Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 04:39 pm BST

PDB ID	:	4RTD
Title	:	Escherichia coli alpha-2-macroglobulin activated by porcine elastase
Authors	:	Fyfe, C.D.; Grinter, R.; Roszak, A.W.; Josts, I.; Cogdell, R.J.; Walker, D.
Deposited on	:	2014-11-14
Resolution	:	3.65 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 following versions of software and data (see references (1)) were used in the production of this report:

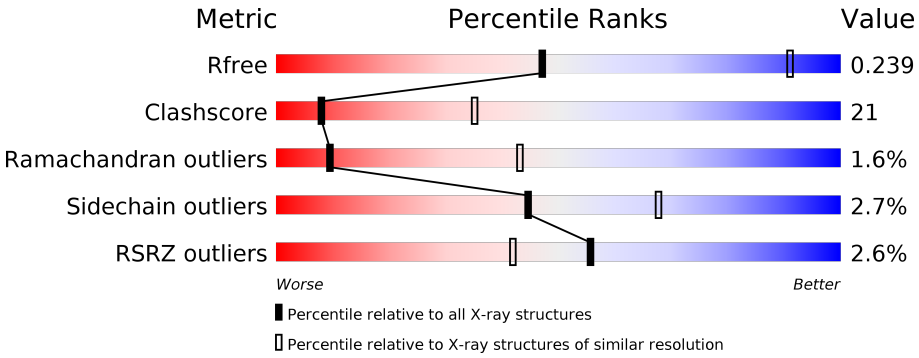
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.65 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	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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 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	1639	2% 43% 24% 32%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8699 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 Uncharacterized lipoprotein YfhM.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1122	Total	C	N	O	S	Se	0	0	0
			8699	5497	1505	1677	1	19			

There are 11 discrepancies between the modelled and reference sequences:

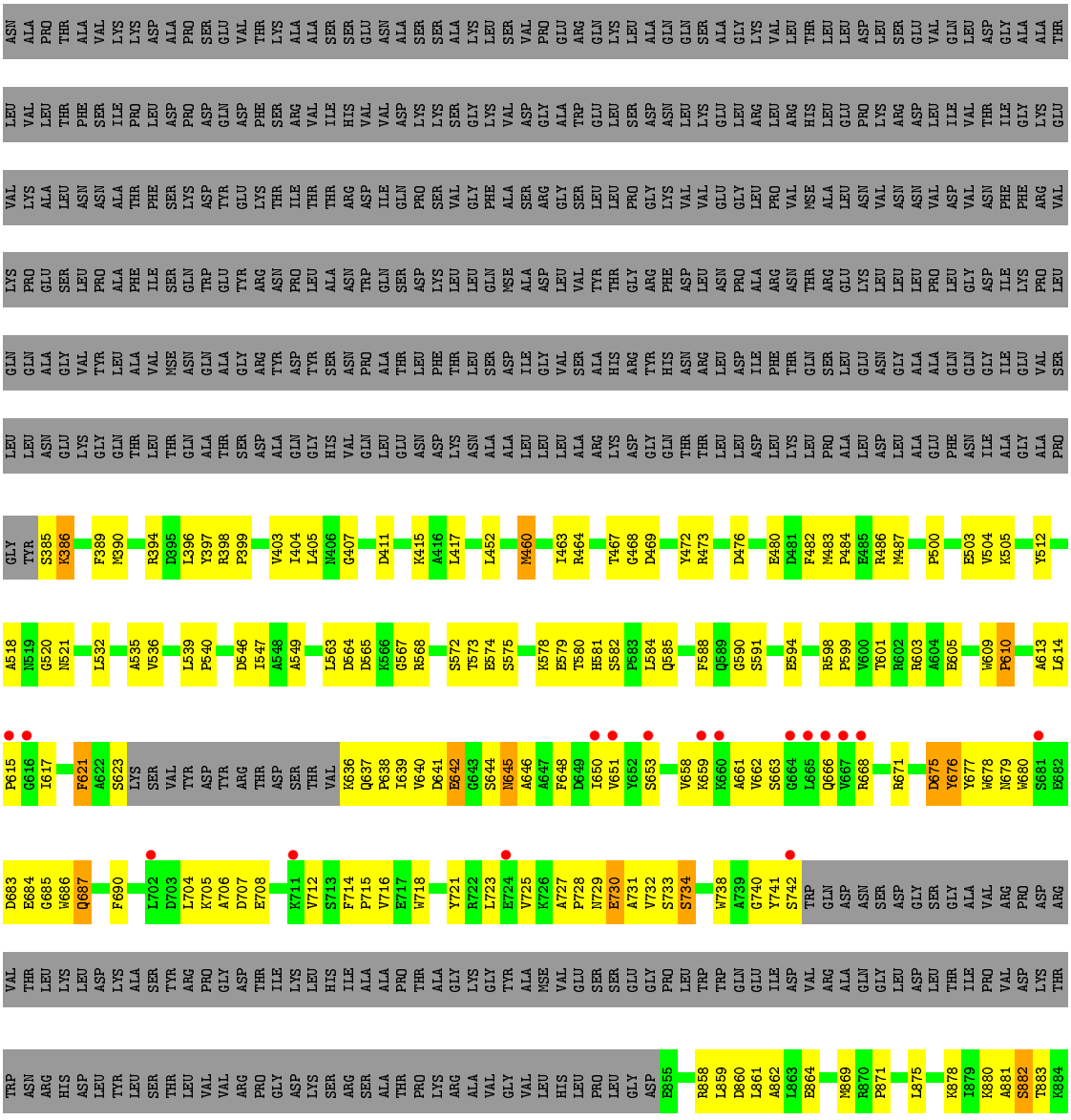
Chain	Residue	Modelled	Actual	Comment	Reference
A	219	PRO	SER	ENGINEERED MUTATION	UNP P76578
A	606	ARG	GLN	ENGINEERED MUTATION	UNP P76578
A	1587	ASN	SER	ENGINEERED MUTATION	UNP P76578
A	1654	LEU	-	EXPRESSION TAG	UNP P76578
A	1655	GLU	-	EXPRESSION TAG	UNP P76578
A	1656	HIS	-	EXPRESSION TAG	UNP P76578
A	1657	HIS	-	EXPRESSION TAG	UNP P76578
A	1658	HIS	-	EXPRESSION TAG	UNP P76578
A	1659	HIS	-	EXPRESSION TAG	UNP P76578
A	1660	HIS	-	EXPRESSION TAG	UNP P76578
A	1661	HIS	-	EXPRESSION TAG	UNP P76578

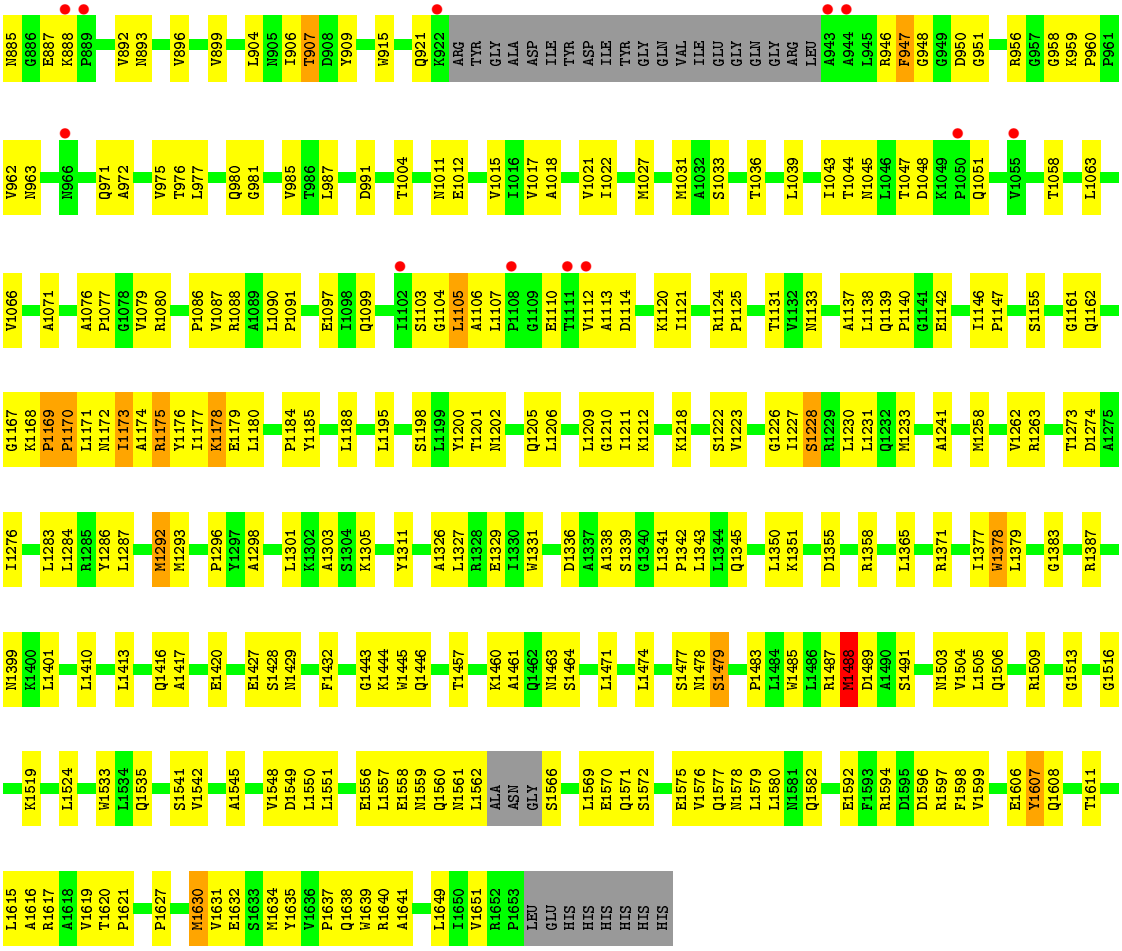
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Uncharacterized lipoprotein YfhM

Chain A:




N885 G886 E887 K888 P889 V892 N893 V896 V899 L904 N905 I906 T907 D908 Y909 W915 Q921 K922 ARG TYR GLY ALA ASP ILE TYR ASP ILE TYR GLY GLN VAL ILE GLU GLY GLN GLY ARG LEU A943 A944 L945 R946 F947 G948 G949 D950 G951 R956 G957 G958 K959 P960 P961
V962 N963 N966 Q971 A972 V975 T976 L977 Q980 G981 V985 T986 L987 D991 T1004 N1011 E1012 V1015 I1016 V1017 A1018 V1021 I1022 M1027 M1031 A1032 S1033 T1036 L1039 I1043 T1044 N1045 L1046 T1047 D1048 K1049 P1050 Q1051 Y1055 T1058 L1063
V1066 A1071 A1076 P1077 G1078 V1079 R1080 P1086 V1087 R1088 A1089 L1090 P1091 E1097 I1098 Q1099 I1102 S1103 G1104 L1105 A1106 L1107 P1108 G1109 E1110 T1111 V1112 A1113 D1114 K1120 I1121 R1124 P1125 T1131 V1132 N1133 A1137 L1138 Q1139 P1140 G1141 E1142 I1146 P1147 S1155 G1161 Q1162
G1167 K1168 P1169 P1170 L1171 N1172 I1173 A1174 R1175 Y1176 I1177 K1178 E1179 L1180 P1184 Y1185 L1188 L1195 S1198 L1199 Y1200 T1201 N1202 Q1205 L1206 L1209 G1210 I1211 K1212 K1218 S1222 V1223 G1226 I1227 S1228 R1229 L1230 L1231 Q1232 M1233 A1241 M1258 V1262 R1263 T1273 D1274 A1275
I1276 L1283 L1284 R1285 Y1286 L1287 M1292 M1293 P1296 Y1297 A1298 L1301 K1302 A1303 S1304 K1305 Y1311 A1326 L1327 R1328 E1329 T1330 W1331 D1336 A1337 A1338 S1339 G1340 L1341 P1342 L1343 L1344 Q1345 L1350 K1351 D1355 R1358 L1365 R1371 I1377 W1378 L1379 G1383 R1387
N1399 K1400 L1401 L1410 L1413 Q1416 A1417 E1420 E1427 S1428 N1429 F1432 G1443 K1444 W1445 Q1446 T1457 K1460 A1461 Q1462 N1463 S1464 L1471 L1474 S1477 N1478 S1479 P1483 L1484 W1485 L1486 R1487 N1488 D1489 A1490 S1491 N1503 V1504 L1505 Q1506 R1509 G1513 G1516
K1519 L1524 W1533 L1534 Q1535 S1541 V1542 A1545 V1548 D1549 L1550 L1551 E1556 L1557 E1558 N1559 Q1560 N1561 L1562 ALA ASN GLY S1566 L1569 E1570 Q1571 S1572 E1575 V1576 Q1577 N1578 L1579 L1580 N1581 Q1582 E1592 F1593 R1594 D1595 D1596 R1597 F1598 V1599 E1606 Y1607 Q1608 T1611
L1615 A1616 R1617 A1618 V1619 T1620 P1621 P1627 M1630 V1631 E1632 S1633 M1634 Y1635 V1636 P1637 Q1638 W1639 R1640 A1641 L1649 I1650 V1651 R1652 P1653 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	176.06Å 176.06Å 161.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.87 – 3.65 46.87 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.87-3.65) 100.0 (46.87-3.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 3.66Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.177 , 0.238 0.183 , 0.239	Depositor DCC
R_{free} test set	1033 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	126.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 113.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8699	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/8863	0.75	3/12024 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	460	MSE	CG-SE-CE	7.75	115.94	98.90
1	A	1105	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	1488	MSE	CA-CB-CG	-5.20	104.46	113.30

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	8699	0	8589	370	0
All	All	8699	0	8589	370	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 21.

All (370) 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:639:ILE:HG21	1:A:738:TRP:O	1.73	0.89
1:A:396:LEU:HD22	1:A:906:ILE:HD11	1.56	0.87
1:A:1045:ASN:OD1	1:A:1047:THR:HG22	1.77	0.84
1:A:1504:VAL:HG21	1:A:1639:TRP:CD1	2.15	0.81
1:A:1106:ALA:HA	1:A:1113:ALA:HA	1.62	0.81
1:A:1578:ASN:HB2	1:A:1579:LEU:HD12	1.64	0.79
1:A:1417:ALA:HA	1:A:1420:GLU:HG3	1.65	0.78
1:A:661:ALA:HB1	1:A:704:LEU:O	1.83	0.78
1:A:1033:SER:HB2	1:A:1091:PRO:HA	1.65	0.78
1:A:1273:THR:O	1:A:1276:ILE:HG22	1.83	0.78
1:A:411:ASP:HB3	1:A:417:LEU:HD11	1.66	0.78
1:A:1488:MSE:HG3	1:A:1489:ASP:N	2.00	0.77
1:A:1509:ARG:NH1	1:A:1549:ASP:OD1	2.19	0.75
1:A:1170:PRO:HG2	1:A:1410:LEU:HD21	1.69	0.75
1:A:658:VAL:HG22	1:A:659:LYS:HG2	1.68	0.75
1:A:1562:LEU:HB2	1:A:1566:SER:OG	1.86	0.74
1:A:946:ARG:NH2	1:A:1545:ALA:O	2.21	0.74
1:A:893:ASN:OD1	1:A:976:THR:HG22	1.86	0.73
1:A:396:LEU:HD22	1:A:906:ILE:CD1	2.18	0.73
1:A:1383:GLY:HA2	1:A:1387:ARG:HD3	1.70	0.73
1:A:1460:LYS:HG3	1:A:1461:ALA:H	1.55	0.72
1:A:864:GLU:HB2	1:A:878:LYS:HB2	1.72	0.72
1:A:882:SER:O	1:A:883:THR:HG22	1.89	0.71
1:A:906:ILE:HD12	1:A:907:THR:N	2.06	0.71
1:A:1021:VAL:HG12	1:A:1045:ASN:HA	1.74	0.70
1:A:500:PRO:HD3	1:A:609:TRP:O	1.92	0.70
1:A:683:ASP:HB3	1:A:685:GLY:O	1.93	0.69
1:A:397:TYR:CE2	1:A:403:VAL:HA	2.28	0.69
1:A:487:MSE:HE2	1:A:512:TYR:CZ	2.29	0.68
1:A:565:ASP:HB3	1:A:568:ARG:O	1.93	0.68
1:A:1173:ILE:HB	1:A:1176:TYR:CD1	2.30	0.67
1:A:875:LEU:HD11	1:A:1015:VAL:HG11	1.76	0.67
1:A:859:LEU:HD13	1:A:888:LYS:HE2	1.77	0.66
1:A:1107:LEU:HD12	1:A:1110:GLU:HB2	1.76	0.66
1:A:1168:LYS:HB2	1:A:1443:GLY:HA2	1.77	0.66
1:A:1175:ARG:NH1	1:A:1210:GLY:O	2.28	0.66
1:A:480:GLU:OE2	1:A:1561:ASN:ND2	2.27	0.66
1:A:661:ALA:HB2	1:A:705:LYS:C	2.17	0.65
1:A:621:PHE:CD2	1:A:638:PRO:HB2	2.32	0.65
1:A:1178:LYS:HB3	1:A:1179:GLU:HA	1.79	0.64
1:A:1011:ASN:OD1	1:A:1012:GLU:N	2.30	0.64
1:A:1582:GLN:OE1	1:A:1611:THR:OG1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:ASN:HB2	1:A:1637:PRO:HG3	1.78	0.64
1:A:1162:GLN:OE1	1:A:1162:GLN:N	2.32	0.63
1:A:1378:TRP:HA	1:A:1378:TRP:CE3	2.34	0.63
1:A:536:VAL:HG11	1:A:539:LEU:HD12	1.80	0.63
1:A:1378:TRP:HA	1:A:1378:TRP:HE3	1.64	0.63
1:A:1569:LEU:HD23	1:A:1570:GLU:N	2.14	0.62
1:A:741:TYR:HD1	1:A:742:SER:HB2	1.63	0.62
1:A:883:THR:HG21	1:A:887:GLU:C	2.19	0.62
1:A:661:ALA:HB2	1:A:706:ALA:N	2.14	0.62
1:A:1558:GLU:CD	1:A:1569:LEU:HD13	2.20	0.62
1:A:1556:GLU:OE2	1:A:1619:VAL:HG21	2.00	0.62
1:A:958:GLY:O	1:A:1597:ARG:NH1	2.31	0.62
1:A:1124:ARG:HG3	1:A:1125:PRO:O	1.99	0.62
1:A:679:ASN:HB3	1:A:687:GLN:HA	1.80	0.62
1:A:1509:ARG:NH2	1:A:1627:PRO:O	2.32	0.62
1:A:1170:PRO:HG2	1:A:1410:LEU:CD2	2.30	0.61
1:A:639:ILE:HG22	1:A:640:VAL:O	2.00	0.61
1:A:678:TRP:HE3	1:A:687:GLN:HB2	1.65	0.61
1:A:869:MSE:SE	1:A:875:LEU:HD12	2.50	0.60
1:A:1200:TYR:OH	1:A:1263:ARG:HD3	2.01	0.60
1:A:1133:ASN:HB2	1:A:1637:PRO:CG	2.30	0.60
1:A:1178:LYS:CD	1:A:1180:LEU:HB2	2.32	0.60
1:A:1178:LYS:HG3	1:A:1211:ILE:HD12	1.84	0.60
1:A:1478:ASN:OD1	1:A:1479:SER:N	2.35	0.60
1:A:1571:GLN:OE1	1:A:1571:GLN:HA	2.02	0.60
1:A:396:LEU:CD2	1:A:906:ILE:HD11	2.28	0.60
1:A:1535:GLN:OE1	1:A:1535:GLN:HA	2.00	0.60
1:A:615:PRO:HG3	1:A:727:ALA:HB2	1.83	0.60
1:A:639:ILE:HG22	1:A:640:VAL:N	2.16	0.60
1:A:1168:LYS:HB3	1:A:1169:PRO:HD3	1.82	0.59
1:A:1104:GLY:O	1:A:1105:LEU:HG	2.02	0.59
1:A:1445:TRP:NE1	1:A:1460:LYS:O	2.30	0.59
1:A:1558:GLU:OE2	1:A:1617:ARG:NE	2.30	0.59
1:A:1177:ILE:O	1:A:1178:LYS:CB	2.50	0.59
1:A:486:ARG:NH2	1:A:594:GLU:OE1	2.36	0.59
1:A:892:VAL:HG11	1:A:977:LEU:HD12	1.83	0.58
1:A:1619:VAL:HG23	1:A:1620:THR:N	2.18	0.58
1:A:1410:LEU:HD23	1:A:1410:LEU:C	2.23	0.58
1:A:1570:GLU:HG2	1:A:1571:GLN:N	2.19	0.58
1:A:1167:GLY:C	1:A:1485:TRP:HZ3	2.07	0.58
1:A:1031:MSE:HE1	1:A:1063:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1632:GLU:HG2	1:A:1640:ARG:HB3	1.85	0.57
1:A:639:ILE:HG12	1:A:738:TRP:O	2.03	0.57
1:A:871:PRO:HD3	1:A:1018:ALA:O	2.03	0.57
1:A:1487:ARG:NH2	1:A:1635:TYR:O	2.33	0.57
1:A:483:MSE:HE2	1:A:963:ASN:HD21	1.70	0.57
1:A:1167:GLY:HA3	1:A:1445:TRP:HB3	1.85	0.57
1:A:638:PRO:O	1:A:639:ILE:HG13	2.04	0.57
1:A:1578:ASN:HB2	1:A:1579:LEU:CD1	2.35	0.56
1:A:1039:LEU:HD13	1:A:1087:VAL:HG21	1.86	0.56
1:A:398:ARG:O	1:A:399:PRO:C	2.44	0.56
1:A:1569:LEU:HD23	1:A:1569:LEU:C	2.26	0.56
1:A:532:LEU:HD12	1:A:585:GLN:HB3	1.87	0.56
1:A:718:TRP:CG	1:A:718:TRP:O	2.59	0.56
1:A:640:VAL:HG11	1:A:716:VAL:CG2	2.35	0.55
1:A:1131:THR:HG23	1:A:1491:SER:OG	2.06	0.55
1:A:1562:LEU:HB2	1:A:1566:SER:CB	2.36	0.55
1:A:1577:GLN:O	1:A:1578:ASN:C	2.45	0.55
1:A:1076:ALA:HB3	1:A:1079:VAL:HG21	1.89	0.55
1:A:1503:ASN:ND2	1:A:1638:GLN:O	2.39	0.55
1:A:460:MSE:CE	1:A:476:ASP:HB3	2.37	0.55
1:A:645:ASN:OD1	1:A:645:ASN:N	2.39	0.55
1:A:1146:ILE:HG13	1:A:1147:PRO:HD2	1.88	0.55
1:A:1177:ILE:O	1:A:1178:LYS:HB2	2.06	0.55
1:A:1506:GLN:HA	1:A:1641:ALA:CB	2.37	0.55
1:A:684:GLU:N	1:A:685:GLY:O	2.39	0.55
1:A:1076:ALA:HB1	1:A:1077:PRO:HD2	1.90	0.54
1:A:658:VAL:CG2	1:A:659:LYS:HG2	2.36	0.54
1:A:1195:LEU:HD22	1:A:1223:VAL:HA	1.88	0.54
1:A:394:ARG:HA	1:A:909:TYR:CE2	2.42	0.54
1:A:1171:LEU:HG	1:A:1173:ILE:HG23	1.89	0.54
1:A:1615:LEU:HD12	1:A:1616:ALA:N	2.22	0.54
1:A:859:LEU:HD13	1:A:888:LYS:CE	2.36	0.54
1:A:858:ARG:HB3	1:A:915:TRP:CD1	2.43	0.54
1:A:959:LYS:HD2	1:A:960:PRO:HD2	1.89	0.54
1:A:1619:VAL:HG23	1:A:1620:THR:H	1.72	0.54
1:A:1139:GLN:HG2	1:A:1140:PRO:HD2	1.90	0.53
1:A:590:GLY:O	1:A:601:THR:HG23	2.09	0.53
1:A:1036:THR:HG22	1:A:1088:ARG:HA	1.90	0.53
1:A:705:LYS:O	1:A:708:GLU:HB3	2.08	0.53
1:A:729:ASN:O	1:A:730:GLU:HB2	2.09	0.53
1:A:1172:ASN:O	1:A:1174:ALA:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1575:GLU:OE1	1:A:1576:VAL:HG13	2.08	0.53
1:A:1177:ILE:O	1:A:1178:LYS:CG	2.56	0.53
1:A:718:TRP:CD1	1:A:718:TRP:O	2.61	0.53
1:A:1350:LEU:O	1:A:1351:LYS:C	2.45	0.53
1:A:581:HIS:HB3	1:A:730:GLU:O	2.08	0.53
1:A:1205:GLN:O	1:A:1209:LEU:HB2	2.09	0.53
1:A:1524:LEU:HD12	1:A:1649:LEU:HD11	1.91	0.53
1:A:505:LYS:HB3	1:A:572:SER:CB	2.39	0.53
1:A:645:ASN:HA	1:A:715:PRO:HA	1.91	0.52
1:A:1562:LEU:CB	1:A:1566:SER:OG	2.56	0.52
1:A:464:ARG:HD2	1:A:472:TYR:HD2	1.73	0.52
1:A:1542:VAL:HG22	1:A:1639:TRP:CZ3	2.45	0.52
1:A:639:ILE:CG2	1:A:640:VAL:N	2.73	0.52
1:A:650:ILE:CD1	1:A:712:VAL:HG22	2.40	0.52
1:A:1607:TYR:CE1	1:A:1608:GLN:HG3	2.45	0.52
1:A:1090:LEU:HB3	1:A:1091:PRO:HD2	1.90	0.52
1:A:1339:SER:HB2	1:A:1371:ARG:HE	1.74	0.52
1:A:1569:LEU:HD21	1:A:1615:LEU:HD23	1.89	0.52
1:A:651:VAL:CG1	1:A:659:LYS:HE3	2.39	0.52
1:A:1413:LEU:HA	1:A:1416:GLN:HG2	1.92	0.51
1:A:1551:LEU:HD11	1:A:1557:LEU:HD13	1.92	0.51
1:A:1176:TYR:C	1:A:1177:ILE:HD12	2.30	0.51
1:A:1417:ALA:HA	1:A:1420:GLU:CG	2.39	0.51
1:A:1463:ASN:OD1	1:A:1464:SER:N	2.44	0.51
1:A:662:VAL:HG12	1:A:663:SER:O	2.10	0.51
1:A:883:THR:HG23	1:A:885:ASN:HB2	1.92	0.51
1:A:1103:SER:HA	1:A:1114:ASP:OD1	2.11	0.51
1:A:662:VAL:HG11	1:A:728:PRO:HG2	1.93	0.51
1:A:1446:GLN:HG2	1:A:1457:THR:HG23	1.91	0.51
1:A:1058:THR:HB	1:A:1099:GLN:HB2	1.93	0.51
1:A:1178:LYS:CD	1:A:1211:ILE:HD12	2.40	0.51
1:A:888:LYS:NZ	1:A:892:VAL:HG13	2.25	0.51
1:A:1228:SER:HA	1:A:1231:LEU:HD12	1.93	0.51
1:A:1341:LEU:O	1:A:1345:GLN:HG3	2.12	0.51
1:A:1188:LEU:HD13	1:A:1233:MSE:SE	2.61	0.50
1:A:1341:LEU:HB3	1:A:1342:PRO:HD3	1.92	0.50
1:A:893:ASN:HA	1:A:975:VAL:O	2.10	0.50
1:A:676:TYR:O	1:A:690:PHE:HA	2.11	0.50
1:A:678:TRP:CE3	1:A:687:GLN:HB2	2.44	0.50
1:A:671:ARG:NH1	1:A:721:TYR:OH	2.44	0.50
1:A:675:ASP:HA	1:A:690:PHE:HE1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:THR:HG21	1:A:584:LEU:HD21	1.94	0.50
1:A:972:ALA:HB2	1:A:987:LEU:HD21	1.94	0.50
1:A:1139:GLN:N	1:A:1142:GLU:OE2	2.45	0.50
1:A:1177:ILE:O	1:A:1178:LYS:HG2	2.12	0.50
1:A:639:ILE:HG12	1:A:738:TRP:N	2.27	0.50
1:A:678:TRP:HZ3	1:A:687:GLN:HG3	1.77	0.50
1:A:500:PRO:O	1:A:575:SER:OG	2.15	0.50
1:A:661:ALA:HB1	1:A:705:LYS:HA	1.93	0.49
1:A:1579:LEU:HD12	1:A:1579:LEU:N	2.27	0.49
1:A:675:ASP:OD1	1:A:675:ASP:N	2.45	0.49
1:A:1331:TRP:CD1	1:A:1358:ARG:HD2	2.48	0.49
1:A:503:GLU:HG2	1:A:574:GLU:HA	1.94	0.49
1:A:1161:GLY:C	1:A:1162:GLN:OE1	2.51	0.49
1:A:588:PHE:O	1:A:603:ARG:HA	2.13	0.49
1:A:1188:LEU:HD22	1:A:1241:ALA:O	2.13	0.49
1:A:386:LYS:O	1:A:473:ARG:NH2	2.46	0.49
1:A:1178:LYS:HD3	1:A:1180:LEU:HB2	1.95	0.49
1:A:1576:VAL:O	1:A:1576:VAL:HG23	2.13	0.49
1:A:396:LEU:HD21	1:A:482:PHE:CG	2.47	0.49
1:A:980:GLN:N	1:A:980:GLN:OE1	2.46	0.49
1:A:1031:MSE:HE2	1:A:1121:ILE:HD13	1.93	0.48
1:A:1533:TRP:CD1	1:A:1579:LEU:HD23	2.47	0.48
1:A:411:ASP:OD1	1:A:415:LYS:N	2.45	0.48
1:A:651:VAL:HG11	1:A:659:LYS:HE3	1.94	0.48
1:A:472:TYR:N	1:A:472:TYR:CD1	2.81	0.48
1:A:1137:ALA:O	1:A:1138:LEU:HD23	2.12	0.48
1:A:1178:LYS:CG	1:A:1211:ILE:HD12	2.42	0.48
1:A:1137:ALA:HB2	1:A:1485:TRP:CD1	2.48	0.48
1:A:467:THR:C	1:A:469:ASP:H	2.17	0.48
1:A:639:ILE:HG12	1:A:738:TRP:H	1.79	0.48
1:A:1201:THR:HG21	1:A:1432:PHE:HZ	1.78	0.47
1:A:1569:LEU:HD21	1:A:1615:LEU:CD2	2.43	0.47
1:A:906:ILE:HD12	1:A:906:ILE:C	2.35	0.47
1:A:1106:ALA:CA	1:A:1113:ALA:HA	2.40	0.47
1:A:1471:LEU:HA	1:A:1474:LEU:HB2	1.96	0.47
1:A:1559:ASN:OD1	1:A:1561:ASN:N	2.46	0.47
1:A:487:MSE:HE2	1:A:512:TYR:CE1	2.49	0.47
1:A:741:TYR:HD1	1:A:742:SER:CB	2.25	0.47
1:A:472:TYR:HD1	1:A:472:TYR:N	2.13	0.47
1:A:532:LEU:HD21	1:A:535:ALA:HA	1.95	0.47
1:A:590:GLY:O	1:A:601:THR:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:THR:HG21	1:A:1051:GLN:HE21	1.78	0.47
1:A:1292:MSE:CG	1:A:1293:MSE:N	2.77	0.47
1:A:1371:ARG:HH12	1:A:1383:GLY:HA3	1.80	0.47
1:A:1387:ARG:HB3	1:A:1427:GLU:HG2	1.97	0.47
1:A:1558:GLU:HB3	1:A:1569:LEU:HD22	1.97	0.47
1:A:1562:LEU:O	1:A:1566:SER:HA	2.15	0.47
1:A:460:MSE:HE2	1:A:476:ASP:HB3	1.95	0.47
1:A:1303:ALA:HB1	1:A:1338:ALA:HB2	1.96	0.47
1:A:599:PRO:HG2	1:A:1617:ARG:HD2	1.97	0.47
1:A:1596:ASP:C	1:A:1597:ARG:HG2	2.34	0.47
1:A:1173:ILE:HD11	1:A:1420:GLU:OE2	2.15	0.47
1:A:1326:ALA:O	1:A:1329:GLU:HG2	2.14	0.47
1:A:599:PRO:HG2	1:A:1617:ARG:CD	2.45	0.47
1:A:598:ARG:NH2	1:A:1027:MSE:O	2.45	0.46
1:A:1139:GLN:HA	1:A:1483:PRO:HB3	1.97	0.46
1:A:1039:LEU:HD13	1:A:1087:VAL:CG2	2.45	0.46
1:A:578:LYS:HG3	1:A:579:GLU:N	2.30	0.46
1:A:880:LYS:HA	1:A:981:GLY:O	2.14	0.46
1:A:1505:LEU:O	1:A:1641:ALA:HB2	2.16	0.46
1:A:1630:MSE:HG3	1:A:1640:ARG:HH21	1.81	0.46
1:A:535:ALA:HB1	1:A:609:TRP:CZ2	2.50	0.46
1:A:723:LEU:O	1:A:734:SER:HA	2.16	0.46
1:A:1168:LYS:CB	1:A:1169:PRO:HD3	2.46	0.46
1:A:861:LEU:HD23	1:A:862:ALA:N	2.31	0.46
1:A:1106:ALA:HA	1:A:1112:VAL:O	2.15	0.46
1:A:1047:THR:HG21	1:A:1051:GLN:HG3	1.98	0.46
1:A:1283:LEU:O	1:A:1286:TYR:HB2	2.16	0.46
1:A:1570:GLU:HG2	1:A:1571:GLN:H	1.81	0.46
1:A:896:VAL:HG11	1:A:985:VAL:HG21	1.98	0.46
1:A:1105:LEU:HD12	1:A:1105:LEU:O	2.16	0.46
1:A:1577:GLN:HA	1:A:1580:LEU:HD12	1.98	0.45
1:A:888:LYS:CE	1:A:892:VAL:HG13	2.46	0.45
1:A:1548:VAL:HG22	1:A:1599:VAL:HG22	1.98	0.45
1:A:1226:GLY:O	1:A:1230:LEU:HG	2.16	0.45
1:A:637:GLN:O	1:A:639:ILE:HD12	2.16	0.45
1:A:892:VAL:HB	1:A:977:LEU:HB2	1.97	0.45
1:A:1503:ASN:OD1	1:A:1504:VAL:HG23	2.16	0.45
1:A:390:MSE:HE1	1:A:473:ARG:O	2.17	0.45
1:A:617:ILE:HD11	1:A:725:VAL:HG23	1.99	0.45
1:A:1202:ASN:OD1	1:A:1202:ASN:N	2.49	0.45
1:A:1410:LEU:HD23	1:A:1410:LEU:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:LYS:CB	1:A:707:ASP:HA	2.46	0.45
1:A:1558:GLU:O	1:A:1560:GLN:NE2	2.50	0.45
1:A:521:ASN:OD1	1:A:1080:ARG:NH2	2.50	0.44
1:A:1169:PRO:HA	1:A:1170:PRO:HD3	1.82	0.44
1:A:1227:ILE:HG22	1:A:1228:SER:N	2.32	0.44
1:A:1578:ASN:CB	1:A:1579:LEU:HD12	2.41	0.44
1:A:1218:LYS:O	1:A:1222:SER:HB2	2.17	0.44
1:A:621:PHE:HD2	1:A:638:PRO:HB2	1.79	0.44
1:A:1097:GLU:HB3	1:A:1120:LYS:HG2	2.00	0.44
1:A:661:ALA:CB	1:A:706:ALA:N	2.80	0.44
1:A:860:ASP:O	1:A:881:ALA:HA	2.17	0.44
1:A:1031:MSE:HE1	1:A:1063:LEU:CD1	2.46	0.44
1:A:1444:LYS:HD3	1:A:1444:LYS:N	2.33	0.44
1:A:1169:PRO:HB2	1:A:1172:ASN:HB3	1.99	0.44
1:A:613:ALA:HB1	1:A:653:SER:O	2.17	0.44
1:A:956:ARG:NH2	1:A:1634:MSE:O	2.51	0.44
1:A:882:SER:O	1:A:883:THR:CG2	2.62	0.44
1:A:1327:LEU:HB3	1:A:1350:LEU:CD2	2.47	0.44
1:A:1178:LYS:HG3	1:A:1211:ILE:CD1	2.46	0.44
1:A:546:ASP:HB3	1:A:549:ALA:HB2	1.99	0.44
1:A:385:SER:O	1:A:386:LYS:HB2	2.18	0.43
1:A:505:LYS:HB3	1:A:572:SER:HB2	2.00	0.43
1:A:1377:ILE:N	1:A:1377:ILE:HD13	2.32	0.43
1:A:1607:TYR:CD1	1:A:1608:GLN:HG3	2.53	0.43
1:A:460:MSE:HE2	1:A:476:ASP:CB	2.49	0.43
1:A:661:ALA:CB	1:A:705:LYS:C	2.86	0.43
1:A:1179:GLU:OE1	1:A:1212:LYS:N	2.52	0.43
1:A:397:TYR:CD2	1:A:403:VAL:HG22	2.53	0.43
1:A:464:ARG:CD	1:A:472:TYR:HD2	2.32	0.43
1:A:504:VAL:O	1:A:572:SER:HA	2.18	0.43
1:A:639:ILE:CG2	1:A:738:TRP:O	2.56	0.43
1:A:888:LYS:HZ3	1:A:1004:THR:CG2	2.31	0.43
1:A:1201:THR:HG22	1:A:1205:GLN:OE1	2.19	0.43
1:A:1177:ILE:C	1:A:1178:LYS:HG2	2.39	0.43
1:A:1178:LYS:HE2	1:A:1211:ILE:HD12	2.01	0.43
1:A:1592:GLU:OE1	1:A:1594:ARG:NH1	2.45	0.43
1:A:614:LEU:HD22	1:A:731:ALA:HB1	2.01	0.43
1:A:623:SER:HA	1:A:636:LYS:HE2	2.01	0.43
1:A:641:ASP:O	1:A:642:GLU:HB2	2.19	0.43
1:A:1428:SER:O	1:A:1429:ASN:C	2.57	0.43
1:A:460:MSE:CE	1:A:476:ASP:CB	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ALA:CB	1:A:705:LYS:HA	2.48	0.43
1:A:729:ASN:O	1:A:730:GLU:CB	2.67	0.43
1:A:1550:LEU:CD2	1:A:1597:ARG:HD2	2.49	0.43
1:A:1571:GLN:OE1	1:A:1571:GLN:CA	2.67	0.42
1:A:1549:ASP:HB3	1:A:1598:PHE:HB3	2.00	0.42
1:A:613:ALA:HB1	1:A:653:SER:C	2.40	0.42
1:A:732:VAL:HG12	1:A:733:SER:N	2.33	0.42
1:A:899:VAL:HG11	1:A:904:LEU:HD21	2.01	0.42
1:A:1184:PRO:HG2	1:A:1185:TYR:CE2	2.54	0.42
1:A:859:LEU:HD22	1:A:888:LYS:HE2	2.01	0.42
1:A:950:ASP:HA	1:A:951:GLY:HA2	1.78	0.42
1:A:405:LEU:HD22	1:A:463:ILE:HG21	2.01	0.42
1:A:520:GLY:HA2	1:A:564:ASP:HA	2.01	0.42
1:A:640:VAL:HG21	1:A:644:SER:C	2.39	0.42
1:A:487:MSE:CE	1:A:512:TYR:CZ	3.02	0.42
1:A:504:VAL:HB	1:A:573:THR:HG22	2.00	0.42
1:A:487:MSE:HE1	1:A:594:GLU:HA	2.01	0.42
1:A:718:TRP:CD1	1:A:740:GLY:HA3	2.54	0.42
1:A:1175:ARG:HG3	1:A:1176:TYR:H	1.84	0.42
1:A:399:PRO:HA	1:A:452:LEU:CD2	2.49	0.42
1:A:680:TRP:NE1	1:A:683:ASP:HA	2.34	0.42
1:A:875:LEU:CD1	1:A:1015:VAL:HG11	2.47	0.42
1:A:1066:VAL:CG1	1:A:1086:PRO:HB2	2.50	0.42
1:A:389:PHE:O	1:A:407:GLY:HA2	2.20	0.42
1:A:483:MSE:HA	1:A:484:PRO:HD2	1.93	0.42
1:A:1063:LEU:HA	1:A:1063:LEU:HD12	1.83	0.42
1:A:1171:LEU:CD2	1:A:1417:ALA:CB	2.98	0.42
1:A:518:ALA:HB1	1:A:521:ASN:HB2	2.02	0.42
1:A:1138:LEU:HB3	1:A:1142:GLU:HB2	2.00	0.42
1:A:1378:TRP:CA	1:A:1378:TRP:CE3	3.03	0.42
1:A:1621:PRO:HA	1:A:1651:VAL:HB	2.01	0.42
1:A:646:ALA:N	1:A:714:PHE:O	2.40	0.42
1:A:1124:ARG:NH1	1:A:1125:PRO:O	2.46	0.42
1:A:1170:PRO:O	1:A:1172:ASN:ND2	2.48	0.42
1:A:677:TYR:CD1	1:A:690:PHE:CZ	3.08	0.42
1:A:1258:MSE:HE2	1:A:1258:MSE:HB2	1.91	0.41
1:A:532:LEU:C	1:A:532:LEU:HD23	2.40	0.41
1:A:591:SER:HB3	1:A:599:PRO:HB3	2.01	0.41
1:A:684:GLU:HA	1:A:684:GLU:OE1	2.20	0.41
1:A:869:MSE:HG3	1:A:1017:VAL:HG22	2.02	0.41
1:A:1137:ALA:HB2	1:A:1485:TRP:HD1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1505:LEU:CD1	1:A:1631:VAL:HG13	2.50	0.41
1:A:1516:GLY:HA3	1:A:1576:VAL:HG11	2.02	0.41
1:A:582:SER:O	1:A:584:LEU:HD13	2.20	0.41
1:A:1206:LEU:HB3	1:A:1211:ILE:O	2.21	0.41
1:A:1298:ALA:HB1	1:A:1379:LEU:HA	2.02	0.41
1:A:1301:LEU:O	1:A:1305:LYS:HG2	2.21	0.41
1:A:1399:ASN:HB3	1:A:1401:LEU:HG	2.02	0.41
1:A:396:LEU:HD21	1:A:482:PHE:CD2	2.55	0.41
1:A:539:LEU:N	1:A:540:PRO:HD3	2.36	0.41
1:A:1044:THR:HA	1:A:1080:ARG:HB3	2.03	0.41
1:A:883:THR:HG21	1:A:887:GLU:O	2.21	0.41
1:A:1262:VAL:HG22	1:A:1276:ILE:HD11	2.03	0.41
1:A:1311:TYR:HA	1:A:1345:GLN:OE1	2.20	0.41
1:A:1606:GLU:O	1:A:1607:TYR:CG	2.73	0.41
1:A:623:SER:H	1:A:636:LYS:HD3	1.84	0.41
1:A:680:TRP:HE1	1:A:683:ASP:HA	1.85	0.41
1:A:991:ASP:OD1	1:A:991:ASP:C	2.59	0.41
1:A:610:PRO:HD2	1:A:614:LEU:HD21	2.03	0.41
1:A:1107:LEU:N	1:A:1112:VAL:O	2.40	0.41
1:A:547:ILE:HG22	1:A:734:SER:HB2	2.02	0.41
1:A:946:ARG:O	1:A:947:PHE:HB3	2.19	0.41
1:A:1022:ILE:O	1:A:1043:ILE:HA	2.21	0.41
1:A:623:SER:N	1:A:636:LYS:HD3	2.36	0.41
1:A:888:LYS:HZ2	1:A:892:VAL:HG13	1.85	0.41
1:A:1562:LEU:HB2	1:A:1566:SER:HB2	2.01	0.41
1:A:1178:LYS:HE3	1:A:1180:LEU:HD22	2.03	0.41
1:A:1284:LEU:O	1:A:1287:LEU:N	2.51	0.41
1:A:1355:ASP:OD2	1:A:1358:ARG:HG3	2.21	0.40
1:A:398:ARG:HB2	1:A:482:PHE:CE1	2.56	0.40
1:A:666:GLN:OE1	1:A:668:ARG:NH2	2.53	0.40
1:A:675:ASP:HA	1:A:690:PHE:CE1	2.55	0.40
1:A:1619:VAL:CG2	1:A:1620:THR:N	2.84	0.40
1:A:1045:ASN:CG	1:A:1047:THR:HG22	2.40	0.40
1:A:1343:LEU:HD13	1:A:1365:LEU:HD23	2.03	0.40
1:A:1548:VAL:O	1:A:1548:VAL:HG12	2.21	0.40
1:A:404:ILE:HG21	1:A:971:GLN:OE1	2.20	0.40
1:A:1513:GLY:CA	1:A:1519:LYS:HG3	2.52	0.40
1:A:648:PHE:CD2	1:A:723:LEU:HD22	2.57	0.40
1:A:639:ILE:CG1	1:A:738:TRP:H	2.34	0.40
1:A:1413:LEU:HD12	1:A:1416:GLN:HG3	2.03	0.40
1:A:1137:ALA:CB	1:A:1485:TRP:CD1	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1112/1639 (68%)	989 (89%)	105 (9%)	18 (2%)	9 43

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	642	GLU
1	A	730	GLU
1	A	1169	PRO
1	A	1178	LYS
1	A	947	PHE
1	A	948	GLY
1	A	687	GLN
1	A	1170	PRO
1	A	386	LYS
1	A	610	PRO
1	A	1071	ALA
1	A	1173	ILE
1	A	1175	ARG
1	A	567	GLY
1	A	676	TYR
1	A	1048	ASP
1	A	1296	PRO
1	A	468	GLY

5.3.2 Protein sidechains

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	927/1340 (69%)	902 (97%)	25 (3%)	44 68

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	563	LEU
1	A	605	GLU
1	A	621	PHE
1	A	645	ASN
1	A	675	ASP
1	A	686	TRP
1	A	734	SER
1	A	882	SER
1	A	907	THR
1	A	921	GLN
1	A	962	VAL
1	A	1155	SER
1	A	1198	SER
1	A	1228	SER
1	A	1274	ASP
1	A	1292	MSE
1	A	1336	ASP
1	A	1378	TRP
1	A	1477	SER
1	A	1479	SER
1	A	1488	MSE
1	A	1541	SER
1	A	1572	SER
1	A	1607	TYR
1	A	1630	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1139	GLN
1	A	1172	ASN
1	A	1470	GLN
1	A	1590	HIS

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1103/1639 (67%)	0.05	29 (2%) 56 42	85, 139, 205, 267	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1108	PRO	4.9
1	A	943	ALA	4.0
1	A	616	GLY	3.3
1	A	615	PRO	3.2
1	A	651	VAL	3.1
1	A	665	LEU	3.1
1	A	653	SER	3.0
1	A	650	ILE	2.9
1	A	1111	THR	2.7
1	A	922	LYS	2.7
1	A	667	VAL	2.6
1	A	702	LEU	2.6
1	A	889	PRO	2.4
1	A	888	LYS	2.4
1	A	664	GLY	2.4
1	A	1112	VAL	2.4
1	A	659	LYS	2.3
1	A	966	ASN	2.3
1	A	666	GLN	2.3
1	A	1102	ILE	2.3
1	A	742	SER	2.3
1	A	1050	PRO	2.2
1	A	668	ARG	2.2
1	A	711	LYS	2.2
1	A	681	SER	2.2
1	A	660	LYS	2.2
1	A	724	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1055	VAL	2.1
1	A	944	ALA	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.