Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 06:20 PM EDT

PDB ID	:	1EG7
Title	:	THE CRYSTAL STRUCTURE OF FORMYLTETRAHYDROFOLATE SYNTHETASE FROM MOORELLA THERMOACETICA
Authors	:	Radfar, R.; Shin, R.; Sheldrick, G.M.; Minor, W.; Lovell, C.R.; Odom, J.D.; Dunlap, R.B.; Lebioda, L.
Deposited on	:	2000-02-14
Resolution	:	2.50 Å(reported)

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

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

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

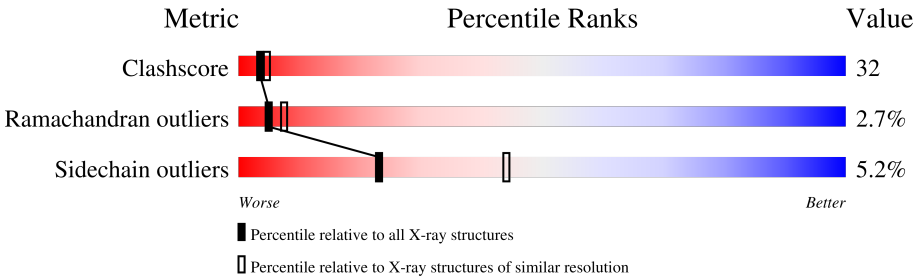
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	557	61% 34%
1	B	557	44% 50% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	3	-	-	X	-
2	SO4	A	5	-	-	X	-
2	SO4	A	7	-	-	X	-
2	SO4	A	8	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8586 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.

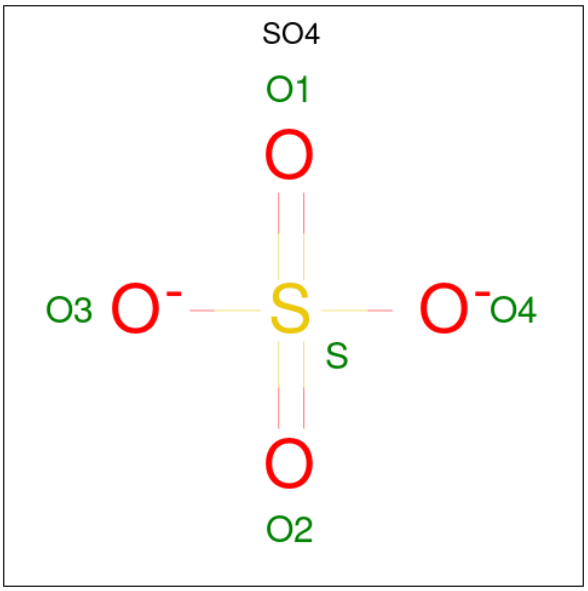
- Molecule 1 is a protein called FORMYLTETRAHYDROFOLATE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4135	2618	716	780	21			
1	B	548	Total	C	N	O	S	0	0	0
			4127	2614	715	777	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1174	GLU	ASP	conflict	UNP P21164
A	1225	LYS	ILE	conflict	UNP P21164
A	?	-	GLU	deletion	UNP P21164
A	?	-	VAL	deletion	UNP P21164
B	1174	GLU	ASP	conflict	UNP P21164
B	1225	LYS	ILE	conflict	UNP P21164
B	?	-	GLU	deletion	UNP P21164
B	?	-	VAL	deletion	UNP P21164

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	198	Total O 198 198	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	71	Total	O	0	0
			71	71		

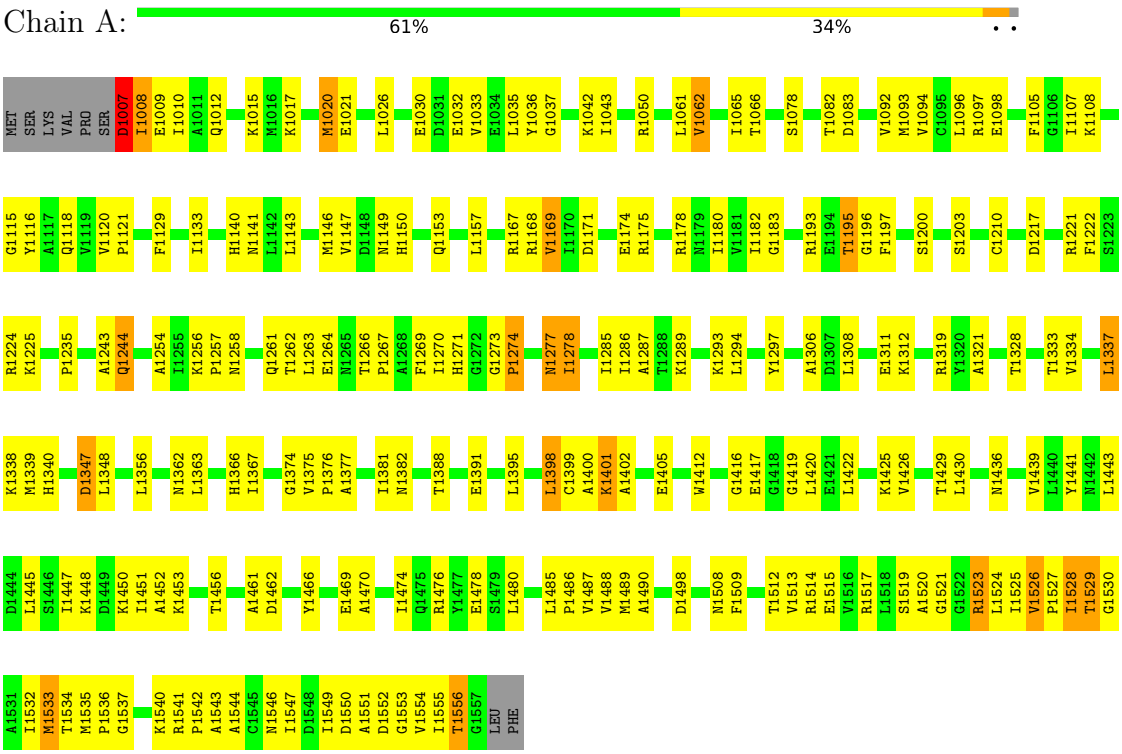
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

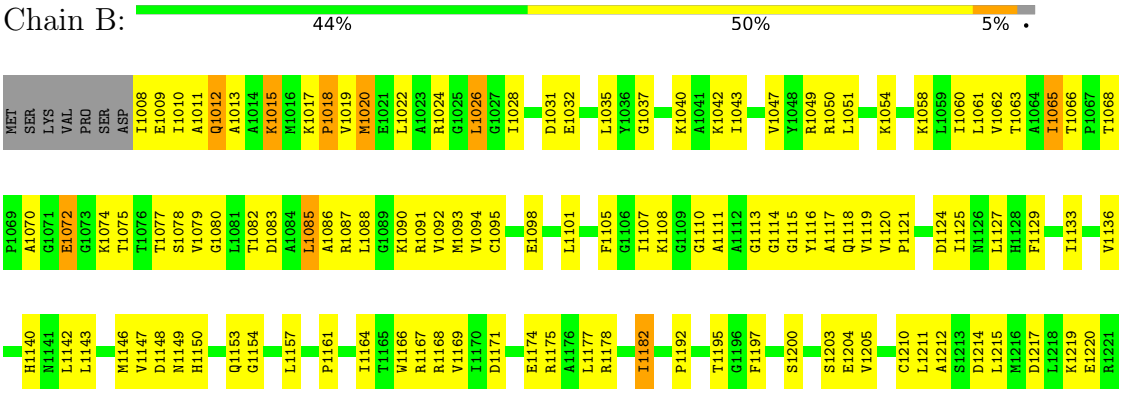
• Molecule 1: FORMYLTETRAHYDROFOLATE SYNTHETASE

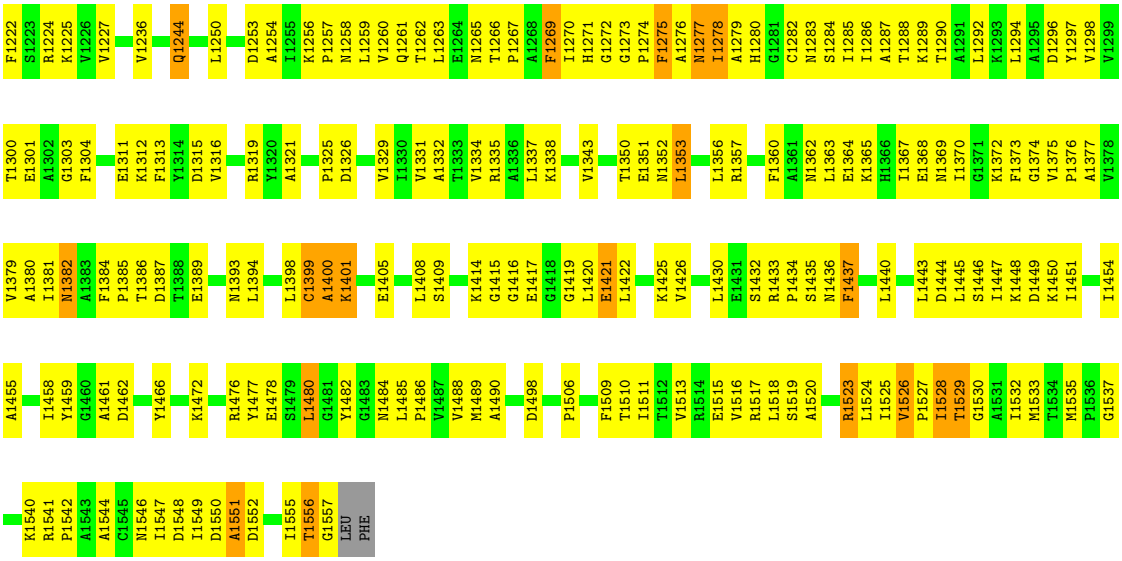
Chain A:



• Molecule 1: FORMYLTETRAHYDROFOLATE SYNTHETASE

Chain B:




F1222 S1223 R1224 K1225 V1226 V1227 V1236 Q1244 L1250 D1253 A1254 I1255 K1256 P1257 N1258 L1259 V1260 Q1261 T1262 L1263 E1264 N1265 T1266 P1267 A1268 F1269 I1270 H1271 G1272 G1273 P1274 F1275 A1276 N1277 I1278 A1279 H1280 G1281 C1282 N1283 S1284 I1285 I1286 A1287 T1288 K1289 T1290 A1291 L1292 K1293 L1294 A1295 D1296 Y1297 V1298 V1299
T1300 E1301 A1302 G1303 F1304 E1311 K1312 F1313 Y1314 D1315 V1316 R1319 Y1320 A1321 P1325 D1326 V1329 I1330 V1331 A1332 T1333 V1334 R1335 A1336 L1337 K1338 V1343 T1350 E1351 N1352 L1353 L1356 R1357 F1360 A1361 N1362 L1363 E1364 K1365 H1366 I1367 E1368 N1369 I1370 G1371 K1372 F1373 G1374 V1375 P1376 A1377 V1378
V1379 A1380 I1381 N1382 A1383 F1384 P1385 T1386 D1387 T1388 E1389 N1393 L1394 L1398 C1399 A1400 K1401 E1405 L1408 S1409 K1414 G1415 G1416 E1417 G1418 G1419 L1420 E1421 L1422 K1425 V1426 L1430 E1431 S1432 R1433 P1434 S1435 N1436 F1437 L1440 L1443 D1444 L1445 S1446 I1447 K1448 D1449 K1450 I1451 I1454
A1455 I1458 Y1459 G1460 A1461 D1462 Y1466 K1472 R1476 Y1477 E1478 S1479 L1480 G1481 Y1482 G1483 N1484 L1485 P1486 V1487 V1488 M1489 A1490 D1498 P1506 F1509 T1510 I1511 T1512 V1513 R1514 E1515 V1516 R1517 L1518 S1519 A1520 R1523 L1524 I1525 V1526 P1527 I1528 T1529 G1530 A1531 I1532 M1533 T1534 M1535 P1536 G1537
K1540 R1541 P1542 A1543 A1544 C1545 N1546 I1547 D1548 I1549 D1550 A1551 D1552 I1555 T1556 G1557 LEU PHE

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	160.88Å 160.88Å 256.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.50	Depositor
% Data completeness (in resolution range)	90.6 (19.99-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.253 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8586	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.43	3/4203 (0.1%)	0.70	7/5691 (0.1%)
1	B	0.39	0/4195	0.64	1/5680 (0.0%)
All	All	0.41	3/8398 (0.0%)	0.67	8/11371 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1008	ILE	N-CA	9.27	1.64	1.46
1	A	1008	ILE	CA-C	5.74	1.67	1.52
1	A	1007	ASP	CA-C	5.03	1.66	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1007	ASP	N-CA-C	7.38	130.92	111.00
1	B	1015	LYS	N-CA-C	7.38	130.92	111.00
1	A	1007	ASP	CA-C-O	-6.80	105.83	120.10
1	A	1008	ILE	CB-CA-C	-6.64	98.32	111.60
1	A	1007	ASP	CB-CA-C	6.52	123.44	110.40
1	A	1008	ILE	N-CA-CB	6.16	124.96	110.80
1	A	1008	ILE	N-CA-C	-6.08	94.59	111.00
1	A	1007	ASP	N-CA-CB	-6.05	99.70	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1007	ASP	Peptide,Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4135	0	4223	218	1
1	B	4127	0	4219	317	0
2	A	35	0	0	12	0
2	B	20	0	0	2	0
3	A	198	0	0	14	0
3	B	71	0	0	4	0
All	All	8586	0	8442	535	1

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 32.

All (535) 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:1009:GLU:OE2	1:B:1111:ALA:HB2	1.33	1.27
1:A:1175:ARG:HD3	2:A:5:SO4:O3	1.55	1.07
1:A:1244:GLN:H	1:A:1244:GLN:NE2	1.55	1.03
1:B:1277:ASN:ND2	1:B:1278:ILE:H	1.59	1.01
1:B:1244:GLN:H	1:B:1244:GLN:NE2	1.59	0.99
1:B:1009:GLU:OE2	1:B:1111:ALA:CB	2.10	0.97
1:B:1517:ARG:HH22	1:B:1532:ILE:HG13	1.28	0.97
1:A:1244:GLN:HE21	1:A:1244:GLN:N	1.62	0.97
1:A:1517:ARG:HH22	1:A:1532:ILE:HG13	1.27	0.96
1:A:1257:PRO:HD3	1:A:1286:ILE:HD13	1.48	0.94
1:B:1277:ASN:HD22	1:B:1278:ILE:H	1.06	0.93
1:A:1277:ASN:HD22	1:A:1278:ILE:H	1.13	0.91
1:B:1212:ALA:O	1:B:1286:ILE:HG23	1.72	0.89
1:A:1533:MET:HB2	2:A:3:SO4:O2	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1353:LEU:HD12	1:B:1353:LEU:H	1.37	0.88
1:B:1498:ASP:CB	1:B:1528:ILE:HG21	2.03	0.88
1:A:1498:ASP:CB	1:A:1528:ILE:HG21	2.04	0.88
1:B:1012:GLN:NE2	1:B:1116:TYR:CE2	2.42	0.88
1:A:1523:ARG:HH11	1:A:1525:ILE:HD11	1.39	0.87
1:B:1394:LEU:O	1:B:1398:LEU:HD23	1.73	0.87
1:B:1149:ASN:O	1:B:1153:GLN:HG2	1.75	0.86
1:B:1244:GLN:H	1:B:1244:GLN:HE21	1.17	0.86
1:B:1557:GLY:HA3	3:B:164:HOH:O	1.77	0.84
1:B:1277:ASN:HD22	1:B:1278:ILE:N	1.74	0.84
1:B:1523:ARG:HH11	1:B:1525:ILE:HD11	1.41	0.84
1:A:1515:GLU:O	1:A:1527:PRO:HD2	1.78	0.83
1:A:1017:LYS:H	1:A:1261:GLN:HE22	1.27	0.83
1:A:1020:MET:HE3	1:A:1030:GLU:HG3	1.60	0.82
1:B:1022:LEU:HD11	1:B:1261:GLN:NE2	1.96	0.80
1:A:1546:ASN:HB3	1:A:1556:THR:HG21	1.63	0.79
1:A:1451:ILE:HG12	1:A:1489:MET:HE1	1.65	0.79
1:B:1498:ASP:HB2	1:B:1528:ILE:HG21	1.65	0.78
1:B:1319:ARG:HE	1:B:1443:LEU:HD13	1.48	0.77
1:A:1286:ILE:HD12	1:A:1286:ILE:C	2.05	0.77
1:A:1244:GLN:H	1:A:1244:GLN:HE21	0.83	0.76
1:A:1512:THR:O	1:A:1528:ILE:HG23	1.86	0.76
1:B:1212:ALA:O	1:B:1286:ILE:CG2	2.33	0.76
1:B:1498:ASP:HB3	1:B:1528:ILE:HG21	1.66	0.76
1:B:1368:GLU:HG2	1:B:1401:LYS:HE2	1.69	0.75
1:B:1443:LEU:HG	1:B:1484:ASN:O	1.87	0.75
1:A:1498:ASP:HB2	1:A:1528:ILE:HG21	1.68	0.75
1:B:1262:THR:HG22	1:B:1263:LEU:H	1.49	0.75
1:A:1082:THR:HG21	1:A:1094:VAL:HG22	1.69	0.75
1:B:1356:LEU:HD12	1:B:1394:LEU:HD23	1.68	0.75
1:B:1049:ARG:HD3	1:B:1049:ARG:C	2.08	0.74
1:A:1277:ASN:HD22	1:A:1278:ILE:N	1.85	0.74
1:A:1277:ASN:ND2	1:A:1278:ILE:H	1.85	0.74
1:B:1523:ARG:NH1	1:B:1525:ILE:HD11	2.03	0.73
1:B:1244:GLN:HE21	1:B:1244:GLN:N	1.87	0.73
1:B:1550:ASP:C	1:B:1552:ASP:H	1.92	0.73
1:A:1195:THR:HG21	3:A:134:HOH:O	1.89	0.72
1:B:1161:PRO:HA	1:B:1164:ILE:HD12	1.70	0.72
1:B:1472:LYS:O	1:B:1476:ARG:HG3	1.90	0.72
1:B:1012:GLN:NE2	1:B:1116:TYR:CD2	2.58	0.72
1:B:1093:MET:HG2	1:B:1267:PRO:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1061:LEU:HD22	1:B:1313:PHE:CD2	2.25	0.71
1:B:1319:ARG:NE	1:B:1443:LEU:HD13	2.03	0.71
1:A:1271:HIS:ND1	1:A:1286:ILE:HD11	2.05	0.71
1:B:1455:ALA:HA	1:B:1459:TYR:HD2	1.54	0.71
1:B:1074:LYS:HB2	1:B:1074:LYS:NZ	2.06	0.70
1:A:1523:ARG:NH1	1:A:1525:ILE:HD11	2.06	0.70
1:B:1373:PHE:O	1:B:1375:VAL:HG13	1.92	0.69
1:B:1149:ASN:ND2	1:B:1153:GLN:HE21	1.90	0.69
1:B:1360:PHE:CE2	1:B:1364:GLU:HB2	2.27	0.69
1:A:1174:GLU:HG3	3:A:237:HOH:O	1.93	0.69
1:A:1150:HIS:HE1	1:A:1157:LEU:H	1.39	0.69
1:B:1074:LYS:HB2	1:B:1074:LYS:HZ2	1.58	0.69
1:B:1090:LYS:HD2	1:B:1297:TYR:HE2	1.57	0.69
1:B:1334:VAL:HB	1:B:1387:ASP:OD1	1.93	0.69
1:A:1277:ASN:HD22	1:A:1277:ASN:H	1.41	0.69
1:B:1175:ARG:HD3	2:B:9:SO4:O3	1.93	0.68
1:B:1079:VAL:HB	1:B:1117:ALA:O	1.94	0.68
1:A:1042:LYS:HE3	1:A:1258:ASN:OD1	1.94	0.68
1:A:1476:ARG:O	1:A:1480:LEU:HB2	1.93	0.68
1:A:1143:LEU:O	1:A:1147:VAL:HG23	1.94	0.68
1:B:1082:THR:HG21	1:B:1094:VAL:HG22	1.76	0.68
1:A:1533:MET:CB	2:A:3:SO4:O2	2.42	0.68
1:A:1486:PRO:HD2	1:A:1523:ARG:HB3	1.75	0.67
1:B:1275:PHE:O	1:B:1279:ALA:HB3	1.94	0.67
1:B:1019:VAL:HG13	1:B:1259:LEU:HG	1.75	0.67
1:B:1353:LEU:HD12	1:B:1353:LEU:N	2.08	0.67
1:B:1075:THR:HG22	1:B:1113:GLY:HA2	1.76	0.67
1:A:1286:ILE:HD12	1:A:1287:ALA:N	2.10	0.66
1:B:1373:PHE:CE2	1:B:1440:LEU:HB2	2.30	0.66
1:B:1517:ARG:NH2	1:B:1532:ILE:HG13	2.07	0.66
1:A:1533:MET:HA	2:A:3:SO4:O4	1.96	0.66
1:B:1477:TYR:HE2	1:B:1516:VAL:HG12	1.60	0.66
1:B:1448:LYS:HE2	1:B:1466:TYR:CD2	2.31	0.66
1:A:1167:ARG:NH2	1:A:1178:ARG:O	2.29	0.66
1:A:1382:ASN:OD1	2:A:7:SO4:O1	2.13	0.66
1:B:1120:VAL:HB	1:B:1121:PRO:HA	1.77	0.66
1:A:1277:ASN:ND2	1:A:1277:ASN:H	1.94	0.65
1:A:1540:LYS:O	1:A:1542:PRO:HD3	1.97	0.65
1:B:1447:ILE:O	1:B:1451:ILE:HG13	1.96	0.65
1:B:1262:THR:HG22	1:B:1263:LEU:N	2.10	0.65
1:B:1546:ASN:HB3	1:B:1556:THR:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:THR:HG21	1:A:1094:VAL:CG2	2.27	0.65
1:A:1032:GLU:OE2	1:A:1050:ARG:NH1	2.30	0.65
1:A:1469:GLU:HG3	3:A:274:HOH:O	1.96	0.65
1:A:1257:PRO:HD3	1:A:1286:ILE:CD1	2.23	0.64
1:A:1009:GLU:HG2	1:A:1115:GLY:H	1.61	0.64
1:A:1169:VAL:HG22	1:A:1200:SER:HA	1.79	0.64
1:B:1312:LYS:HD3	1:B:1488:VAL:HG13	1.79	0.64
1:A:1417:GLU:HA	1:A:1420:LEU:CD2	2.27	0.64
1:A:1020:MET:CE	1:A:1030:GLU:HG3	2.28	0.64
1:B:1482:TYR:HB3	1:B:1485:LEU:HD12	1.80	0.64
1:B:1161:PRO:HA	1:B:1164:ILE:CD1	2.27	0.64
1:B:1445:LEU:O	1:B:1450:LYS:HE3	1.96	0.64
1:B:1315:ASP:O	1:B:1319:ARG:HD2	1.98	0.63
1:B:1384:PHE:CD1	1:B:1385:PRO:HD2	2.33	0.63
1:B:1446:SER:HB3	1:B:1449:ASP:OD2	1.97	0.63
1:A:1169:VAL:CG2	1:A:1200:SER:HA	2.29	0.63
1:A:1412:TRP:CG	2:A:7:SO4:O4	2.51	0.63
1:B:1417:GLU:HA	1:B:1420:LEU:HD23	1.81	0.63
1:A:1035:LEU:HD22	1:A:1037:GLY:O	1.98	0.63
1:B:1051:LEU:HD22	1:B:1054:LYS:HG3	1.80	0.63
1:B:1082:THR:HG21	1:B:1094:VAL:CG2	2.29	0.63
1:A:1381:ILE:HD12	1:A:1395:LEU:HD21	1.80	0.62
1:B:1277:ASN:ND2	1:B:1278:ILE:N	2.37	0.62
1:A:1262:THR:HG22	1:A:1263:LEU:N	2.13	0.62
1:A:1417:GLU:HA	1:A:1420:LEU:HD23	1.81	0.62
1:B:1062:VAL:HG13	1:B:1301:GLU:HB3	1.80	0.62
1:A:1093:MET:HG2	1:A:1267:PRO:HB2	1.82	0.62
1:B:1042:LYS:NZ	1:B:1254:ALA:HA	2.14	0.62
1:B:1303:GLY:HA2	2:B:2:SO4:O1	2.00	0.62
1:B:1490:ALA:O	1:B:1527:PRO:HA	1.99	0.62
1:A:1020:MET:HE1	1:A:1030:GLU:HA	1.82	0.62
1:B:1105:PHE:HB3	1:B:1544:ALA:HB2	1.82	0.62
1:A:1066:THR:H	1:A:1362:ASN:HD21	1.48	0.62
1:A:1554:VAL:HG12	1:A:1555:ILE:N	2.14	0.62
1:B:1326:ASP:O	1:B:1376:PRO:HG2	2.00	0.61
1:B:1066:THR:H	1:B:1362:ASN:HD21	1.47	0.61
1:B:1142:LEU:O	1:B:1146:MET:HG3	2.00	0.61
1:B:1074:LYS:NZ	1:B:1074:LYS:CB	2.62	0.61
1:B:1353:LEU:H	1:B:1353:LEU:CD1	2.10	0.61
1:B:1417:GLU:HA	1:B:1420:LEU:CD2	2.30	0.61
1:A:1533:MET:CA	2:A:3:SO4:O2	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1363:LEU:O	1:B:1367:ILE:HG12	2.00	0.61
1:A:1043:ILE:HD12	1:A:1269:PHE:HE1	1.65	0.60
1:B:1042:LYS:HD3	1:B:1256:LYS:HB2	1.83	0.60
1:B:1337:LEU:HD23	1:B:1360:PHE:HA	1.83	0.60
1:B:1086:ALA:HB2	1:B:1092:VAL:HG12	1.83	0.60
1:B:1140:HIS:HD2	1:B:1203:SER:OG	1.85	0.60
1:A:1487:VAL:HG12	1:A:1489:MET:HE2	1.83	0.60
1:B:1488:VAL:CG2	1:B:1523:ARG:HD3	2.31	0.60
1:B:1528:ILE:HG22	1:B:1529:THR:N	2.17	0.60
1:A:1517:ARG:NH2	1:A:1532:ILE:HG13	2.08	0.60
1:B:1331:VAL:HG12	1:B:1332:ALA:N	2.17	0.60
1:A:1133:ILE:HG21	1:A:1171:ASP:OD1	2.01	0.59
1:A:1140:HIS:HD2	1:A:1203:SER:OG	1.85	0.59
1:B:1083:ASP:OD2	1:B:1262:THR:HG21	2.02	0.59
1:A:1513:VAL:HB	1:A:1526:VAL:HG23	1.84	0.59
1:B:1082:THR:HG22	1:B:1266:THR:HG21	1.84	0.59
1:A:1319:ARG:NH2	1:A:1439:VAL:HG21	2.18	0.59
1:A:1486:PRO:O	1:A:1523:ARG:HB2	2.02	0.59
1:B:1062:VAL:HG11	1:B:1078:SER:OG	2.02	0.59
1:A:1082:THR:HG22	1:A:1266:THR:HG21	1.84	0.59
1:B:1009:GLU:OE1	1:B:1114:GLY:HA2	2.03	0.59
1:A:1107:ILE:O	1:A:1108:LYS:HB2	2.02	0.59
1:A:1398:LEU:C	1:A:1400:ALA:H	2.06	0.58
1:A:1319:ARG:NH2	1:A:1441:TYR:O	2.33	0.58
1:B:1107:ILE:O	1:B:1108:LYS:HB2	2.02	0.58
1:A:1363:LEU:O	1:A:1367:ILE:HG12	2.03	0.58
1:A:1533:MET:HA	2:A:3:SO4:S	2.43	0.58
1:B:1133:ILE:HG21	1:B:1171:ASP:OD1	2.03	0.58
1:B:1365:LYS:HE3	1:B:1369:ASN:HD21	1.67	0.58
1:B:1555:ILE:HG23	1:B:1555:ILE:O	2.04	0.58
1:B:1020:MET:O	1:B:1024:ARG:HG3	2.02	0.58
1:A:1222:PHE:HA	1:A:1225:LYS:HD2	1.85	0.58
1:B:1110:GLY:HA2	3:B:191:HOH:O	2.03	0.58
1:B:1546:ASN:C	1:B:1556:THR:HG21	2.23	0.58
1:A:1462:ASP:OD2	1:A:1508:ASN:HA	2.03	0.58
1:B:1515:GLU:O	1:B:1527:PRO:HD2	2.03	0.58
1:A:1036:TYR:CE1	1:A:1042:LYS:HG3	2.39	0.58
1:B:1026:LEU:HD23	1:B:1028:ILE:HD11	1.84	0.58
1:B:1092:VAL:HG23	1:B:1297:TYR:O	2.03	0.58
1:B:1550:ASP:C	1:B:1552:ASP:N	2.54	0.58
1:A:1222:PHE:HA	1:A:1225:LYS:CD	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1042:LYS:HE2	1:B:1258:ASN:OD1	2.03	0.58
1:B:1175:ARG:HG2	1:B:1178:ARG:CZ	2.34	0.57
1:B:1283:ASN:ND2	1:B:1300:THR:OG1	2.36	0.57
1:B:1353:LEU:HB3	1:B:1394:LEU:HD22	1.86	0.57
1:A:1120:VAL:HB	1:A:1121:PRO:HA	1.86	0.57
1:A:1083:ASP:OD2	1:A:1262:THR:HG21	2.05	0.57
1:B:1277:ASN:ND2	1:B:1277:ASN:H	2.03	0.57
1:B:1376:PRO:HD3	1:B:1435:SER:HB3	1.86	0.57
1:A:1532:ILE:HG12	1:A:1532:ILE:O	2.04	0.56
1:B:1169:VAL:HG13	1:B:1200:SER:HA	1.86	0.56
1:A:1554:VAL:HG12	1:A:1555:ILE:H	1.69	0.56
1:A:1405:GLU:HG3	1:A:1425:LYS:HB2	1.88	0.56
1:A:1523:ARG:HD2	1:A:1523:ARG:N	2.19	0.56
1:B:1331:VAL:HG12	1:B:1332:ALA:H	1.70	0.56
1:A:1514:ARG:HD3	3:A:295:HOH:O	2.05	0.56
1:A:1083:ASP:OD1	1:A:1262:THR:HG21	2.06	0.56
1:A:1010:ILE:C	1:A:1012:GLN:H	2.07	0.56
1:A:1150:HIS:CE1	1:A:1157:LEU:H	2.23	0.56
1:B:1515:GLU:HB3	1:B:1527:PRO:CG	2.36	0.56
1:B:1515:GLU:HB3	1:B:1527:PRO:HG2	1.87	0.56
1:B:1370:ILE:HG21	1:B:1377:ALA:HB2	1.88	0.56
1:A:1092:VAL:HG23	1:A:1297:TYR:O	2.06	0.55
1:A:1116:TYR:CZ	2:A:8:SO4:O1	2.59	0.55
1:B:1043:ILE:HD11	1:B:1259:LEU:HD22	1.88	0.55
1:B:1408:LEU:HD13	1:B:1414:LYS:NZ	2.21	0.55
1:B:1416:GLY:O	1:B:1420:LEU:HD22	2.06	0.55
1:A:1083:ASP:CG	1:A:1262:THR:HG21	2.27	0.55
1:B:1043:ILE:HD12	1:B:1269:PHE:CZ	2.41	0.55
1:B:1476:ARG:O	1:B:1480:LEU:HD13	2.05	0.55
1:B:1275:PHE:HD2	1:B:1277:ASN:HD21	1.55	0.55
1:B:1285:ILE:HD13	1:B:1321:ALA:HB2	1.89	0.55
1:A:1333:THR:HG22	1:A:1382:ASN:HB3	1.89	0.55
1:A:1445:LEU:O	1:A:1450:LYS:HE3	2.07	0.55
1:B:1284:SER:HB2	3:B:283:HOH:O	2.06	0.55
1:B:1288:THR:O	1:B:1292:LEU:HG	2.06	0.55
1:B:1422:LEU:O	1:B:1426:VAL:HG23	2.07	0.55
1:A:1140:HIS:HE1	1:A:1167:ARG:O	1.90	0.54
1:A:1533:MET:HA	2:A:3:SO4:O2	2.07	0.54
1:B:1498:ASP:HB2	1:B:1528:ILE:CG2	2.36	0.54
1:B:1095:CYS:O	1:B:1283:ASN:ND2	2.41	0.54
1:B:1547:ILE:HA	1:B:1556:THR:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1286:ILE:C	1:B:1286:ILE:HD12	2.28	0.54
1:A:1007:ASP:OD2	3:A:131:HOH:O	2.19	0.54
1:A:1217:ASP:O	1:A:1221:ARG:HG3	2.07	0.53
1:B:1058:LYS:HB2	1:B:1297:TYR:HD1	1.73	0.53
1:B:1214:ASP:O	1:B:1217:ASP:N	2.33	0.53
1:A:1550:ASP:OD1	1:A:1551:ALA:N	2.41	0.53
1:A:1556:THR:O	1:A:1556:THR:HG22	2.09	0.53
1:B:1049:ARG:HD3	1:B:1049:ARG:O	2.08	0.53
1:B:1280:HIS:CD2	1:B:1282:CYS:HB2	2.43	0.53
1:A:1417:GLU:O	1:A:1420:LEU:HD23	2.08	0.53
1:B:1555:ILE:O	1:B:1556:THR:CB	2.55	0.53
1:A:1082:THR:CG2	1:A:1094:VAL:HG22	2.38	0.53
1:A:1140:HIS:CD2	1:A:1203:SER:OG	2.62	0.53
1:B:1088:LEU:HD21	1:B:1420:LEU:HD12	1.91	0.53
1:B:1019:VAL:CG1	1:B:1259:LEU:HG	2.37	0.53
1:A:1174:GLU:HA	3:A:214:HOH:O	2.09	0.53
1:A:1141:ASN:OD1	1:A:1168:ARG:HG3	2.09	0.53
1:B:1174:GLU:HG3	3:B:298:HOH:O	2.09	0.53
1:B:1286:ILE:HD12	1:B:1287:ALA:N	2.23	0.53
1:B:1286:ILE:HA	1:B:1289:LYS:HE2	1.91	0.53
1:B:1448:LYS:HE2	1:B:1466:TYR:CG	2.44	0.53
1:B:1271:HIS:CE1	1:B:1286:ILE:HD11	2.44	0.53
1:B:1211:LEU:HD21	1:B:1280:HIS:NE2	2.24	0.52
1:B:1510:THR:HG22	1:B:1511:ILE:N	2.23	0.52
1:B:1080:GLY:HA3	1:B:1409:SER:HB3	1.92	0.52
1:B:1222:PHE:HA	1:B:1225:LYS:HD2	1.91	0.52
1:B:1414:LYS:O	1:B:1417:GLU:HB3	2.09	0.52
1:B:1540:LYS:C	1:B:1542:PRO:HD3	2.30	0.52
1:B:1149:ASN:ND2	1:B:1153:GLN:NE2	2.56	0.52
1:B:1150:HIS:HE1	1:B:1157:LEU:H	1.57	0.52
1:A:1175:ARG:HG2	1:A:1178:ARG:CZ	2.39	0.52
1:B:1350:THR:HG22	1:B:1351:GLU:N	2.25	0.52
1:B:1083:ASP:O	1:B:1087:ARG:HB2	2.09	0.52
1:B:1214:ASP:O	1:B:1215:LEU:C	2.48	0.52
1:A:1017:LYS:H	1:A:1261:GLN:NE2	2.01	0.52
1:B:1405:GLU:HG3	1:B:1425:LYS:HB2	1.92	0.52
1:A:1182:ILE:CG2	1:A:1183:GLY:N	2.72	0.51
1:B:1374:GLY:O	1:B:1435:SER:HB2	2.09	0.51
1:A:1017:LYS:HD3	1:A:1021:GLU:OE2	2.10	0.51
1:A:1540:LYS:HG3	1:A:1541:ARG:N	2.25	0.51
1:B:1488:VAL:HG21	1:B:1523:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1526:VAL:O	1:B:1526:VAL:HG22	2.09	0.51
1:A:1530:GLY:C	1:A:1532:ILE:H	2.13	0.51
1:A:1485:LEU:HD13	1:A:1523:ARG:HA	1.91	0.51
1:B:1008:ILE:HG13	1:B:1011:ALA:HB2	1.92	0.51
1:A:1461:ALA:HB2	1:A:1509:PHE:CE1	2.45	0.51
1:B:1204:GLU:HB3	1:B:1225:LYS:NZ	2.25	0.51
1:A:1347:ASP:OD2	1:A:1347:ASP:N	2.43	0.51
1:B:1062:VAL:HG12	1:B:1300:THR:O	2.11	0.51
1:B:1092:VAL:HA	1:B:1297:TYR:O	2.11	0.51
1:B:1143:LEU:HD23	1:B:1166:TRP:CE2	2.45	0.51
1:B:1405:GLU:OE1	1:B:1421:GLU:HG2	2.10	0.51
1:A:1277:ASN:HD22	1:A:1277:ASN:N	2.04	0.51
1:A:1334:VAL:O	1:A:1338:LYS:HG3	2.11	0.51
1:A:1425:LYS:O	1:A:1429:THR:HG23	2.10	0.51
1:B:1518:LEU:HD12	1:B:1519:SER:N	2.26	0.51
1:B:1523:ARG:H	1:B:1523:ARG:HD2	1.76	0.50
1:A:1062:VAL:HG11	1:A:1078:SER:OG	2.11	0.50
1:A:1405:GLU:OE2	1:A:1425:LYS:HD3	2.11	0.50
1:B:1061:LEU:HD13	1:B:1313:PHE:CE1	2.46	0.50
1:A:1523:ARG:HD2	1:A:1523:ARG:H	1.76	0.50
1:B:1040:LYS:HE2	1:B:1124:ASP:OD2	2.11	0.50
1:A:1540:LYS:C	1:A:1542:PRO:HD3	2.31	0.50
1:B:1417:GLU:C	1:B:1419:GLY:H	2.15	0.50
1:B:1517:ARG:HH22	1:B:1532:ILE:CG1	2.10	0.50
1:A:1262:THR:CG2	1:A:1263:LEU:N	2.75	0.50
1:B:1149:ASN:HD21	1:B:1153:GLN:NE2	2.09	0.50
1:A:1451:ILE:HG12	1:A:1489:MET:CE	2.40	0.50
1:A:1377:ALA:O	1:A:1402:ALA:HB1	2.12	0.50
1:A:1447:ILE:O	1:A:1451:ILE:HG13	2.12	0.50
1:B:1050:ARG:HG3	1:B:1051:LEU:N	2.26	0.50
1:A:1517:ARG:HH22	1:A:1532:ILE:CG1	2.13	0.50
1:B:1011:ALA:C	1:B:1013:ALA:H	2.14	0.50
1:B:1169:VAL:CG1	1:B:1200:SER:HA	2.41	0.50
1:B:1047:VAL:CG1	1:B:1294:LEU:HD21	2.42	0.49
1:B:1225:LYS:HA	1:B:1520:ALA:HB3	1.94	0.49
1:B:1436:ASN:O	1:B:1436:ASN:CG	2.50	0.49
1:B:1523:ARG:HD2	1:B:1523:ARG:N	2.27	0.49
1:A:1149:ASN:O	1:A:1153:GLN:HG2	2.12	0.49
1:B:1149:ASN:HD21	1:B:1153:GLN:HE21	1.58	0.49
1:B:1177:LEU:HB3	1:B:1197:PHE:HB2	1.93	0.49
1:B:1210:CYS:O	1:B:1211:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1219:LYS:O	1:B:1222:PHE:HB2	2.11	0.49
1:A:1210:CYS:SG	1:A:1274:PRO:HD3	2.51	0.49
1:A:1398:LEU:O	1:A:1400:ALA:N	2.43	0.49
1:B:1115:GLY:O	1:B:1118:GLN:HG2	2.13	0.49
1:B:1515:GLU:HG2	1:B:1516:VAL:H	1.76	0.49
1:A:1043:ILE:HD12	1:A:1269:PHE:CE1	2.47	0.49
1:A:1381:ILE:HD12	1:A:1395:LEU:CD2	2.43	0.49
1:A:1168:ARG:HG2	1:A:1197:PHE:CE2	2.48	0.49
1:B:1010:ILE:C	1:B:1012:GLN:N	2.63	0.49
1:A:1065:ILE:CD1	1:A:1337:LEU:HD13	2.42	0.49
1:B:1136:VAL:HG13	1:B:1205:VAL:CG1	2.43	0.49
1:B:1244:GLN:NE2	1:B:1244:GLN:N	2.42	0.49
1:B:1550:ASP:O	1:B:1552:ASP:N	2.46	0.49
1:A:1490:ALA:O	1:A:1527:PRO:HA	2.13	0.49
1:B:1455:ALA:HA	1:B:1459:TYR:CD2	2.41	0.49
1:B:1530:GLY:C	1:B:1532:ILE:H	2.15	0.49
1:A:1474:ILE:O	1:A:1478:GLU:HG3	2.13	0.49
1:B:1335:ARG:HH21	1:B:1386:THR:HG21	1.78	0.49
1:B:1459:TYR:HE2	1:B:1489:MET:HG3	1.78	0.49
1:A:1339:MET:HG2	1:A:1348:LEU:HD21	1.95	0.48
1:A:1550:ASP:C	1:A:1552:ASP:H	2.15	0.48
1:A:1116:TYR:CE1	2:A:8:SO4:O1	2.66	0.48
1:B:1042:LYS:NZ	1:B:1253:ASP:O	2.42	0.48
1:B:1148:ASP:OD2	1:B:1168:ARG:NH2	2.46	0.48
1:B:1488:VAL:HG23	1:B:1523:ARG:HD3	1.94	0.48
1:B:1182:ILE:O	1:B:1192:PRO:HA	2.13	0.48
1:B:1398:LEU:C	1:B:1400:ALA:H	2.17	0.48
1:A:1042:LYS:NZ	1:A:1254:ALA:HA	2.28	0.48
1:B:1370:ILE:CG2	1:B:1377:ALA:HB2	2.43	0.48
1:B:1486:PRO:HD2	1:B:1523:ARG:HB3	1.95	0.48
1:A:1010:ILE:C	1:A:1012:GLN:N	2.67	0.47
1:B:1440:LEU:HD22	1:B:1458:ILE:HD11	1.96	0.47
1:A:1129:PHE:CZ	1:A:1270:ILE:HG21	2.49	0.47
1:A:1182:ILE:HG22	1:A:1183:GLY:N	2.29	0.47
1:B:1277:ASN:ND2	1:B:1277:ASN:N	2.62	0.47
1:B:1292:LEU:HD23	1:B:1298:VAL:HG21	1.96	0.47
1:B:1380:ALA:O	1:B:1381:ILE:HD13	2.13	0.47
1:B:1220:GLU:O	1:B:1224:ARG:HG3	2.15	0.47
1:A:1277:ASN:ND2	1:A:1278:ILE:N	2.53	0.47
1:A:1417:GLU:CA	1:A:1420:LEU:HD23	2.45	0.47
1:B:1058:LYS:N	1:B:1296:ASP:O	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:PHE:HB3	1:A:1544:ALA:HB2	1.96	0.47
1:A:1270:ILE:HG23	1:A:1270:ILE:O	2.15	0.47
1:B:1031:ASP:OD2	1:B:1032:GLU:HG3	2.15	0.47
1:B:1222:PHE:HA	1:B:1225:LYS:CD	2.44	0.47
1:B:1375:VAL:CG1	1:B:1437:PHE:HD2	2.28	0.47
1:B:1210:CYS:SG	1:B:1274:PRO:HD3	2.55	0.47
1:B:1515:GLU:C	1:B:1527:PRO:HD2	2.35	0.47
1:B:1098:GLU:N	1:B:1272:GLY:O	2.37	0.47
1:A:1096:LEU:O	1:A:1270:ILE:HA	2.15	0.46
1:A:1532:ILE:O	1:A:1534:THR:N	2.47	0.46
1:B:1091:ARG:HB3	1:B:1296:ASP:H	1.80	0.46
1:B:1204:GLU:HB3	1:B:1225:LYS:HZ1	1.79	0.46
1:B:1278:ILE:HD12	1:B:1490:ALA:HB1	1.97	0.46
1:B:1338:LYS:HB3	1:B:1343:VAL:HG21	1.97	0.46
1:A:1285:ILE:HD13	1:A:1321:ALA:HB2	1.96	0.46
1:A:1476:ARG:HD3	3:A:148:HOH:O	2.16	0.46
1:A:1523:ARG:N	1:A:1523:ARG:CD	2.77	0.46
1:B:1203:SER:OG	1:B:1205:VAL:HB	2.15	0.46
1:B:1376:PRO:HB3	1:B:1433:ARG:HG2	1.97	0.46
1:B:1482:TYR:HB3	1:B:1485:LEU:CD1	2.46	0.46
1:B:1550:ASP:OD1	1:B:1551:ALA:N	2.49	0.46
1:B:1257:PRO:HD3	1:B:1286:ILE:HD13	1.97	0.46
1:A:1417:GLU:HA	1:A:1420:LEU:HD21	1.97	0.46
1:A:1487:VAL:CG1	1:A:1489:MET:HE2	2.45	0.46
1:B:1271:HIS:ND1	1:B:1286:ILE:HD11	2.31	0.46
1:B:1523:ARG:HB2	1:B:1524:LEU:H	1.52	0.46
1:B:1506:PRO:HB2	1:B:1509:PHE:CD2	2.51	0.46
1:B:1549:ILE:HG23	1:B:1549:ILE:O	2.16	0.46
1:B:1375:VAL:HG23	1:B:1375:VAL:O	2.15	0.46
1:A:1419:GLY:HA2	3:A:310:HOH:O	2.15	0.45
1:B:1140:HIS:HE1	1:B:1167:ARG:O	1.98	0.45
1:B:1394:LEU:C	1:B:1398:LEU:HD23	2.35	0.45
1:B:1448:LYS:HG2	1:B:1466:TYR:CE2	2.51	0.45
1:A:1555:ILE:O	1:A:1556:THR:CB	2.64	0.45
1:B:1042:LYS:HZ3	1:B:1254:ALA:HA	1.82	0.45
1:B:1065:ILE:HG23	1:B:1332:ALA:HB2	1.99	0.45
1:A:1550:ASP:C	1:A:1552:ASP:N	2.70	0.45
1:B:1368:GLU:O	1:B:1372:LYS:HG3	2.15	0.45
1:B:1079:VAL:CB	1:B:1117:ALA:O	2.64	0.45
1:B:1515:GLU:O	1:B:1516:VAL:HG23	2.16	0.45
1:B:1548:ASP:OD1	1:B:1549:ILE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:GLU:HG2	1:A:1115:GLY:N	2.31	0.45
1:A:1543:ALA:O	1:A:1547:ILE:HG12	2.17	0.45
1:B:1061:LEU:HD22	1:B:1313:PHE:CE2	2.52	0.45
1:B:1262:THR:CG2	1:B:1263:LEU:H	2.26	0.45
1:A:1098:GLU:HA	1:A:1270:ILE:HD11	1.97	0.45
1:A:1519:SER:C	1:A:1521:GLY:H	2.20	0.45
1:B:1432:SER:O	1:B:1434:PRO:HD3	2.17	0.45
1:B:1447:ILE:HG13	1:B:1478:GLU:OE1	2.17	0.45
1:A:1498:ASP:OD2	1:A:1528:ILE:HG21	2.17	0.45
1:B:1356:LEU:HD13	1:B:1356:LEU:C	2.38	0.45
1:B:1459:TYR:CE2	1:B:1489:MET:HG3	2.52	0.45
1:B:1466:TYR:CE2	1:B:1513:VAL:HG11	2.52	0.45
1:A:1308:LEU:O	1:A:1312:LYS:HG3	2.16	0.44
1:B:1143:LEU:O	1:B:1147:VAL:HG23	2.17	0.44
1:B:1379:VAL:HG21	1:B:1399:CYS:SG	2.56	0.44
1:B:1379:VAL:HG12	1:B:1380:ALA:N	2.31	0.44
1:A:1065:ILE:HB	1:A:1362:ASN:ND2	2.33	0.44
1:A:1178:ARG:NH2	2:A:5:SO4:O2	2.49	0.44
1:A:1235:PRO:HG3	1:A:1480:LEU:HD21	1.99	0.44
1:B:1058:LYS:HB3	1:B:1430:LEU:HD21	1.99	0.44
1:B:1114:GLY:O	1:B:1115:GLY:C	2.55	0.44
1:B:1125:ILE:HA	1:B:1129:PHE:CD1	2.51	0.44
1:B:1382:ASN:HD22	1:B:1382:ASN:HA	1.56	0.44
1:B:1032:GLU:OE1	1:B:1050:ARG:NH1	2.47	0.44
1:B:1523:ARG:N	1:B:1523:ARG:CD	2.76	0.44
1:A:1517:ARG:HH12	1:A:1532:ILE:HD12	1.83	0.44
1:B:1222:PHE:HD2	1:B:1225:LYS:HD2	1.83	0.44
1:A:1020:MET:CE	1:A:1033:VAL:HB	2.48	0.44
1:B:1227:VAL:HG22	1:B:1236:VAL:O	2.18	0.44
1:A:1319:ARG:HA	3:A:352:HOH:O	2.17	0.44
1:B:1408:LEU:HD13	1:B:1414:LYS:CE	2.47	0.44
1:A:1092:VAL:HG22	1:A:1093:MET:N	2.33	0.43
1:A:1398:LEU:HD13	1:A:1398:LEU:HA	1.86	0.43
1:A:1416:GLY:O	1:A:1420:LEU:CD2	2.66	0.43
1:A:1498:ASP:HB3	1:A:1528:ILE:HG21	1.93	0.43
1:B:1276:ALA:HB3	1:B:1304:PHE:CE2	2.53	0.43
1:A:1175:ARG:HG2	1:A:1178:ARG:NH2	2.33	0.43
1:A:1277:ASN:ND2	1:A:1277:ASN:N	2.56	0.43
1:A:1374:GLY:HA3	1:A:1436:ASN:O	2.18	0.43
1:B:1024:ARG:C	1:B:1026:LEU:H	2.21	0.43
1:B:1035:LEU:HB3	1:B:1037:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1389:GLU:O	1:B:1393:ASN:ND2	2.51	0.43
1:B:1417:GLU:C	1:B:1419:GLY:N	2.71	0.43
1:B:1488:VAL:HB	1:B:1525:ILE:HD13	1.99	0.43
1:A:1175:ARG:HG3	1:A:1537:GLY:HA3	2.00	0.43
1:A:1286:ILE:C	1:A:1286:ILE:CD1	2.77	0.43
1:B:1008:ILE:CG1	1:B:1011:ALA:HB2	2.49	0.43
1:B:1095:CYS:SG	1:B:1288:THR:HA	2.57	0.43
1:A:1544:ALA:HA	1:A:1547:ILE:HG12	2.01	0.43
1:B:1376:PRO:CD	1:B:1435:SER:HB3	2.49	0.43
1:A:1061:LEU:O	1:A:1328:THR:HA	2.19	0.43
1:A:1422:LEU:O	1:A:1426:VAL:HG23	2.19	0.43
1:A:1488:VAL:CG2	1:A:1523:ARG:HD3	2.48	0.43
1:B:1451:ILE:HG23	1:B:1489:MET:CE	2.49	0.43
1:A:1066:THR:HB	1:A:1340:HIS:CE1	2.53	0.43
1:B:1357:ARG:O	1:B:1360:PHE:HB3	2.19	0.43
1:A:1042:LYS:HZ3	1:A:1254:ALA:HA	1.84	0.43
1:A:1498:ASP:HB2	1:A:1528:ILE:CG2	2.44	0.43
1:B:1262:THR:CG2	1:B:1263:LEU:N	2.81	0.43
1:B:1454:ILE:O	1:B:1458:ILE:HB	2.17	0.43
1:B:1068:THR:C	1:B:1070:ALA:H	2.21	0.43
1:B:1075:THR:HA	1:B:1301:GLU:OE2	2.18	0.43
1:A:1333:THR:O	1:A:1337:LEU:HB2	2.18	0.43
1:B:1335:ARG:NH2	1:B:1386:THR:HG21	2.33	0.43
1:A:1271:HIS:CE1	1:A:1286:ILE:HD11	2.53	0.42
1:B:1062:VAL:CG1	1:B:1301:GLU:HB3	2.46	0.42
1:B:1092:VAL:HG23	1:B:1297:TYR:C	2.39	0.42
1:B:1175:ARG:HG3	1:B:1537:GLY:HA3	2.00	0.42
1:A:1549:ILE:HG23	1:A:1549:ILE:O	2.19	0.42
1:B:1337:LEU:HD21	1:B:1363:LEU:HB2	2.01	0.42
1:B:1555:ILE:O	1:B:1556:THR:HB	2.18	0.42
1:A:1257:PRO:HB3	1:A:1286:ILE:CD1	2.50	0.42
1:A:1376:PRO:HA	3:A:202:HOH:O	2.18	0.42
1:A:1448:LYS:HG3	3:A:173:HOH:O	2.18	0.42
1:B:1101:LEU:HD13	1:B:1127:LEU:HA	2.01	0.42
1:B:1312:LYS:O	1:B:1316:VAL:HB	2.19	0.42
1:B:1461:ALA:HB2	1:B:1511:ILE:HG12	2.01	0.42
1:A:1312:LYS:HD3	1:A:1488:VAL:HG13	2.01	0.42
1:A:1533:MET:SD	1:A:1536:PRO:HA	2.59	0.42
1:B:1376:PRO:HB3	1:B:1433:ARG:CG	2.50	0.42
1:B:1513:VAL:CG2	1:B:1526:VAL:HG23	2.49	0.42
1:A:1398:LEU:C	1:A:1400:ALA:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1546:ASN:CB	1:A:1556:THR:HG21	2.43	0.42
1:A:1118:GLN:HG2	1:A:1263:LEU:HD11	2.02	0.42
1:A:1400:ALA:O	1:A:1401:LYS:HB2	2.20	0.42
1:A:1417:GLU:C	1:A:1420:LEU:HD23	2.39	0.42
1:B:1026:LEU:HG	1:B:1294:LEU:HB3	2.02	0.42
1:A:1167:ARG:NH2	1:A:1196:GLY:HA3	2.35	0.42
1:B:1062:VAL:HG13	1:B:1301:GLU:CB	2.46	0.42
1:A:1286:ILE:HG23	3:A:169:HOH:O	2.18	0.42
1:A:1416:GLY:O	1:A:1420:LEU:HD22	2.20	0.42
1:A:1466:TYR:CD2	1:A:1513:VAL:HG22	2.55	0.41
1:B:1040:LYS:HB2	1:B:1040:LYS:NZ	2.35	0.41
1:B:1257:PRO:HA	1:B:1271:HIS:CG	2.55	0.41
1:A:1097:ARG:HG3	3:A:102:HOH:O	2.21	0.41
1:A:1289:LYS:O	1:A:1293:LYS:HD3	2.21	0.41
1:A:1528:ILE:HB	1:A:1529:THR:H	1.66	0.41
1:A:1529:THR:HB	1:A:1530:GLY:H	1.76	0.41
1:A:1550:ASP:N	1:A:1553:GLY:O	2.53	0.41
1:B:1010:ILE:C	1:B:1012:GLN:H	2.22	0.41
1:B:1047:VAL:HG11	1:B:1294:LEU:HD21	2.02	0.41
1:A:1306:ALA:HB3	1:A:1366:HIS:ND1	2.36	0.41
1:A:1441:TYR:HB3	1:A:1453:LYS:HD3	2.02	0.41
1:A:1470:ALA:O	1:A:1474:ILE:HG13	2.20	0.41
1:A:1523:ARG:HB2	1:A:1524:LEU:H	1.62	0.41
1:B:1011:ALA:O	1:B:1013:ALA:N	2.47	0.41
1:B:1032:GLU:CD	1:B:1050:ARG:HH12	2.24	0.41
1:B:1506:PRO:HG2	1:B:1509:PHE:CE2	2.55	0.41
1:A:1180:ILE:HG12	1:A:1196:GLY:HA2	2.01	0.41
1:B:1488:VAL:HB	1:B:1525:ILE:CD1	2.49	0.41
1:B:1400:ALA:O	1:B:1401:LYS:HB2	2.20	0.41
1:B:1541:ARG:N	1:B:1542:PRO:HD3	2.35	0.41
1:A:1042:LYS:HE2	1:A:1256:LYS:O	2.20	0.41
1:A:1388:THR:OG1	1:A:1391:GLU:HG3	2.21	0.41
1:A:1007:ASP:CG	3:A:131:HOH:O	2.59	0.41
1:B:1369:ASN:O	1:B:1372:LYS:HB2	2.21	0.41
1:B:1415:GLY:C	1:B:1417:GLU:N	2.74	0.41
1:A:1452:ALA:O	1:A:1456:THR:HB	2.21	0.41
1:A:1488:VAL:HG23	1:A:1523:ARG:HD3	2.02	0.41
1:B:1017:LYS:HA	1:B:1018:PRO:HD3	1.97	0.41
1:B:1043:ILE:HD12	1:B:1269:PHE:HZ	1.83	0.41
1:B:1061:LEU:HD13	1:B:1313:PHE:CZ	2.56	0.41
1:B:1063:THR:N	1:B:1329:VAL:O	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1085:LEU:CD2	1:B:1090:LYS:HG3	2.50	0.41
1:B:1169:VAL:CG1	1:B:1200:SER:OG	2.68	0.41
1:B:1215:LEU:HD23	1:B:1215:LEU:HA	1.85	0.41
1:B:1287:ALA:O	1:B:1290:THR:HB	2.20	0.41
1:B:1350:THR:CG2	1:B:1351:GLU:N	2.84	0.41
1:B:1376:PRO:HB3	1:B:1433:ARG:HD3	2.03	0.41
1:B:1482:TYR:CD1	1:B:1482:TYR:N	2.89	0.41
1:A:1146:MET:SD	1:A:1243:ALA:HB2	2.61	0.41
1:B:1119:VAL:HG13	1:B:1261:GLN:O	2.21	0.41
1:B:1373:PHE:CZ	1:B:1440:LEU:HB2	2.56	0.41
1:B:1394:LEU:CD1	1:B:1398:LEU:HD21	2.51	0.41
1:A:1262:THR:HG22	1:A:1263:LEU:H	1.86	0.40
1:A:1554:VAL:CG1	1:A:1555:ILE:N	2.82	0.40
1:B:1277:ASN:HD22	1:B:1277:ASN:N	2.17	0.40
1:A:1026:LEU:HG	1:A:1294:LEU:HB3	2.04	0.40
1:B:1060:ILE:HG22	1:B:1060:ILE:O	2.21	0.40
1:B:1082:THR:CG2	1:B:1094:VAL:HG22	2.48	0.40
1:B:1085:LEU:HD22	1:B:1090:LYS:HB2	2.04	0.40
1:B:1270:ILE:HG23	1:B:1270:ILE:O	2.20	0.40
1:B:1010:ILE:O	1:B:1012:GLN:N	2.54	0.40
1:B:1167:ARG:NH2	1:B:1178:ARG:O	2.53	0.40
1:B:1312:LYS:CD	1:B:1488:VAL:HG13	2.49	0.40
1:B:1405:GLU:HG3	1:B:1425:LYS:CB	2.52	0.40
1:B:1466:TYR:CD2	1:B:1513:VAL:HG11	2.56	0.40
1:A:1262:THR:HG22	1:A:1264:GLU:H	1.86	0.40
1:A:1490:ALA:HB3	1:A:1527:PRO:HB3	2.04	0.40
1:B:1043:ILE:HD12	1:B:1269:PHE:CE1	2.56	0.40
1:B:1415:GLY:O	1:B:1417:GLU:N	2.54	0.40
1:B:1455:ALA:O	1:B:1459:TYR:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1462:ASP:O	1:A:1462:ASP:O[12_555]	2.02	0.18

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	547/557 (98%)	485 (89%)	54 (10%)	8 (2%)	10 18
1	B	546/557 (98%)	444 (81%)	81 (15%)	21 (4%)	3 4
All	All	1093/1114 (98%)	929 (85%)	135 (12%)	29 (3%)	5 7

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1015	LYS
1	A	1401	LYS
1	B	1015	LYS
1	A	1399	CYS
1	B	1065	ILE
1	B	1352	ASN
1	B	1401	LYS
1	B	1529	THR
1	B	1556	THR
1	B	1018	PRO
1	B	1273	GLY
1	B	1400	ALA
1	B	1437	PHE
1	A	1520	ALA
1	A	1529	THR
1	B	1072	GLU
1	B	1325	PRO
1	B	1551	ALA
1	A	1556	THR
1	B	1265	ASN
1	B	1399	CYS
1	B	1421	GLU
1	B	1528	ILE
1	B	1026	LEU
1	B	1077	THR

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Mol	Chain	Res	Type
1	A	1528	ILE
1	B	1154	GLY
1	A	1273	GLY
1	B	1260	VAL

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	432/440 (98%)	409 (95%)	23 (5%)	22 43
1	B	431/440 (98%)	409 (95%)	22 (5%)	24 45
All	All	863/880 (98%)	818 (95%)	45 (5%)	23 44

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1008	ILE
1	A	1020	MET
1	A	1062	VAL
1	A	1169	VAL
1	A	1193	ARG
1	A	1195	THR
1	A	1224	ARG
1	A	1244	GLN
1	A	1274	PRO
1	A	1277	ASN
1	A	1278	ILE
1	A	1311	GLU
1	A	1337	LEU
1	A	1347	ASP
1	A	1356	LEU
1	A	1375	VAL
1	A	1398	LEU
1	A	1430	LEU
1	A	1443	LEU

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Mol	Chain	Res	Type
1	A	1523	ARG
1	A	1526	VAL
1	A	1533	MET
1	A	1535	MET
1	B	1012	GLN
1	B	1020	MET
1	B	1072	GLU
1	B	1085	LEU
1	B	1182	ILE
1	B	1195	THR
1	B	1244	GLN
1	B	1250	LEU
1	B	1269	PHE
1	B	1275	PHE
1	B	1277	ASN
1	B	1278	ILE
1	B	1311	GLU
1	B	1353	LEU
1	B	1382	ASN
1	B	1444	ASP
1	B	1462	ASP
1	B	1480	LEU
1	B	1523	ARG
1	B	1526	VAL
1	B	1533	MET
1	B	1535	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1029	GLN
1	A	1140	HIS
1	A	1149	ASN
1	A	1150	HIS
1	A	1158	ASN
1	A	1244	GLN
1	A	1261	GLN
1	A	1265	ASN
1	A	1277	ASN
1	A	1362	ASN
1	A	1382	ASN
1	A	1465	ASN

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Mol	Chain	Res	Type
1	A	1484	ASN
1	B	1029	GLN
1	B	1140	HIS
1	B	1149	ASN
1	B	1150	HIS
1	B	1158	ASN
1	B	1189	ASN
1	B	1244	GLN
1	B	1277	ASN
1	B	1283	ASN
1	B	1362	ASN
1	B	1369	ASN
1	B	1382	ASN
1	B	1393	ASN
1	B	1465	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	1	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	A	3	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	B	2	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	A	5	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	A	6	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	A	4	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	B	11	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	B	9	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	B	10	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	A	7	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	A	8	-	4,4,4	0.82	0	6,6,6	0.50	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3	SO4	6	0
2	B	2	SO4	1	0
2	A	5	SO4	2	0
2	B	9	SO4	1	0
2	A	7	SO4	2	0
2	A	8	SO4	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.