Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:48 PM GMT

PDB ID	:	1CJY
Title	:	HUMAN CYTOSOLIC PHOSPHOLIPASE A2
Authors	:	Dessen, A.; Tang, J.; Schmidt, H.; Stahl, M.; Clark, J.D.; Seehra, J.; Somers, W.S.
Deposited on	:	1999-04-20
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

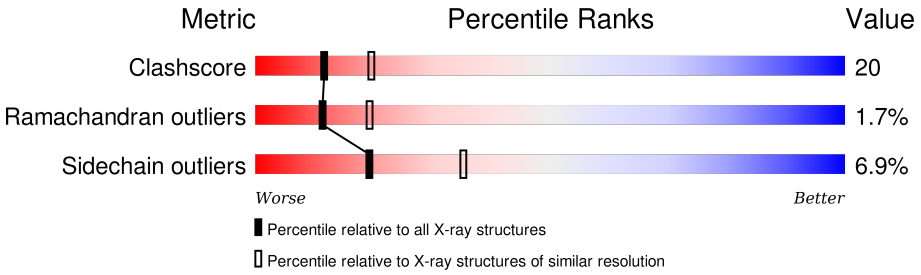
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	749	53% 27% • 15%
1	B	749	52% 26% 5% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9706 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.

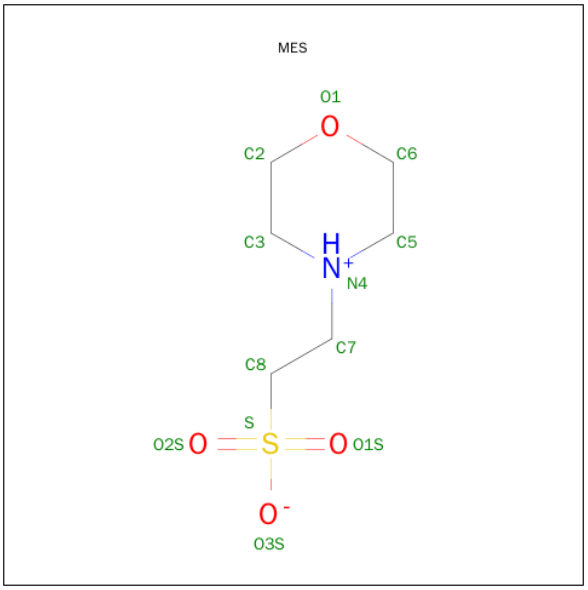
- Molecule 1 is a protein called PROTEIN (CYTOSOLIC PHOSPHOLIPASE A2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	0	0
			4876	3144	804	895	33			
1	B	614	Total	C	N	O	S	0	0	0
			4744	3066	773	871	34			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	26	Total	O	0	0
			26	26		

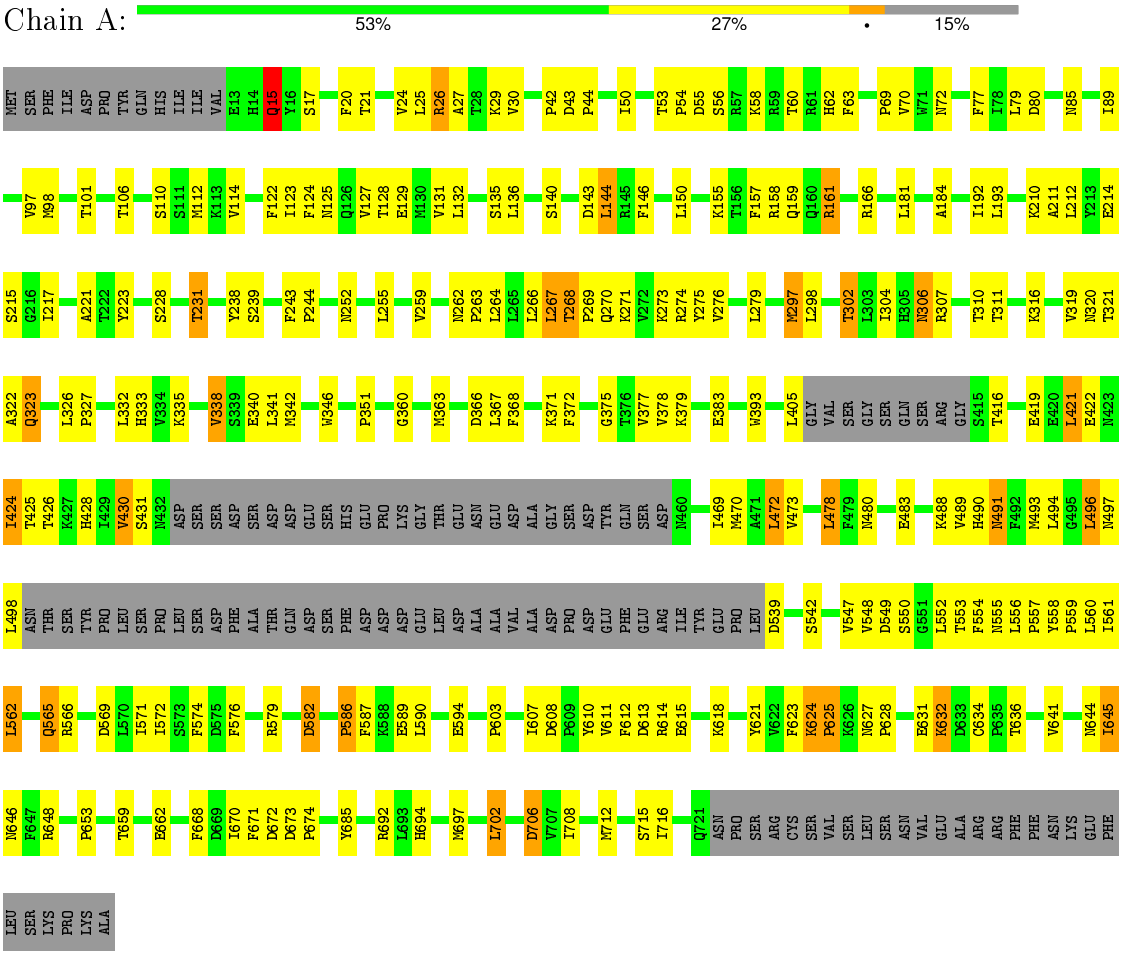
3 Residue-property plots (i)

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

Note EDS was not executed.

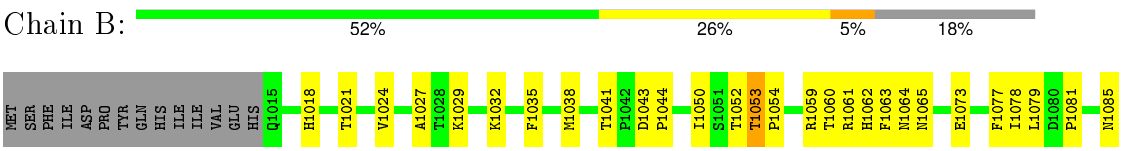
- Molecule 1: PROTEIN (CYTOSOLIC PHOSPHOLIPASE A2)

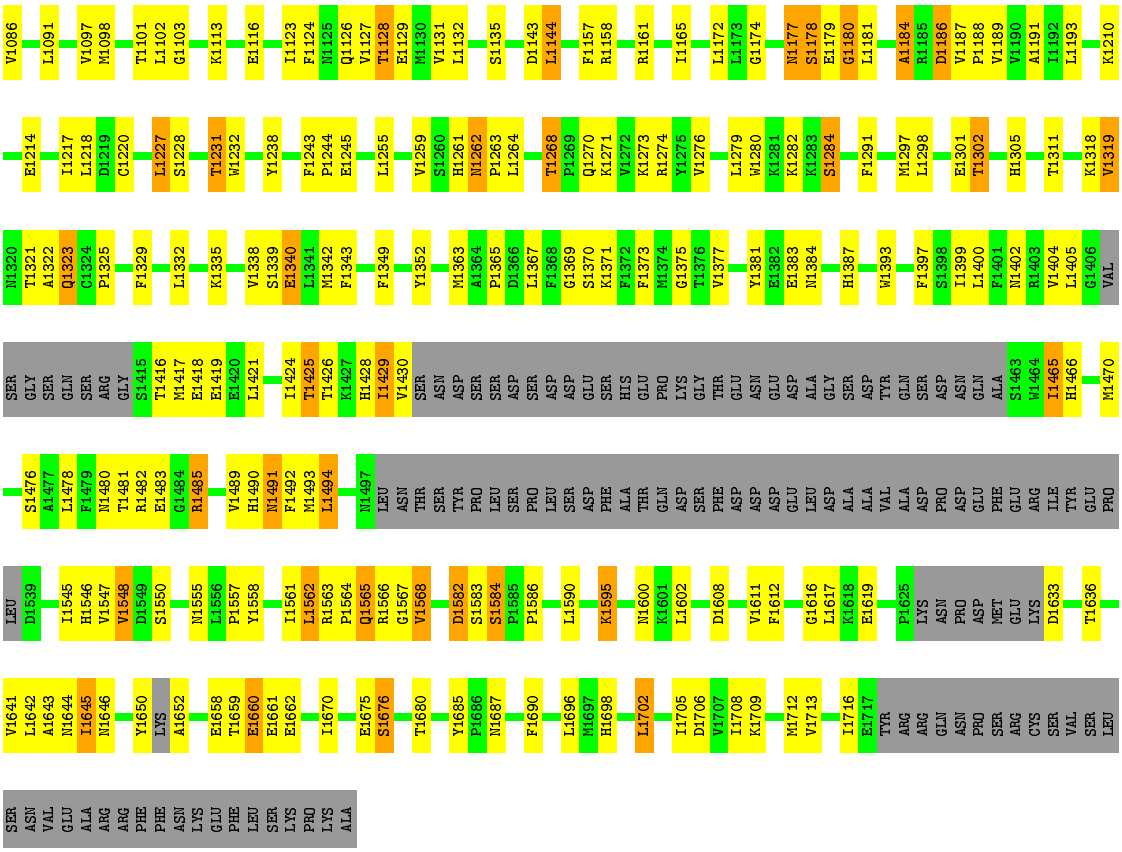
Chain A:



- Molecule 1: PROTEIN (CYTOSOLIC PHOSPHOLIPASE A2)

Chain B:




V1086 L1091 V1097 M1098 T1101 L1102 G1103 K1113 E1116 I1123 F1124 N1125 Q1126 V1127 T1128 E1129 M1130 V1131 L1132 S1135 D1143 L1144 F1157 R1158 R1161 I1165 L1172 L1173 G1174 N1177 S1178 E1179 G1180 L1181 A1184 R1185 D1186 V1187 P1188 V1189 V1190 A1191 I1192 L1193 K1210
E1214 I1217 L1218 D1219 C1220 L1227 S1228 T1231 W1232 Y1238 F1243 P1244 E1245 L1255 V1259 S1260 H1261 N1262 P1263 L1264 T1268 P1269 Q1270 K1271 V1272 K1273 R1274 Y1275 V1276 L1279 W1280 K1281 K1282 K1283 S1284 F1291 M1297 L1298 E1301 T1302 H1305 T1311 K1318 V1319
N1320 T1321 A1322 Q1323 C1324 P1325 F1329 L1332 K1335 V1338 S1339 E1340 L1341 M1342 F1343 F1349 Y1352 M1363 A1364 P1365 D1366 L1367 F1368 G1369 S1370 K1371 F1372 F1373 M1374 G1375 T1376 V1377 Y1381 E1382 E1383 N1384 H1387 W1393 F1397 S1398 I1399 L1400 F1401 N1402 R1403 V1404 L1405 G1406 VAL
SER GLY SER GLN SER ARG GLY S1415 T1416 M1417 E1418 E1419 E1420 L1421 I1424 T1425 T1426 K1427 H1428 I1429 V1430 SER ASN ASP SER SER ASP SER ASP ASP GLU SER HIS GLU PRO LYS GLY THR GLU ASN GLU ASP ALA GLY SER ASP TYR GLN SER ASP ASN GLN ALA S1463 W1464 I1465 H1466 M1470
S1476 A1477 L1478 F1479 N1480 T1481 R1482 E1483 G1484 R1485 V1489 H1490 N1491 F1492 M1493 L1494 N1497 LEU ASN THR SER TYR PRO LEU SER PRO LEU SER ASP PHE ALA THR GLN ASP SER PHE ASP ASP ASP GLU LEU ASP ALA ALA VAL ALA ASP PRO ASP GLU PHE GLU ARG ILE TYR GLU PRO
LEU D1539 I1545 H1546 V1547 V1548 D1549 S1550 N1555 L1556 P1557 Y1558 I1561 L1562 R1563 P1564 Q1565 R1566 G1567 V1568 D1582 S1583 S1584 P1585 P1586 L1590 K1595 N1600 K1601 L1602 D1608 V1611 F1612 G1616 L1617 K1618 E1619 P1625 LYS ASN PRO ASP MET GLU LYS D1633 T1636
V1641 L1642 A1643 N1644 I1645 N1646 Y1650 LYS A1652 E1658 T1659 E1660 E1661 E1662 I1670 E1675 S1676 T1680 Y1685 P1686 N1687 F1690 L1696 M1697 H1698 L1702 I1705 D1706 V1707 I1708 K1709 M1712 V1713 I1716 E1717 TYR ARG ARG GLN ASN PRO SER ARG CYS SER VAL SER LEU
SER ASN VAL GLU ALA ARG ARG PHE PHE ASN LYS GLU PHE LEU SER LYS PRO LYS ALA

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	153.59Å 95.49Å 139.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.50	Depositor
% Data completeness (in resolution range)	93.3 (12.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.229 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9706	wwPDB-VP
Average B, all atoms (Å^2)	51.0	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: CA, MES

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	0.39	0/4999	0.63	0/6796
1	B	0.40	0/4862	0.64	1/6603 (0.0%)
All	All	0.39	0/9861	0.63	1/13399 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1227	LEU	CA-CB-CG	5.49	127.94	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	4876	0	4668	203	0
1	B	4744	0	4576	181	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	12	0	13	0	0
3	B	12	0	13	1	0
4	A	32	0	0	1	0
4	B	26	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9706	0	9270	384	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 20.

All (384) 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:323:GLN:N	1:A:323:GLN:HE21	1.54	1.04
1:A:79:LEU:HD22	1:A:85:ASN:HD22	1.23	1.03
1:A:323:GLN:NE2	1:A:323:GLN:H	1.59	0.99
1:B:1323:GLN:HE21	1:B:1323:GLN:H	1.08	0.98
1:B:1465:ILE:HD12	1:B:1465:ILE:H	1.26	0.97
1:A:565:GLN:H	1:A:565:GLN:NE2	1.64	0.95
1:B:1429:ILE:HD12	1:B:1548:VAL:HG11	1.51	0.91
1:B:1323:GLN:NE2	1:B:1323:GLN:H	1.69	0.90
1:A:425:THR:HG23	1:A:428:HIS:H	1.37	0.89
1:B:1262:ASN:HD21	1:B:1264:LEU:HD23	1.37	0.89
1:A:268:THR:HG22	1:A:271:LYS:H	1.38	0.87
1:A:193:LEU:HD11	1:A:561:ILE:HD13	1.54	0.87
1:A:608:ASP:OD1	1:A:611:VAL:HB	1.75	0.87
1:B:1323:GLN:HE21	1:B:1323:GLN:N	1.74	0.85
1:B:1491:ASN:ND2	1:B:1493:MET:H	1.76	0.83
1:A:323:GLN:HE21	1:A:323:GLN:H	0.86	0.83
1:A:97:VAL:HG23	1:A:98:MET:H	1.45	0.81
1:B:1029:LYS:O	1:B:1128:THR:HB	1.81	0.81
1:A:26:ARG:HB2	1:A:69:PRO:O	1.82	0.80
1:A:79:LEU:HD22	1:A:85:ASN:ND2	1.98	0.79
1:B:1268:THR:HG22	1:B:1271:LYS:H	1.49	0.77
1:A:363:MET:HE2	1:A:368:PHE:HA	1.66	0.76
1:A:306:ASN:HD21	1:A:307:ARG:HH11	1.32	0.76
1:A:238:TYR:CE2	1:A:327:PRO:HG3	2.21	0.75
1:B:1187:VAL:HG12	1:B:1188:PRO:HD2	1.67	0.75
1:A:321:THR:H	1:A:323:GLN:HE22	1.31	0.75
1:B:1321:THR:H	1:B:1323:GLN:HE22	1.33	0.75
1:A:29:LYS:O	1:A:128:THR:HB	1.86	0.74
1:A:298:LEU:O	1:A:302:THR:HG23	1.88	0.74
1:B:1097:VAL:HG23	1:B:1098:MET:H	1.53	0.73
1:B:1187:VAL:CG1	1:B:1188:PRO:HD2	2.18	0.73
1:A:157:PHE:CE1	1:A:319:VAL:HG23	2.23	0.73
1:A:15:GLN:NE2	1:A:17:SER:H	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1425:THR:HB	1:B:1428:HIS:H	1.53	0.71
1:B:1024:VAL:HA	1:B:1132:LEU:HD22	1.72	0.71
1:A:155:LYS:O	1:A:159:GLN:HG3	1.91	0.70
1:B:1608:ASP:O	1:B:1611:VAL:HG23	1.91	0.70
1:B:1264:LEU:H	1:B:1264:LEU:HD22	1.56	0.69
1:A:316:LYS:HE3	1:A:351:PRO:O	1.91	0.69
1:B:1268:THR:CG2	1:B:1271:LYS:H	2.05	0.69
1:A:306:ASN:ND2	1:A:307:ARG:HG2	2.07	0.69
1:B:1645:ILE:HG22	1:B:1646:ASN:N	2.08	0.69
1:A:556:LEU:HD11	1:A:589:GLU:HG2	1.75	0.68
1:A:565:GLN:H	1:A:565:GLN:HE21	1.41	0.68
1:A:279:LEU:HG	1:A:297:MET:HE2	1.74	0.68
1:A:306:ASN:HD21	1:A:307:ARG:NH1	1.90	0.68
1:A:210:LYS:O	1:A:214:GLU:HG3	1.94	0.68
1:A:366:ASP:HA	1:A:383:GLU:HG3	1.75	0.68
1:B:1430:VAL:HG13	1:B:1546:HIS:CE1	2.30	0.67
1:A:181:LEU:HA	1:A:184:ALA:HB2	1.75	0.67
1:B:1113:LYS:O	1:B:1116:GLU:HB3	1.95	0.66
1:B:1298:LEU:O	1:B:1302:THR:HG23	1.95	0.66
1:B:1645:ILE:HG22	1:B:1646:ASN:H	1.59	0.66
1:A:491:ASN:ND2	1:A:493:MET:H	1.94	0.65
1:A:15:GLN:HE22	1:A:17:SER:H	1.42	0.65
1:A:269:PRO:O	1:A:273:LYS:HG3	1.97	0.65
1:B:1342:MET:HE2	1:B:1595:LYS:HG2	1.77	0.65
1:B:1097:VAL:HG23	1:B:1098:MET:N	2.12	0.65
1:B:1405:LEU:HD12	1:B:1466:HIS:HB2	1.79	0.65
1:A:161:ARG:HB2	1:A:322:ALA:HB1	1.79	0.64
1:B:1144:LEU:HD22	1:B:1375:GLY:HA2	1.80	0.64
1:A:610:TYR:O	1:A:614:ARG:HG2	1.98	0.64
1:A:144:LEU:HD22	1:A:375:GLY:HA2	1.79	0.63
1:B:1702:LEU:HD12	1:B:1705:ILE:HD11	1.80	0.63
1:B:1218:LEU:HD22	1:B:1325:PRO:HG2	1.80	0.63
1:A:193:LEU:CD1	1:A:561:ILE:HD13	2.27	0.63
1:B:1311:THR:HB	1:B:1383:GLU:OE2	2.00	0.62
1:A:158:ARG:HH21	1:A:566:ARG:HA	1.64	0.61
1:A:416:THR:OG1	1:A:419:GLU:HG3	2.00	0.61
1:B:1123:ILE:HD12	1:B:1128:THR:O	2.01	0.61
1:A:603:PRO:HB3	1:A:634:CYS:HB2	1.82	0.61
1:B:1078:ILE:HG22	1:B:1373:PHE:HD2	1.64	0.61
1:A:89:ILE:HD13	1:A:132:LEU:HD12	1.83	0.61
1:B:1255:LEU:HD12	1:B:1690:PHE:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1465:ILE:CD1	1:B:1465:ILE:H	2.02	0.61
1:B:1187:VAL:HG12	1:B:1188:PRO:CD	2.31	0.60
1:A:89:ILE:HD13	1:A:132:LEU:CD1	2.31	0.60
1:B:1369:GLY:HA2	1:B:1489:VAL:HG22	1.83	0.60
1:A:579:ARG:HD3	1:A:586:PRO:HB3	1.83	0.60
1:B:1255:LEU:HD12	1:B:1690:PHE:HE1	1.65	0.60
1:B:1387:HIS:HD2	4:B:77:HOH:O	1.85	0.60
1:A:275:TYR:HA	1:A:297:MET:HE1	1.82	0.60
1:A:161:ARG:NH1	1:A:221:ALA:O	2.34	0.60
1:B:1369:GLY:HA2	1:B:1489:VAL:CG2	2.30	0.60
1:A:548:VAL:HG22	1:A:549:ASP:N	2.15	0.60
1:B:1565:GLN:H	1:B:1565:GLN:NE2	2.00	0.60
1:B:1018:HIS:CE1	1:B:1081:PRO:HB3	2.36	0.60
1:B:1425:THR:HB	1:B:1428:HIS:N	2.15	0.60
1:B:1228:SER:O	1:B:1231:THR:HB	2.02	0.60
1:A:228:SER:O	1:A:231:THR:HB	2.02	0.59
1:A:125:ASN:O	1:A:127:VAL:HG23	2.02	0.59
1:A:97:VAL:HG23	1:A:98:MET:N	2.16	0.58
1:A:53:THR:HG23	1:A:54:PRO:HD2	1.85	0.58
1:A:21:THR:HB	1:A:135:SER:HB2	1.84	0.58
1:A:645:ILE:O	1:A:648:ARG:HG3	2.03	0.58
1:A:553:THR:HG22	1:A:554:PHE:CD2	2.38	0.58
1:A:25:LEU:HA	1:A:72:ASN:HD22	1.67	0.58
1:A:558:TYR:HB3	1:A:562:LEU:HD22	1.84	0.58
1:A:166:ARG:HH12	1:A:184:ALA:HB3	1.69	0.57
1:B:1582:ASP:O	1:B:1617:LEU:HD22	2.03	0.57
1:A:426:THR:O	1:A:430:VAL:HG22	2.04	0.57
1:A:430:VAL:HG23	1:A:431:SER:H	1.70	0.57
1:B:1021:THR:HB	1:B:1135:SER:HB2	1.86	0.57
1:B:1416:THR:OG1	1:B:1419:GLU:HG3	2.05	0.57
1:A:627:ASN:N	1:A:628:PRO:HD2	2.20	0.57
1:A:15:GLN:HA	1:A:497:ASN:CG	2.24	0.57
1:B:1189:VAL:HB	1:B:1568:VAL:HA	1.86	0.57
1:B:1157:PHE:CE1	1:B:1319:VAL:HG22	2.40	0.56
1:A:470:MET:HA	1:A:470:MET:HE2	1.86	0.56
1:A:319:VAL:O	1:A:319:VAL:HG22	2.06	0.56
1:A:659:THR:OG1	1:A:662:GLU:HG3	2.06	0.56
1:B:1264:LEU:N	1:B:1264:LEU:HD22	2.21	0.56
1:B:1127:VAL:HB	4:B:62:HOH:O	2.04	0.56
1:A:430:VAL:HG23	1:A:431:SER:N	2.21	0.56
1:A:493:MET:O	1:A:496:LEU:HD23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ASN:O	1:A:483:GLU:HG2	2.06	0.56
1:B:1259:VAL:HG12	1:B:1685:TYR:HB2	1.87	0.55
1:A:366:ASP:OD2	1:A:367:LEU:HD13	2.05	0.55
1:A:335:LYS:NZ	1:A:539:ASP:HB2	2.20	0.55
1:A:498:LEU:C	1:A:498:LEU:HD13	2.27	0.55
1:B:1583:SER:O	1:B:1584:SER:O	2.24	0.55
1:A:157:PHE:CD1	1:A:319:VAL:HG23	2.41	0.55
1:B:1259:VAL:O	1:B:1259:VAL:HG12	2.04	0.55
1:B:1174:GLY:O	1:B:1177:ASN:ND2	2.40	0.55
1:B:1184:ALA:HB1	1:B:1186:ASP:O	2.08	0.54
1:A:332:LEU:O	1:A:547:VAL:HA	2.07	0.54
1:B:1332:LEU:HG	1:B:1550:SER:HA	1.88	0.54
1:B:1650:TYR:O	1:B:1652:ALA:N	2.40	0.54
1:A:259:VAL:HG12	1:A:685:TYR:HB2	1.90	0.54
1:B:1321:THR:OG1	1:B:1323:GLN:NE2	2.41	0.54
1:A:181:LEU:HA	1:A:184:ALA:CB	2.37	0.54
1:A:158:ARG:NH2	1:A:566:ARG:O	2.40	0.54
1:B:1335:LYS:O	1:B:1338:VAL:HG22	2.08	0.54
1:B:1238:TYR:O	1:B:1318:LYS:HG3	2.07	0.53
1:B:1268:THR:HG22	1:B:1271:LYS:CB	2.38	0.53
1:A:363:MET:HE2	1:A:368:PHE:CA	2.35	0.53
1:A:335:LYS:O	1:A:338:VAL:HG12	2.08	0.53
1:B:1158:ARG:NH2	1:B:1566:ARG:O	2.39	0.53
1:B:1054:PRO:HG2	1:B:1494:LEU:HD13	1.89	0.53
1:A:79:LEU:HB3	1:A:85:ASN:ND2	2.24	0.53
1:B:1424:ILE:HD12	1:B:1424:ILE:O	2.08	0.53
1:B:1400:LEU:O	1:B:1404:VAL:HG23	2.08	0.53
1:A:419:GLU:O	1:A:422:GLU:HG2	2.09	0.53
1:B:1165:ILE:HD12	1:B:1220:CYS:O	2.08	0.53
1:A:556:LEU:CD1	1:A:589:GLU:HG2	2.39	0.52
1:B:1480:ASN:CG	1:B:1482:ARG:H	2.12	0.52
1:B:1131:VAL:O	1:B:1132:LEU:HD23	2.09	0.52
1:A:469:ILE:HG22	1:A:470:MET:HE3	1.92	0.52
1:B:1243:PHE:CD1	1:B:1244:PRO:HA	2.44	0.52
1:A:631:GLU:O	1:A:632:LYS:O	2.27	0.52
1:A:306:ASN:HD22	1:A:306:ASN:C	2.13	0.52
1:B:1027:ALA:HA	1:B:1129:GLU:O	2.09	0.52
1:A:589:GLU:OE2	1:A:589:GLU:N	2.34	0.52
1:A:469:ILE:HG22	1:A:470:MET:CE	2.41	0.51
1:A:607:ILE:HG23	1:A:623:PHE:CE2	2.45	0.51
1:A:252:ASN:HD22	1:A:694:HIS:HE1	1.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1659:THR:O	1:B:1662:GLU:N	2.38	0.51
1:B:1329:PHE:HB2	1:B:1349:PHE:HB2	1.93	0.51
1:B:1465:ILE:N	1:B:1465:ILE:HD12	2.09	0.51
1:A:268:THR:CG2	1:A:271:LYS:H	2.18	0.51
1:B:1371:LYS:HE2	1:B:1490:HIS:CE1	2.46	0.51
1:B:1210:LYS:O	1:B:1214:GLU:HG3	2.10	0.51
1:B:1231:THR:CG2	1:B:1393:TRP:HE3	2.23	0.51
1:B:1264:LEU:H	1:B:1264:LEU:CD2	2.23	0.51
1:B:1491:ASN:HD22	1:B:1491:ASN:C	2.12	0.51
1:B:1491:ASN:ND2	1:B:1491:ASN:C	2.64	0.51
1:B:1262:ASN:HD22	1:B:1262:ASN:C	2.14	0.51
1:B:1259:VAL:CG1	1:B:1685:TYR:HB2	2.41	0.51
1:A:708:ILE:HG22	1:A:712:MET:HE3	1.93	0.50
1:A:332:LEU:HG	1:A:550:SER:HA	1.93	0.50
1:B:1301:GLU:O	1:B:1305:HIS:HB3	2.11	0.50
1:A:259:VAL:O	1:A:259:VAL:HG12	2.10	0.50
1:B:1035:PHE:HA	1:B:1038:MET:HE3	1.93	0.50
1:A:587:PHE:HE2	1:A:612:PHE:HB2	1.77	0.50
1:B:1041:THR:HG22	1:B:1065:ASN:HA	1.93	0.50
1:A:181:LEU:HG	1:A:716:ILE:HD13	1.93	0.50
1:B:1078:ILE:HG22	1:B:1373:PHE:CD2	2.46	0.50
1:B:1191:ALA:CB	1:B:1561:ILE:HG12	2.42	0.50
1:B:1282:LYS:NZ	1:B:1384:ASN:HD21	2.09	0.50
1:B:1231:THR:HG23	1:B:1393:TRP:HE3	1.76	0.50
1:B:1279:LEU:HG	1:B:1297:MET:CE	2.42	0.50
1:A:306:ASN:HD21	1:A:307:ARG:HG2	1.77	0.49
1:B:1712:MET:O	1:B:1716:ILE:HG13	2.12	0.49
1:A:30:VAL:HG11	1:A:44:PRO:HG3	1.93	0.49
1:A:215:SER:OG	1:A:217:ILE:HG12	2.13	0.49
1:A:469:ILE:O	1:A:473:VAL:HG23	2.12	0.49
1:A:143:ASP:OD2	1:A:377:VAL:HG13	2.12	0.49
1:B:1645:ILE:CG2	1:B:1646:ASN:H	2.22	0.49
1:A:548:VAL:HG22	1:A:549:ASP:H	1.75	0.49
1:A:123:ILE:HD12	1:A:123:ILE:N	2.27	0.49
1:B:1043:ASP:HA	1:B:1063:PHE:O	2.13	0.49
1:B:1123:ILE:HD11	1:B:1126:GLN:C	2.32	0.49
1:A:238:TYR:CZ	1:A:327:PRO:HG3	2.48	0.49
1:B:1421:LEU:O	1:B:1421:LEU:HD23	2.13	0.49
1:A:306:ASN:HD22	1:A:307:ARG:N	2.11	0.49
1:A:20:PHE:HD1	1:A:135:SER:O	1.96	0.49
1:A:122:PHE:C	1:A:123:ILE:HD12	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1079:LEU:HB3	1:B:1085:ASN:OD1	2.12	0.49
1:A:211:ALA:HB1	1:A:702:LEU:HD13	1.95	0.49
1:B:1143:ASP:OD2	1:B:1377:VAL:HG13	2.13	0.49
1:B:1421:LEU:HA	1:B:1424:ILE:CG2	2.43	0.48
1:B:1659:THR:O	1:B:1660:GLU:C	2.50	0.48
1:A:624:LYS:HG3	1:A:625:PRO:HD2	1.94	0.48
1:B:1231:THR:HG23	1:B:1393:TRP:CE3	2.48	0.48
1:A:212:LEU:HD22	1:A:217:ILE:HG21	1.95	0.48
1:A:668:PHE:CD2	1:A:692:ARG:HD3	2.48	0.48
1:A:611:VAL:O	1:A:615:GLU:HB2	2.14	0.48
1:A:279:LEU:HG	1:A:297:MET:CE	2.44	0.48
1:B:1650:TYR:HB3	1:B:1652:ALA:O	2.14	0.48
1:B:1399:ILE:HA	1:B:1485:ARG:HG3	1.94	0.48
1:B:1430:VAL:HG13	1:B:1546:HIS:HE1	1.79	0.48
1:B:1561:ILE:HG13	1:B:1568:VAL:HG11	1.95	0.48
1:B:1178:SER:O	1:B:1180:GLY:N	2.47	0.48
1:B:1480:ASN:HD21	1:B:1482:ARG:CB	2.26	0.48
1:A:239:SER:HB2	1:A:310:THR:HG21	1.96	0.48
1:B:1231:THR:HG21	1:B:1393:TRP:HB2	1.96	0.47
1:B:1321:THR:N	1:B:1323:GLN:HE22	2.08	0.47
1:A:610:TYR:HA	1:A:613:ASP:OD1	2.13	0.47
1:B:1032:LYS:HG2	1:B:1102:LEU:HD22	1.96	0.47
1:A:150:LEU:CD1	1:A:158:ARG:HE	2.26	0.47
1:B:1214:GLU:OE1	1:B:1698:HIS:HE1	1.97	0.47
1:A:645:ILE:HG22	1:A:646:ASN:N	2.29	0.47
1:B:1193:LEU:HG	1:B:1557:PRO:HG2	1.96	0.47
1:A:311:THR:HB	1:A:383:GLU:OE2	2.14	0.47
1:B:1387:HIS:CD2	4:B:77:HOH:O	2.63	0.47
1:B:1421:LEU:C	1:B:1421:LEU:HD23	2.34	0.47
1:A:333:HIS:HE1	4:A:3029:HOH:O	1.98	0.47
1:B:1687:ASN:N	1:B:1687:ASN:HD22	2.12	0.47
1:A:24:VAL:HA	1:A:132:LEU:HD23	1.97	0.47
1:A:670:ILE:N	1:A:670:ILE:HD12	2.30	0.47
1:B:1491:ASN:HB2	1:B:1545:ILE:HG23	1.96	0.46
1:B:1261:HIS:O	1:B:1263:PRO:HD3	2.15	0.46
1:A:708:ILE:HG22	1:A:712:MET:CE	2.45	0.46
1:B:1165:ILE:HD12	1:B:1220:CYS:C	2.36	0.46
1:A:670:ILE:HG22	1:A:671:PHE:CD1	2.50	0.46
1:A:421:LEU:O	1:A:424:ILE:HG22	2.15	0.46
1:B:1370:SER:HA	1:B:1381:TYR:CD1	2.51	0.46
1:A:268:THR:HG23	1:A:270:GLN:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PHE:O	1:A:128:THR:HG22	2.16	0.46
1:B:1558:TYR:HB3	1:B:1562:LEU:HD22	1.98	0.46
1:B:1268:THR:HG22	1:B:1271:LYS:HB2	1.97	0.46
1:A:586:PRO:CB	1:A:641:VAL:HG21	2.45	0.46
1:B:1332:LEU:O	1:B:1547:VAL:HA	2.16	0.46
1:A:576:PHE:HE2	1:A:697:MET:HG3	1.81	0.46
1:A:491:ASN:HD21	1:A:493:MET:HB2	1.80	0.46
1:A:24:VAL:HG11	1:A:60:THR:HG21	1.98	0.46
1:B:1157:PHE:CE1	1:B:1319:VAL:CG2	2.98	0.46
1:A:15:GLN:NE2	1:A:17:SER:N	2.61	0.46
1:B:1675:GLU:O	1:B:1676:SER:O	2.34	0.46
1:A:561:ILE:HD12	1:A:571:ILE:HG12	1.98	0.45
1:B:1491:ASN:HD22	1:B:1492:PHE:N	2.13	0.45
1:A:346:TRP:CE2	1:A:559:PRO:HG2	2.52	0.45
1:B:1280:TRP:O	1:B:1284:SER:HB2	2.16	0.45
1:A:306:ASN:ND2	1:A:306:ASN:C	2.68	0.45
1:A:25:LEU:HD12	1:A:131:VAL:HG12	1.98	0.45
1:A:712:MET:O	1:A:716:ILE:HG13	2.16	0.45
1:A:267:LEU:HD11	1:A:298:LEU:HD22	1.98	0.45
1:A:231:THR:HG23	1:A:393:TRP:CE3	2.51	0.45
1:A:594:GLU:OE1	1:A:607:ILE:HG12	2.17	0.45
1:A:157:PHE:CD1	1:A:319:VAL:CG2	3.00	0.45
1:A:346:TRP:CD2	1:A:559:PRO:HG2	2.51	0.45
1:B:1244:PRO:O	1:B:1245:GLU:C	2.55	0.45
1:A:706:ASP:OD1	1:A:706:ASP:N	2.47	0.45
1:B:1274:ARG:HG2	1:B:1274:ARG:HH11	1.82	0.45
1:A:262:ASN:HD22	1:A:263:PRO:CD	2.29	0.45
1:A:335:LYS:HZ2	1:A:539:ASP:HB2	1.82	0.45
1:B:1633:ASP:N	1:B:1633:ASP:OD1	2.50	0.45
1:A:263:PRO:O	1:A:266:LEU:HB2	2.17	0.45
1:A:223:TYR:CZ	1:A:566:ARG:HD3	2.52	0.45
1:B:1053:THR:HG22	1:B:1054:PRO:HD2	1.98	0.45
1:B:1659:THR:O	1:B:1661:GLU:N	2.50	0.44
1:A:340:GLU:OE1	1:A:342:MET:HB3	2.16	0.44
1:A:553:THR:HG22	1:A:554:PHE:HD2	1.79	0.44
1:B:1491:ASN:HD21	1:B:1493:MET:HB2	1.82	0.44
1:A:231:THR:CG2	1:A:393:TRP:CE3	3.00	0.44
1:B:1566:ARG:O	1:B:1567:GLY:C	2.55	0.44
1:B:1050:ILE:HD12	1:B:1077:PHE:CD1	2.52	0.44
1:A:124:PHE:HB2	1:A:128:THR:HG23	1.99	0.44
1:A:618:LYS:HG3	1:A:621:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1612:PHE:O	1:B:1616:GLY:N	2.45	0.44
1:A:243:PHE:CD1	1:A:244:PRO:HA	2.53	0.44
1:A:378:VAL:HG23	1:A:379:LYS:N	2.32	0.44
1:A:342:MET:HG3	1:A:342:MET:O	2.17	0.44
1:A:621:TYR:CD1	1:A:621:TYR:N	2.86	0.44
1:B:1352:TYR:O	1:B:1365:PRO:HD3	2.18	0.44
1:A:56:SER:O	1:A:58:LYS:HG3	2.17	0.44
1:B:1644:ASN:HA	1:B:1696:LEU:HD11	2.00	0.44
1:A:558:TYR:N	1:A:559:PRO:CD	2.80	0.44
1:B:1617:LEU:HD21	1:B:1643:ALA:CB	2.47	0.44
1:A:274:ARG:HH11	1:A:274:ARG:HG2	1.82	0.44
1:B:1273:LYS:HB2	1:B:1273:LYS:HE3	1.90	0.44
1:A:97:VAL:CG2	1:A:98:MET:H	2.25	0.43
1:A:25:LEU:HD23	1:A:72:ASN:ND2	2.32	0.43
1:B:1123:ILE:HD11	1:B:1127:VAL:N	2.33	0.43
1:B:1035:PHE:HA	1:B:1038:MET:CE	2.47	0.43
1:B:1642:LEU:HG	1:B:1670:ILE:HD13	2.00	0.43
1:A:341:LEU:HD13	1:A:552:LEU:HB3	1.99	0.43
1:B:1619:GLU:OE2	1:B:1646:ASN:HB2	2.19	0.43
1:B:1231:THR:CG2	1:B:1393:TRP:CE3	3.01	0.43
1:A:582:ASP:OD1	1:A:672:ASP:N	2.51	0.43
1:B:1708:ILE:O	1:B:1712:MET:HG3	2.18	0.43
1:A:44:PRO:O	1:A:62:HIS:HA	2.18	0.43
1:A:114:VAL:HA	1:A:136:LEU:O	2.18	0.43
1:A:146:PHE:HA	1:A:360:GLY:O	2.19	0.43
1:A:231:THR:CG2	1:A:393:TRP:HE3	2.32	0.43
1:A:590:LEU:O	1:A:590:LEU:HD23	2.18	0.43
1:B:1060:THR:HB	1:B:1073:GLU:OE2	2.19	0.43
1:B:1259:VAL:O	1:B:1259:VAL:CG1	2.66	0.42
1:B:1161:ARG:HB2	1:B:1322:ALA:HB1	2.01	0.42
1:A:304:ILE:HB	1:A:307:ARG:HG3	2.02	0.42
1:A:557:PRO:HB2	1:A:560:LEU:HD12	2.01	0.42
1:A:192:ILE:N	1:A:192:ILE:HD12	2.35	0.42
1:B:1645:ILE:CG2	1:B:1646:ASN:N	2.74	0.42
1:B:1698:HIS:CE1	1:B:1702:LEU:HD22	2.54	0.42
1:A:43:ASP:HA	1:A:63:PHE:O	2.19	0.42
1:B:1600:ASN:O	1:B:1602:LEU:HD22	2.20	0.42
1:A:712:MET:O	1:A:715:SER:HB2	2.20	0.42
1:A:259:VAL:CG1	1:A:685:TYR:HB2	2.49	0.42
1:B:1274:ARG:HG2	1:B:1274:ARG:NH1	2.34	0.42
1:A:80:ASP:OD1	1:A:80:ASP:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1177:ASN:O	1:B:1178:SER:C	2.57	0.42
1:B:1641:VAL:CG1	1:B:1642:LEU:N	2.82	0.42
1:A:110:SER:C	1:A:112:MET:H	2.21	0.42
1:A:548:VAL:CG2	1:A:549:ASP:N	2.83	0.42
1:B:1231:THR:HG22	1:B:1232:TRP:N	2.33	0.42
1:A:42:PRO:C	1:A:44:PRO:HD3	2.40	0.42
1:A:264:LEU:CD2	1:A:405:LEU:HD23	2.50	0.42
1:A:267:LEU:HD13	1:A:469:ILE:HD11	2.00	0.42
1:B:1172:LEU:CD2	1:B:1217:ILE:HD13	2.50	0.42
1:A:50:ILE:HD12	1:A:77:PHE:CD2	2.55	0.42
1:A:371:LYS:NZ	1:A:490:HIS:NE2	2.67	0.42
1:A:193:LEU:HD11	1:A:561:ILE:CD1	2.36	0.42
1:B:1097:VAL:CG2	1:B:1098:MET:H	2.28	0.42
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.85	0.42
1:B:1181:LEU:HG	1:B:1716:ILE:HD13	2.02	0.42
1:B:1397:PHE:CE2	1:B:1417:MET:HE3	2.55	0.42
1:A:27:ALA:HA	1:A:129:GLU:O	2.19	0.42
1:B:1262:ASN:HD21	1:B:1264:LEU:CD2	2.20	0.42
1:A:472:LEU:HD12	1:A:472:LEU:HA	1.85	0.42
1:A:425:THR:HG23	1:A:428:HIS:N	2.18	0.42
1:A:326:LEU:HA	1:A:327:PRO:HD3	1.94	0.42
1:A:430:VAL:CG2	1:A:431:SER:H	2.29	0.42
1:B:1421:LEU:HA	1:B:1424:ILE:HG21	2.01	0.42
1:B:1262:ASN:HD22	1:B:1263:PRO:N	2.18	0.41
1:B:1363:MET:HE3	1:B:1492:PHE:CD2	2.55	0.41
1:A:166:ARG:NH1	1:A:184:ALA:HB3	2.35	0.41
1:B:1064:ASN:OD1	3:B:4000:MES:H31	2.20	0.41
1:B:1262:ASN:ND2	1:B:1262:ASN:C	2.74	0.41
1:B:1268:THR:HG23	1:B:1270:GLN:H	1.84	0.41
1:A:589:GLU:CD	1:A:589:GLU:H	2.19	0.41
1:B:1489:VAL:HG22	4:B:74:HOH:O	2.19	0.41
1:B:1044:PRO:O	1:B:1062:HIS:HA	2.20	0.41
1:A:26:ARG:CB	1:A:70:VAL:HA	2.50	0.41
1:A:26:ARG:HB3	1:A:70:VAL:HA	2.01	0.41
1:A:319:VAL:O	1:A:319:VAL:CG2	2.68	0.41
1:A:320:ASN:OD1	1:A:321:THR:HG23	2.21	0.41
1:B:1617:LEU:HD21	1:B:1643:ALA:HB1	2.02	0.41
1:A:192:ILE:N	1:A:192:ILE:CD1	2.83	0.41
1:A:15:GLN:HA	1:A:497:ASN:OD1	2.20	0.41
1:B:1052:THR:OG1	1:B:1085:ASN:ND2	2.54	0.41
1:B:1276:VAL:HG11	1:B:1476:SER:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:MET:CE	1:A:470:MET:HA	2.49	0.41
1:B:1086:VAL:HG23	1:B:1086:VAL:O	2.20	0.41
1:B:1339:SER:HA	1:B:1426:THR:HG21	2.02	0.41
1:B:1103:GLY:HA3	1:B:1124:PHE:HD2	1.86	0.41
1:A:266:LEU:HD12	1:A:302:THR:HG22	2.02	0.41
1:A:572:ILE:HG22	1:A:574:PHE:CE1	2.55	0.41
1:B:1279:LEU:HG	1:B:1297:MET:HE2	2.02	0.41
1:B:1709:LYS:O	1:B:1713:VAL:HG23	2.21	0.41
1:A:673:ASP:OD1	1:A:674:PRO:HD2	2.21	0.41
1:B:1480:ASN:ND2	1:B:1483:GLU:N	2.69	0.40
1:A:274:ARG:NH1	1:A:274:ARG:HG2	2.35	0.40
1:B:1563:ARG:HA	1:B:1564:PRO:HD2	1.90	0.40
1:B:1291:PHE:CE1	1:B:1470:MET:HE3	2.56	0.40
1:A:262:ASN:HD22	1:A:263:PRO:HD2	1.85	0.40
1:A:372:PHE:CE1	1:A:377:VAL:HG12	2.56	0.40
1:A:276:VAL:HG13	1:A:478:LEU:HG	2.02	0.40
1:A:702:LEU:HA	1:A:702:LEU:HD12	1.94	0.40
1:B:1061:ARG:HG2	1:B:1061:ARG:HH11	1.86	0.40
1:B:1340:GLU:HB3	1:B:1343:PHE:HD2	1.87	0.40
1:A:608:ASP:OD2	1:A:614:ARG:NH1	2.53	0.40
1:A:124:PHE:HB2	1:A:128:THR:CG2	2.52	0.40
1:B:1417:MET:HG2	1:B:1680:THR:HG21	2.04	0.40
1:B:1418:GLU:H	1:B:1418:GLU:CD	2.24	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	625/749 (83%)	565 (90%)	48 (8%)	12 (2%)	10	16
1	B	602/749 (80%)	553 (92%)	40 (7%)	9 (2%)	13	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1227/1498 (82%)	1118 (91%)	88 (7%)	21 (2%)	11 19

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	430	VAL
1	A	625	PRO
1	A	632	LYS
1	B	1178	SER
1	B	1584	SER
1	B	1660	GLU
1	B	1676	SER
1	A	15	GLN
1	A	424	ILE
1	B	1179	GLU
1	A	267	LEU
1	A	542	SER
1	B	1180	GLY
1	A	140	SER
1	A	338	VAL
1	B	1184	ALA
1	B	1645	ILE
1	A	55	ASP
1	A	586	PRO
1	B	1177	ASN
1	A	645	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	519/677 (77%)	487 (94%)	32 (6%)	23 41
1	B	511/677 (76%)	472 (92%)	39 (8%)	16 30
All	All	1030/1354 (76%)	959 (93%)	71 (7%)	19 35

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	26	ARG
1	A	101	THR
1	A	106	THR
1	A	144	LEU
1	A	161	ARG
1	A	231	THR
1	A	255	LEU
1	A	268	THR
1	A	297	MET
1	A	302	THR
1	A	306	ASN
1	A	323	GLN
1	A	421	LEU
1	A	472	LEU
1	A	478	LEU
1	A	488	LYS
1	A	489	VAL
1	A	491	ASN
1	A	494	LEU
1	A	496	LEU
1	A	555	ASN
1	A	562	LEU
1	A	565	GLN
1	A	569	ASP
1	A	582	ASP
1	A	624	LYS
1	A	636	THR
1	A	644	ASN
1	A	653	PRO
1	A	702	LEU
1	A	706	ASP
1	B	1053	THR
1	B	1059	ARG
1	B	1091	LEU
1	B	1101	THR
1	B	1128	THR
1	B	1144	LEU
1	B	1186	ASP
1	B	1227	LEU
1	B	1231	THR
1	B	1262	ASN

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Mol	Chain	Res	Type
1	B	1268	THR
1	B	1284	SER
1	B	1302	THR
1	B	1319	VAL
1	B	1323	GLN
1	B	1340	GLU
1	B	1367	LEU
1	B	1402	ASN
1	B	1425	THR
1	B	1429	ILE
1	B	1465	ILE
1	B	1478	LEU
1	B	1481	THR
1	B	1485	ARG
1	B	1491	ASN
1	B	1494	LEU
1	B	1548	VAL
1	B	1555	ASN
1	B	1562	LEU
1	B	1565	GLN
1	B	1568	VAL
1	B	1582	ASP
1	B	1586	PRO
1	B	1590	LEU
1	B	1595	LYS
1	B	1636	THR
1	B	1658	GLU
1	B	1702	LEU
1	B	1706	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	72	ASN
1	A	82	ASN
1	A	85	ASN
1	A	153	GLN
1	A	258	ASN
1	A	262	ASN
1	A	306	ASN
1	A	323	GLN

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Mol	Chain	Res	Type
1	A	461	GLN
1	A	491	ASN
1	A	565	GLN
1	A	627	ASN
1	A	644	ASN
1	A	684	GLN
1	A	687	ASN
1	A	694	HIS
1	A	704	ASN
1	B	1018	HIS
1	B	1072	ASN
1	B	1082	ASN
1	B	1085	ASN
1	B	1258	ASN
1	B	1262	ASN
1	B	1287	GLN
1	B	1309	ASN
1	B	1323	GLN
1	B	1384	ASN
1	B	1387	HIS
1	B	1480	ASN
1	B	1491	ASN
1	B	1565	GLN
1	B	1684	GLN
1	B	1687	ASN
1	B	1694	HIS
1	B	1698	HIS
1	B	1703	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	MES	A	3000	2	11,12,12	6.39	7 (63%)	14,16,16	2.94	6 (42%)
3	MES	B	4000	2	11,12,12	6.24	7 (63%)	14,16,16	2.90	6 (42%)

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
3	MES	A	3000	2	-	0/6/14/14	0/1/1/1
3	MES	B	4000	2	-	0/6/14/14	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3000	MES	C7-C8	-3.77	1.39	1.52
3	B	4000	MES	C7-C8	-3.69	1.39	1.52
3	A	3000	MES	C3-C2	-3.01	1.38	1.50
3	B	4000	MES	C3-C2	-2.95	1.38	1.50
3	B	4000	MES	C7-N4	-2.49	1.41	1.47
3	A	3000	MES	C7-N4	-2.39	1.41	1.47
3	B	4000	MES	C5-C6	-2.25	1.41	1.50
3	A	3000	MES	C5-C6	-2.21	1.41	1.50
3	B	4000	MES	O1S-S	10.58	1.78	1.45
3	A	3000	MES	O2S-S	10.76	1.78	1.45
3	B	4000	MES	O2S-S	10.94	1.79	1.45
3	A	3000	MES	O1S-S	11.17	1.80	1.45
3	B	4000	MES	O3S-S	12.48	1.78	1.46
3	A	3000	MES	O3S-S	12.90	1.79	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3000	MES	O3S-S-O2S	-3.33	103.87	111.61
3	B	4000	MES	O3S-S-O2S	-2.78	105.13	111.61
3	B	4000	MES	O3S-S-O1S	-2.72	105.27	111.61
3	A	3000	MES	O3S-S-O1S	-2.55	105.67	111.61
3	B	4000	MES	O1-C2-C3	-2.49	106.13	111.84
3	A	3000	MES	O1-C2-C3	-2.48	106.15	111.84
3	B	4000	MES	C7-C8-S	3.52	123.41	112.51
3	A	3000	MES	C7-C8-S	3.83	124.37	112.51
3	A	3000	MES	O2S-S-C8	4.58	110.82	106.91
3	B	4000	MES	O2S-S-C8	4.98	111.15	106.91
3	B	4000	MES	O1S-S-C8	7.15	113.01	106.91
3	A	3000	MES	O1S-S-C8	7.43	113.24	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4000	MES	1	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.