU:C	1:B:1201:LEU:CD1	2.78	0.46
1:A:1222:LEU:HB2	1:A:1224:LEU:CD1	2.45	0.46
1:A:1504:GLU:HG2	1:A:1580:VAL:HG23	1.98	0.46
1:A:1583:PHE:CD2	1:A:1584:ASN:HB2	2.50	0.46
1:B:1280:TYR:CD2	1:B:1280:TYR:C	2.88	0.46
1:A:1160:LEU:CD2	1:A:1497:LEU:CD2	2.89	0.46
1:A:1185:THR:HG21	1:A:1454:PHE:HB3	1.98	0.46
1:A:1193:LYS:NZ	1:B:1578:CYS:HB2	2.29	0.46
1:A:1566:ARG:NH1	1:A:1570:GLU:OE1	2.49	0.46
1:B:1160:LEU:CD2	1:B:1497:LEU:CD2	2.90	0.46
1:A:1330:THR:O	1:A:1331:ASN:HB2	2.15	0.46
1:B:1243:VAL:HG12	1:B:1277:ILE:CG1	2.46	0.46
1:B:1253:SER:O	1:B:1438:TRP:CZ2	2.69	0.46
1:A:1258:ASP:OD1	1:A:1262:THR:N	2.48	0.45
1:A:1373:MET:CE	1:A:1393:ASN:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1564:GLN:O	1:A:1621:GLN:HA	2.16	0.45
1:B:1243:VAL:HG12	1:B:1277:ILE:HG12	1.98	0.45
1:B:1559:LYS:HD3	1:B:1559:LYS:HA	1.80	0.45
1:A:1176:LEU:HB3	1:A:1180:LYS:HB2	1.99	0.45
1:B:1185:THR:HG21	1:B:1454:PHE:HB3	1.98	0.45
1:B:1361:ASN:C	1:B:1361:ASN:OD1	2.54	0.45
1:B:1176:LEU:N	1:B:1176:LEU:CD1	2.78	0.45
1:B:1257:TRP:CD2	1:B:1264:GLN:HG3	2.51	0.45
1:A:1447:SER:CB	1:A:1449:ILE:HG13	2.39	0.45
1:A:1523:ARG:HD2	1:B:1258:ASP:OD2	2.16	0.45
1:B:1372:GLY:CA	1:B:1377:GLN:CG	2.94	0.45
1:B:1449:ILE:HA	1:B:1450:PRO:HD3	1.83	0.45
1:B:1566:ARG:HD2	1:B:1622:TYR:CZ	2.51	0.45
1:A:1353:PHE:CE1	1:A:1354:MET:HE3	2.52	0.45
1:A:1257:TRP:CZ3	1:A:1264:GLN:HG3	2.51	0.45
1:B:1222:LEU:HB2	1:B:1224:LEU:HD12	1.98	0.45
1:B:1361:ASN:O	1:B:1364:SER:HB2	2.17	0.45
1:B:1383:PRO:HD3	1:B:1477:TRP:CE2	2.52	0.45
1:B:1454:PHE:HE1	1:B:1462:VAL:HG22	1.80	0.45
1:B:1575:CYS:SG	1:B:1577:GLU:HG2	2.56	0.45
1:A:1339:ARG:NH1	1:A:1339:ARG:CG	2.75	0.45
1:A:1511:ILE:HA	1:A:1511:ILE:HD13	1.34	0.45
1:A:1519:TRP:CE2	1:A:1540:LEU:CD2	2.98	0.45
1:A:1529:ASP:OD2	1:A:1532:LEU:N	2.35	0.45
1:B:1201:LEU:HD12	1:B:1202:LEU:N	2.32	0.45
1:B:1457:ARG:O	1:B:1460:ASP:HB2	2.17	0.45
1:B:1566:ARG:HD3	1:B:1622:TYR:OH	2.16	0.45
1:A:1383:PRO:HD3	1:A:1477:TRP:CE2	2.52	0.45
1:A:1402:ASN:OD1	1:A:1404:GLY:N	2.50	0.45
1:A:1588:VAL:CG1	1:A:1598:TYR:HD1	2.29	0.45
1:B:1253:SER:O	1:B:1438:TRP:HZ2	2.00	0.45
1:B:1381:LYS:CD	1:B:1474:ALA:HB2	2.46	0.45
1:B:1381:LYS:HD2	1:B:1474:ALA:HB2	1.99	0.45
1:B:1589:THR:O	1:B:1598:TYR:HA	2.17	0.45
1:A:1283:TYR:CE2	1:A:1382:VAL:HG11	2.52	0.45
1:A:1440:ILE:O	1:A:1443:ASP:HB2	2.16	0.45
1:A:1441:LEU:HB3	1:A:1445:TYR:CE2	2.52	0.45
1:A:1401:ILE:CG1	1:A:1461:LEU:HD12	2.47	0.44
1:B:1255:GLU:HB2	1:B:1257:TRP:HE1	1.81	0.44
1:B:1362:MET:HE3	1:B:1487:PRO:O	2.18	0.44
1:A:1526:LYS:HB3	1:A:1637:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1253:SER:HB2	1:B:1411:PHE:CZ	2.49	0.44
1:B:1597:THR:O	1:B:1597:THR:HG22	2.16	0.44
1:A:1500:TYR:CD1	1:A:1514:MET:HB2	2.51	0.44
1:A:1536:ILE:HG13	1:A:1634:PHE:HE2	1.83	0.44
1:A:1166:VAL:HG21	1:A:1490:ALA:HB3	2.00	0.44
1:B:1207:ASP:OD1	1:B:1208:PRO:HD2	2.18	0.44
1:A:1485:VAL:O	1:A:1485:VAL:HG23	2.18	0.44
1:A:1554:LEU:HD23	1:A:1554:LEU:HA	1.71	0.44
1:A:1585:ILE:H	1:A:1585:ILE:HG13	1.62	0.44
1:A:1625:GLU:O	1:A:1626:GLU:C	2.55	0.44
1:B:1542:GLN:O	1:B:1546[A]:HIS:CD2	2.71	0.44
1:B:1190:LEU:HD23	1:B:1190:LEU:HA	1.62	0.44
1:A:1529:ASP:OD2	1:A:1532:LEU:CB	2.65	0.44
1:A:1566:ARG:HH11	1:A:1566:ARG:CB	2.31	0.44
1:A:1582:VAL:HG11	1:A:1586:LEU:HD22	1.98	0.44
1:A:1222:LEU:HB2	1:A:1224:LEU:HD12	1.98	0.44
1:A:1244:GLU:OE2	1:A:1331:ASN:OD1	2.36	0.44
1:A:1370:ILE:CG2	1:A:1511:ILE:HG23	2.45	0.44
1:A:1577:GLU:N	1:A:1577:GLU:CD	2.70	0.44
1:B:1331:ASN:CA	1:B:1377:GLN:NE2	2.79	0.44
1:A:1160:LEU:HG	1:A:1497:LEU:CD2	2.35	0.43
1:A:1568:LYS:HE3	1:A:1568:LYS:HB3	1.76	0.43
1:A:1372:GLY:CA	1:A:1377:GLN:HG2	2.47	0.43
1:A:1454:PHE:HE1	1:A:1462:VAL:HG22	1.83	0.43
1:A:1276:THR:H	1:A:1279:LYS:HE3	1.82	0.43
1:B:1511:ILE:HA	1:B:1511:ILE:HD13	1.42	0.43
1:A:1161:SER:HB3	1:A:1164:GLN:HG3	2.01	0.43
1:B:1215:ILE:HD11	1:B:1461:LEU:H	1.82	0.43
1:B:1378:LEU:HG	1:B:1379:TYR:N	2.33	0.43
1:A:1567:VAL:O	1:B:1263:ARG:NH1	2.46	0.43
1:B:1492:GLN:CA	1:B:1492:GLN:NE2	2.81	0.43
1:B:1506:LYS:HD3	1:B:1506:LYS:HA	1.82	0.43
1:A:1225:ASN:O	1:A:1228:LEU:HD12	2.18	0.43
1:B:1566:ARG:NH1	1:B:1570:GLU:CD	2.72	0.43
1:A:1183:PRO:HD2	1:A:1451:VAL:O	2.19	0.43
1:A:1210:ASN:HA	1:A:1211:PRO:HD2	1.87	0.43
1:B:1245:VAL:HG11	1:B:1327:LYS:HE2	2.01	0.43
1:A:1176:LEU:HB3	1:A:1180:LYS:CG	2.49	0.42
1:A:1536:ILE:HD12	1:A:1537:LYS:N	2.30	0.42
1:B:1161:SER:HB3	1:B:1164:GLN:HG3	2.00	0.42
1:B:1519:TRP:CD2	1:B:1540:LEU:CD2	3.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1554:LEU:CD1	1:B:1618:VAL:HG21	2.49	0.42
1:A:1178:ARG:C	1:A:1178:ARG:CD	2.88	0.42
1:B:1215:ILE:HD13	1:B:1218:LEU:HB2	1.96	0.42
1:A:1202:LEU:HD13	1:A:1353:PHE:CD2	2.54	0.42
1:A:1279:LYS:O	1:A:1282:GLN:CB	2.67	0.42
1:A:1457:ARG:O	1:A:1460:ASP:HB2	2.18	0.42
1:A:1565:GLY:O	1:A:1566:ARG:HG2	2.18	0.42
1:B:1164:GLN:HE22	1:B:1534:LYS:CG	2.18	0.42
1:B:1410:TRP:O	1:B:1453:ARG:HA	2.20	0.42
1:B:1504:GLU:HG2	1:B:1580:VAL:HG23	2.02	0.42
1:A:1193:LYS:H	1:A:1193:LYS:HG2	1.68	0.42
1:A:1215:ILE:HD13	1:A:1218:LEU:HB2	1.96	0.42
1:A:1349:LYS:HD3	1:B:1507:ASN:OD1	2.19	0.42
1:B:1193:LYS:O	1:B:1196:ALA:N	2.52	0.42
1:B:1373:MET:HA	1:B:1484:ASN:HB2	2.00	0.42
1:B:1275:THR:HG23	1:B:1276:THR:N	2.35	0.42
1:A:1257:TRP:CE2	1:A:1264:GLN:CG	3.02	0.42
1:A:1563:TYR:CE1	1:A:1623:ARG:HG2	2.55	0.42
1:B:1215:ILE:CD1	1:B:1218:LEU:HB2	2.47	0.42
1:B:1440:ILE:O	1:B:1443:ASP:HB2	2.20	0.42
1:A:1505:VAL:HG12	1:A:1506:LYS:N	2.33	0.42
1:A:1410:TRP:O	1:A:1453:ARG:HA	2.20	0.42
1:A:1575:CYS:SG	1:A:1577:GLU:HG2	2.59	0.42
1:B:1283:TYR:O	1:B:1287:SER:HB3	2.20	0.42
1:B:1527:ILE:HD13	1:B:1533:PHE:CD1	2.51	0.42
1:A:1275:THR:HG23	1:A:1276:THR:N	2.35	0.41
1:B:1215:ILE:HG12	1:B:1218:LEU:HD13	2.02	0.41
1:B:1253:SER:N	1:B:1473:GLN:NE2	2.68	0.41
1:B:1508:VAL:HG12	1:B:1509:LYS:N	2.34	0.41
1:B:1536:ILE:HG13	1:B:1634:PHE:HE2	1.83	0.41
1:B:1402:ASN:HB2	1:B:1456:GLN:OE1	2.20	0.41
1:A:1197:PHE:CE1	1:A:1351:PRO:HA	2.55	0.41
1:A:1272:ARG:NH1	1:A:1272:ARG:CG	2.82	0.41
1:B:1566:ARG:HG2	1:B:1621:GLN:HB3	2.00	0.41
1:A:1255:GLU:HB2	1:A:1257:TRP:CD1	2.56	0.41
1:A:1356:VAL:HG22	1:A:1483:TRP:CD1	2.56	0.41
1:B:1532:LEU:O	1:B:1536:ILE:HG23	2.20	0.41
1:B:1597:THR:O	1:B:1597:THR:CG2	2.68	0.41
1:A:1542:GLN:O	1:A:1546[A]:HIS:CD2	2.73	0.41
1:B:1183:PRO:HD2	1:B:1451:VAL:O	2.20	0.41
1:B:1441:LEU:HB3	1:B:1445:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1564:GLN:O	1:A:1565:GLY:O	2.39	0.41
1:B:1188:ILE:HD12	1:B:1188:ILE:HA	1.76	0.41
1:B:1369:THR:CG2	1:B:1375:THR:CG2	2.99	0.41
1:A:1373:MET:HA	1:A:1484:ASN:HB2	2.01	0.41
1:B:1243:VAL:HG11	1:B:1277:ILE:CG1	2.44	0.41
1:B:1570:GLU:HA	1:B:1571:PRO:HD2	1.81	0.41
1:A:1255:GLU:HB3	1:A:1264:GLN:OE1	2.20	0.41
1:B:1177:PRO:CB	1:B:1179:GLU:OE2	2.69	0.41
1:B:1529:ASP:OD2	1:B:1532:LEU:HB2	2.21	0.41
1:B:1625:GLU:O	1:B:1626:GLU:C	2.57	0.41
1:A:1256:ASN:O	1:A:1264:GLN:HG2	2.20	0.41
1:A:1405:PRO:O	1:A:1458:PRO:CG	2.69	0.40
1:B:1214:VAL:HG11	1:B:1216:ARG:NH1	2.37	0.40
1:B:1284:GLN:NE2	1:B:1380:MET:HB3	2.33	0.40
1:B:1339:ARG:HH21	1:B:1339:ARG:HB3	1.83	0.40
1:A:1214:VAL:HG11	1:A:1216:ARG:NH1	2.37	0.40
1:A:1257:TRP:CD2	1:A:1264:GLN:CG	3.01	0.40
1:A:1279:LYS:O	1:A:1282:GLN:HB2	2.21	0.40
1:A:1280:TYR:HE2	1:A:1284:GLN:NE2	2.16	0.40
1:B:1222:LEU:HD23	1:B:1222:LEU:HA	1.84	0.40
1:B:1492:GLN:NE2	1:B:1492:GLN:HA	2.36	0.40
1:B:1554:LEU:HA	1:B:1554:LEU:HD23	1.74	0.40
1:A:1231:THR:OG1	1:A:1380:MET:HE2	2.20	0.40
1:B:1252:PRO:HB2	1:B:1255:GLU:CG	2.52	0.40
1:B:1369:THR:HG23	1:B:1375:THR:CG2	2.51	0.40
1:B:1601:HIS:HB2	1:B:1606:ALA:HB2	2.04	0.40
1:A:1170:ILE:C	1:A:1172:THR:H	2.25	0.40
1:A:1565:GLY:C	1:A:1566:ARG:HG3	2.42	0.40
1:A:1566:ARG:NH1	1:A:1621:GLN:NE2	2.69	0.40
1:B:1361:ASN:HA	1:B:1486:GLY:O	2.22	0.40
1:B:1519:TRP:CE2	1:B:1540:LEU:CD2	3.02	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	443/486 (91%)	420 (95%)	23 (5%)	0	100	100
1	B	440/486 (90%)	421 (96%)	19 (4%)	0	100	100
All	All	883/972 (91%)	841 (95%)	42 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	398/424 (94%)	334 (84%)	64 (16%)	2	12
1	B	396/424 (93%)	335 (85%)	61 (15%)	2	13
All	All	794/848 (94%)	669 (84%)	125 (16%)	2	13

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1157	GLU
1	A	1171	ASN
1	A	1176	LEU
1	A	1178	ARG
1	A	1179	GLU
1	A	1185	THR
1	A	1187	SER
1	A	1188	ILE
1	A	1200	VAL
1	A	1201	LEU
1	A	1215	ILE
1	A	1218	LEU
1	A	1243	VAL
1	A	1244	GLU
1	A	1249	VAL

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Mol	Chain	Res	Type
1	A	1254	ASP
1	A	1262	THR
1	A	1263	ARG
1	A	1270	SER
1	A	1272	ARG
1	A	1273	SER
1	A	1287	SER
1	A	1290	GLU
1	A	1292	LEU
1	A	1295	GLU
1	A	1325	ILE
1	A	1332	ILE
1	A	1333	ASP
1	A	1338	LYS
1	A	1339	ARG
1	A	1345	GLN
1	A	1347	LEU
1	A	1371	LEU
1	A	1378	LEU
1	A	1411	PHE
1	A	1419	GLU
1	A	1420	THR
1	A	1426	ASP
1	A	1442	ASP
1	A	1453	ARG
1	A	1457	ARG
1	A	1499	ARG
1	A	1505	VAL
1	A	1508	VAL
1	A	1511	ILE
1	A	1520	ASN
1	A	1523	ARG
1	A	1524	THR
1	A	1525	VAL
1	A	1528	SER
1	A	1534	LYS
1	A	1536	ILE
1	A	1548	GLN
1	A	1552	GLU
1	A	1560	LYS
1	A	1566	ARG
1	A	1577	GLU

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Mol	Chain	Res	Type
1	A	1584	ASN
1	A	1591	GLU
1	A	1599	LEU
1	A	1619	LEU
1	A	1624	THR
1	A	1632	ASP
1	A	1635	THR
1	B	1157	GLU
1	B	1176	LEU
1	B	1179	GLU
1	B	1185	THR
1	B	1187	SER
1	B	1188	ILE
1	B	1194	ARG
1	B	1200	VAL
1	B	1201	LEU
1	B	1209	ARG
1	B	1215	ILE
1	B	1218	LEU
1	B	1224	LEU
1	B	1243	VAL
1	B	1246	ARG
1	B	1249	VAL
1	B	1254	ASP
1	B	1263	ARG
1	B	1270	SER
1	B	1272	ARG
1	B	1273	SER
1	B	1287	SER
1	B	1292	LEU
1	B	1325	ILE
1	B	1327	LYS
1	B	1338	LYS
1	B	1339	ARG
1	B	1345	GLN
1	B	1347	LEU
1	B	1371	LEU
1	B	1377	GLN
1	B	1378	LEU
1	B	1419	GLU
1	B	1420	THR
1	B	1426	ASP

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Mol	Chain	Res	Type
1	B	1442	ASP
1	B	1453	ARG
1	B	1457	ARG
1	B	1481	ILE
1	B	1499	ARG
1	B	1511	ILE
1	B	1523	ARG
1	B	1524	THR
1	B	1525	VAL
1	B	1528	SER
1	B	1536	ILE
1	B	1537	LYS
1	B	1548	GLN
1	B	1552	GLU
1	B	1560	LYS
1	B	1563	TYR
1	B	1564	GLN
1	B	1568	LYS
1	B	1577	GLU
1	B	1586	LEU
1	B	1599	LEU
1	B	1607	ARG
1	B	1619	LEU
1	B	1624	THR
1	B	1632	ASP
1	B	1635	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1164	GLN
1	A	1171	ASN
1	A	1284	GLN
1	A	1331	ASN
1	A	1345	GLN
1	A	1377	GLN
1	A	1473	GLN
1	A	1584	ASN
1	A	1621	GLN
1	B	1164	GLN
1	B	1284	GLN
1	B	1377	GLN

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Mol	Chain	Res	Type
1	B	1473	GLN
1	B	1507	ASN
1	B	1520	ASN
1	B	1564	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

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OGA	B	1701	3	9,9,9	1.13	0	10,11,11	1.22	1 (10%)
2	OGA	A	1701	3	9,9,9	1.07	0	10,11,11	1.23	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OGA	B	1701	3	-	0/8/9/9	-
2	OGA	A	1701	3	-	0/8/9/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1701	OGA	O2-C1-C2	2.35	120.06	113.15
2	B	1701	OGA	O2-C1-C2	2.17	119.55	113.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1701	OGA	1	0
2	A	1701	OGA	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	448/486 (92%)	0.31	33 (7%)	14	4	24, 58, 98, 141	0
1	B	447/486 (91%)	0.21	24 (5%)	25	9	26, 57, 100, 148	0
All	All	895/972 (92%)	0.26	57 (6%)	19	6	24, 57, 100, 148	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1613	LEU	7.5
1	B	1170	ILE	6.1
1	B	1613	LEU	6.0
1	A	1615	GLY	5.7
1	B	1323	HIS	4.9
1	A	1616	VAL	4.7
1	A	1612	GLY	4.7
1	B	1615	GLY	4.5
1	A	1172	THR	4.3
1	B	1614	GLN	4.3
1	A	1614	GLN	4.1
1	A	1563	TYR	3.8
1	B	1290	GLU	3.7
1	B	1294	GLU	3.7
1	A	1554	LEU	3.6
1	B	1610	SER	3.6
1	B	1174	GLU	3.5
1	B	1257	TRP	3.3
1	A	1564	GLN	3.3
1	A	1599	LEU	3.3
1	A	1601	HIS	3.3
1	B	1591	GLU	3.1
1	A	1257	TRP	3.1
1	A	1610	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1170	ILE	3.1
1	A	1555	VAL	3.0
1	A	1585	ILE	3.0
1	B	1553	SER	2.9
1	A	1406	GLY	2.9
1	A	1560	LYS	2.9
1	A	1174	GLU	2.9
1	A	1617	VAL	2.9
1	B	1612	GLY	2.9
1	A	1559	LYS	2.8
1	A	1600	VAL	2.7
1	B	1560	LYS	2.7
1	A	1557	ALA	2.6
1	B	1616	VAL	2.6
1	B	1563	TYR	2.6
1	B	1555	VAL	2.5
1	A	1286	SER	2.4
1	A	1553	SER	2.4
1	B	1253	SER	2.4
1	A	1587	PHE	2.4
1	B	1597	THR	2.3
1	A	1565	GLY	2.3
1	A	1481	ILE	2.3
1	A	1289	GLN	2.3
1	A	1606	ALA	2.2
1	B	1558	GLY	2.2
1	B	1557	ALA	2.1
1	A	1562	ALA	2.1
1	B	1599	LEU	2.0
1	B	1324	HIS	2.0
1	A	1294	GLU	2.0
1	A	1611	ALA	2.0
1	B	1617	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
2	OGA	B	1701	10/10	0.92	0.22	20,20,20,20	0
2	OGA	A	1701	10/10	0.93	0.27	41,60,68,86	0
3	NI	A	1702	1/1	0.94	0.20	46,46,46,46	0
3	NI	B	1702	1/1	0.97	0.21	41,41,41,41	0
4	ZN	B	1703	1/1	0.97	0.14	73,73,73,73	0
4	ZN	A	1703	1/1	0.99	0.05	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.