



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:45 PM GMT

PDB ID : 1CB6
Title : STRUCTURE OF HUMAN APOLACTOFERRIN AT 2.0 Å RESOLUTION.
Authors : Jameson, G.B.; Anderson, B.F.; Norris, G.E.; Thomas, D.H.; Baker, E.N.
Deposited on : 1999-03-01
Resolution : 2.00 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

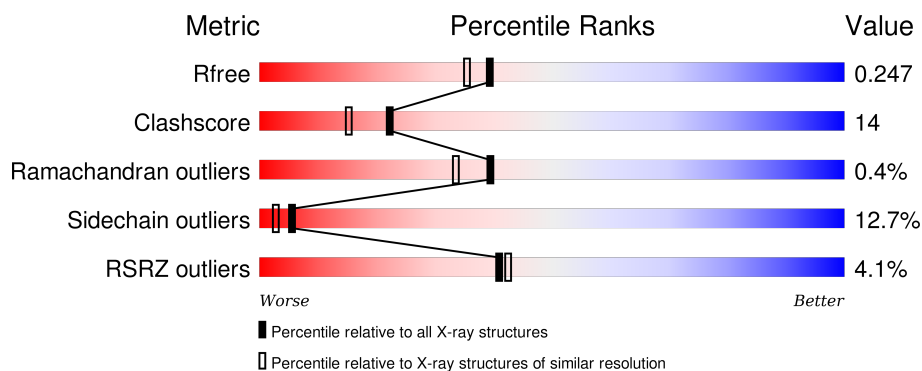
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	691	<div> <div>4%</div> <div>70%</div> <div>23%</div> <div>7%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5727 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 (LACTOFERRIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	4	0
			5368	3353	960	1017	38			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	SEE REMARK 999	UNP P02788

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		

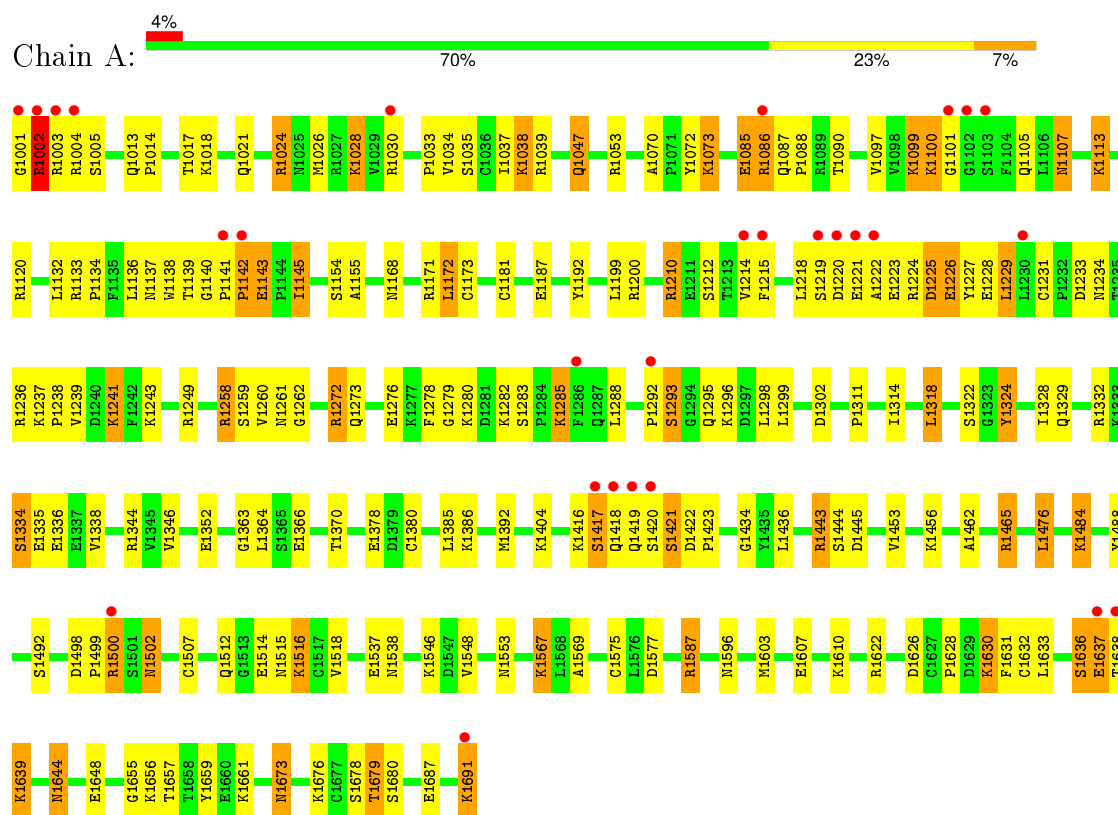
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	357	Total	O	0	0
			357	357		

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.

• Molecule 1: PROTEIN (LACTOFERRIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.09 Å 94.58 Å 55.79 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 16.99 – 1.99	Depositor EDS
% Data completeness (in resolution range)	92.0 (10.00-2.00) 89.1 (16.99-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.99 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.201 , 0.286 0.178 , 0.247	Depositor DCC
R_{free} test set	2133 reflections (4.54%)	DCC
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 86.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53852 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5727	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.26	0/5490	0.53	0/7423

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1492	SER	Peptide

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	5368	0	5230	146	0
2	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	357	0	0	25	0
All	All	5727	0	5230	146	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 14.

All (146) 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:1292:PRO:HG2	1:A:1295:GLN:HG3	1.60	0.82
1:A:1334:SER:HB2	1:A:1336:GLU:HG2	1.60	0.82
1:A:1223:GLU:O	1:A:1226:GLU:HG3	1.82	0.79
1:A:1318:LEU:HD12	1:A:1386:LYS:HD2	1.65	0.78
1:A:1276:GLU:O	1:A:1282:LYS:HE2	1.84	0.78
1:A:1107:ASN:HD22	1:A:1107:ASN:H	1.32	0.78
1:A:1436:LEU:HD11	1:A:1587:ARG:HE	1.50	0.77
1:A:1416:LYS:HD3	1:A:1421:SER:HB3	1.66	0.76
1:A:1516:LYS:HD2	3:A:2196:HOH:O	1.88	0.74
1:A:1210:ARG:HD2	1:A:1212:SER:OG	1.89	0.72
1:A:1200:ARG:HG2	1:A:1227:TYR:OH	1.90	0.72
1:A:1436:LEU:HD11	1:A:1587:ARG:NE	2.05	0.71
1:A:1017:THR:O	1:A:1021:GLN:HG2	1.90	0.71
1:A:1296:LYS:HD3	1:A:1302:ASP:OD2	1.92	0.69
1:A:1003:ARG:HD3	1:A:1005:SER:OG	1.92	0.67
1:A:1003:ARG:HG2	1:A:1004:ARG:H	1.59	0.67
1:A:1631:PHE:HA	3:A:2066:HOH:O	1.95	0.66
1:A:1113:LYS:HE3	3:A:2018:HOH:O	1.94	0.66
1:A:1636:SER:HB2	1:A:1639:LYS:HB2	1.77	0.66
1:A:1155:ALA:HB1	1:A:1172:LEU:HD21	1.78	0.65
1:A:1636:SER:O	1:A:1639:LYS:HG3	1.97	0.65
1:A:1173:CYS:HB3	1:A:1187:GLU:OE1	1.99	0.63
1:A:1238:PRO:HD2	1:A:1241:LYS:HG3	1.80	0.63
1:A:1229:LEU:HD22	1:A:1239:VAL:HA	1.81	0.62
1:A:1028:LYS:HE2	1:A:1285:LYS:HE2	1.81	0.62
1:A:1105:GLN:HB2	1:A:1107:ASN:ND2	2.15	0.61
1:A:1443:ARG:HD3	3:A:2111:HOH:O	2.02	0.60
1:A:1037:ILE:HD12	1:A:1039:ARG:NH1	2.17	0.59
1:A:1622:ARG:HD2	1:A:1648:GLU:HA	1.83	0.59
1:A:1024:ARG:N	1:A:1024:ARG:HD3	2.17	0.58
1:A:1626:ASP:OD1	1:A:1630:LYS:HE3	2.03	0.57
1:A:1546:LYS:HE3	1:A:1548[B]:VAL:CG2	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1168:ASN:HA	1:A:1171:ARG:HG3	1.87	0.56
1:A:1155:ALA:CB	1:A:1172:LEU:HD21	2.34	0.56
1:A:1603:MET:HE1	3:A:2039:HOH:O	2.05	0.56
1:A:1587:ARG:HD2	3:A:2301:HOH:O	2.05	0.56
1:A:1218:LEU:HD22	1:A:1223:GLU:HB3	1.88	0.56
1:A:1515:ASN:O	1:A:1518:VAL:HG22	2.05	0.56
1:A:1656:LYS:HA	1:A:1661:LYS:HZ2	1.72	0.55
1:A:1107:ASN:HD22	1:A:1107:ASN:N	2.00	0.55
1:A:1214:VAL:O	1:A:1218:LEU:HB2	2.06	0.55
1:A:1273:GLN:OE1	1:A:1273:GLN:HA	2.07	0.54
1:A:1324:TYR:CE1	1:A:1328:ILE:HD11	2.42	0.54
1:A:1346:VAL:HG22	1:A:1370:THR:CG2	2.37	0.54
1:A:1659:TYR:HB3	3:A:2231:HOH:O	2.07	0.54
1:A:1138:TRP:HE1	1:A:1143:GLU:HG3	1.72	0.53
1:A:1233:ASP:O	1:A:1234:ASN:HB2	2.08	0.52
1:A:1673:ASN:HD22	1:A:1673:ASN:N	2.06	0.52
1:A:1085:GLU:O	1:A:1086:ARG:HG2	2.10	0.52
1:A:1456:LYS:HD2	3:A:2187:HOH:O	2.09	0.52
1:A:1322:SER:HB3	1:A:1385:LEU:O	2.09	0.52
1:A:1001:GLY:O	1:A:1002:ARG:HB2	2.09	0.52
1:A:1311:PRO:HD2	1:A:1314:ILE:HD12	1.91	0.52
1:A:1292:PRO:HG2	1:A:1295:GLN:CG	2.36	0.51
1:A:1260:VAL:O	1:A:1260:VAL:HG23	2.11	0.51
1:A:1005:SER:HA	1:A:1033:PRO:HG2	1.93	0.51
1:A:1229:LEU:CD2	1:A:1239:VAL:HA	2.40	0.50
1:A:1335:GLU:HG2	3:A:2224:HOH:O	2.10	0.50
1:A:1013:GLN:HB3	1:A:1014:PRO:HD3	1.93	0.50
1:A:1105:GLN:HB2	1:A:1107:ASN:HD21	1.76	0.50
1:A:1628:PRO:HA	1:A:1632:CYS:SG	2.52	0.50
1:A:1260:VAL:O	1:A:1261:ASN:HB2	2.12	0.50
1:A:1638:THR:HG22	1:A:1638:THR:O	2.12	0.49
1:A:1097:VAL:O	1:A:1199:LEU:HD22	2.12	0.49
1:A:1026:MET:SD	1:A:1278:PHE:HE2	2.36	0.49
1:A:1192:TYR:CE1	1:A:1210:ARG:HG2	2.48	0.49
1:A:1507:CYS:O	1:A:1516:LYS:HE2	2.13	0.48
1:A:1038:LYS:HD3	1:A:1039:ARG:O	2.13	0.48
1:A:1047:GLN:HB3	3:A:2007:HOH:O	2.13	0.48
1:A:1607:GLU:HG2	3:A:2199:HOH:O	2.12	0.48
1:A:1222:ALA:HA	1:A:1225:ASP:OD1	2.14	0.48
1:A:1272:ARG:HG2	3:A:2243:HOH:O	2.13	0.48
1:A:1218:LEU:CD1	1:A:1224:ARG:HG2	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1434:GLY:HA2	1:A:1596:ASN:OD1	2.14	0.47
1:A:1445:ASP:HB3	3:A:2114:HOH:O	2.14	0.47
1:A:1018:LYS:HA	1:A:1021:GLN:HG3	1.97	0.47
1:A:1622:ARG:HG3	1:A:1622:ARG:HH11	1.80	0.47
1:A:1673:ASN:O	1:A:1676:LYS:HB2	2.16	0.46
1:A:1037:ILE:HD12	1:A:1039:ARG:CZ	2.45	0.46
1:A:1105:GLN:HE22	1:A:1236:ARG:HG3	1.80	0.46
1:A:1039:ARG:HH21	1:A:1053:ARG:NH1	2.14	0.46
1:A:1655:GLY:O	1:A:1661:LYS:NZ	2.49	0.46
1:A:1258:ARG:HG2	1:A:1262:GLY:HA2	1.98	0.46
1:A:1215:PHE:CZ	1:A:1239:VAL:HG23	2.51	0.46
1:A:1086:ARG:HE	1:A:1086:ARG:HB3	1.39	0.46
1:A:1639:LYS:HE3	1:A:1639:LYS:HB3	1.64	0.45
1:A:1154:SER:O	1:A:1168:ASN:ND2	2.50	0.45
1:A:1352:GLU:OE1	1:A:1352:GLU:N	2.50	0.45
1:A:1691:LYS:HZ3	1:A:1691:LYS:C	2.19	0.45
1:A:1233:ASP:HB3	1:A:1603:MET:HB3	1.98	0.45
1:A:1224:ARG:NH2	3:A:2085:HOH:O	2.47	0.45
1:A:1436:LEU:HD11	1:A:1587:ARG:CD	2.46	0.45
1:A:1298:LEU:O	1:A:1299:LEU:HB2	2.16	0.45
1:A:1132:LEU:O	1:A:1136:LEU:HG	2.16	0.45
1:A:1644:ASN:ND2	3:A:2054:HOH:O	2.50	0.45
1:A:1476:LEU:HA	1:A:1476:LEU:HD12	1.81	0.45
1:A:1138:TRP:NE1	1:A:1143:GLU:HG3	2.33	0.44
1:A:1047:GLN:HG3	1:A:1072:TYR:CE1	2.52	0.44
1:A:1085:GLU:O	1:A:1086:ARG:CG	2.65	0.44
1:A:1087:GLN:N	1:A:1088:PRO:HD3	2.32	0.44
1:A:1498:ASP:OD1	1:A:1500:ARG:NH2	2.50	0.44
1:A:1610:LYS:NZ	3:A:2362:HOH:O	2.50	0.44
1:A:1462:ALA:HB3	1:A:1465:ARG:HG3	1.99	0.44
1:A:1476:LEU:HB3	1:A:1488:TYR:CE2	2.53	0.44
1:A:1145:ILE:H	1:A:1145:ILE:HG12	1.48	0.44
1:A:1553:ASN:OD1	1:A:1638:THR:HG21	2.17	0.43
1:A:1334:SER:O	1:A:1338:VAL:HG23	2.18	0.43
1:A:1679:THR:OG1	1:A:1680:SER:N	2.50	0.43
1:A:1231:CYS:HB2	1:A:1233:ASP:OD1	2.18	0.43
1:A:1655:GLY:C	1:A:1657:THR:HG23	2.37	0.43
1:A:1546:LYS:HE3	1:A:1548[B]:VAL:HG22	2.01	0.43
1:A:1636:SER:HA	3:A:2238:HOH:O	2.19	0.43
1:A:1417:SER:OG	1:A:1418:GLN:N	2.50	0.43
1:A:1443:ARG:HD3	1:A:1569:ALA:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1567:LYS:HB3	3:A:2214:HOH:O	2.19	0.42
1:A:1249:ARG:HG2	1:A:1249:ARG:HH11	1.84	0.42
1:A:1484:LYS:HD2	1:A:1484:LYS:HA	1.61	0.42
1:A:1422:ASP:HB3	1:A:1423:PRO:HD2	2.01	0.42
1:A:1366:GLU:HG3	3:A:2183:HOH:O	2.20	0.42
1:A:1378:GLU:HG3	3:A:2203:HOH:O	2.19	0.42
1:A:1107:ASN:ND2	1:A:1107:ASN:H	2.09	0.42
1:A:1099:LYS:HG2	1:A:1227:TYR:CE1	2.54	0.42
1:A:1637:GLU:O	1:A:1637:GLU:HG2	2.19	0.42
1:A:1293:SER:HB3	3:A:2221:HOH:O	2.20	0.42
1:A:1053:ARG:HD3	3:A:2302:HOH:O	2.19	0.42
1:A:1136:LEU:HD23	1:A:1136:LEU:HA	1.86	0.41
1:A:1363:GLY:HA3	3:A:2182:HOH:O	2.19	0.41
1:A:1537:GLU:O	1:A:1538:ASN:HB2	2.20	0.41
1:A:1575:CYS:HB2	1:A:1577:ASP:OD1	2.20	0.41
1:A:1139:THR:HG22	1:A:1140:GLY:N	2.34	0.41
1:A:1514:GLU:HG3	3:A:2262:HOH:O	2.19	0.41
1:A:1034:VAL:HG13	1:A:1034:VAL:O	2.20	0.41
1:A:1404:LYS:HD3	1:A:1659:TYR:OH	2.21	0.41
1:A:1292:PRO:HD2	1:A:1298:LEU:CD1	2.51	0.41
1:A:1636:SER:O	1:A:1637:GLU:HG2	2.20	0.41
1:A:1380:CYS:HB3	1:A:1392:MET:SD	2.61	0.41
1:A:1502:ASN:HA	1:A:1502:ASN:HD22	1.53	0.41
1:A:1100:LYS:HD2	1:A:1101:GLY:N	2.35	0.41
1:A:1346:VAL:HG22	1:A:1370:THR:HG22	2.02	0.41
1:A:1498:ASP:OD1	1:A:1499:PRO:HD2	2.21	0.41
1:A:1070:ALA:HB2	1:A:1073:LYS:CE	2.50	0.40
1:A:1133:ARG:N	1:A:1134:PRO:HD2	2.36	0.40
1:A:1003:ARG:HG2	1:A:1004:ARG:N	2.32	0.40
1:A:1141:PRO:N	1:A:1142:PRO:HD2	2.37	0.40
1:A:1225:ASP:N	1:A:1225:ASP:OD1	2.48	0.40
1:A:1332:ARG:NH1	3:A:2294:HOH:O	2.54	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	693/691 (100%)	662 (96%)	28 (4%)	3 (0%)	39 33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1002	ARG
1	A	1279	GLY
1	A	1142	PRO

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	578/574 (101%)	505 (87%)	73 (13%)	5 3

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1002	ARG
1	A	1024	ARG
1	A	1028	LYS
1	A	1030	ARG
1	A	1035	SER
1	A	1038	LYS
1	A	1047	GLN
1	A	1073	LYS
1	A	1085	GLU
1	A	1086	ARG
1	A	1090	THR
1	A	1099	LYS
1	A	1100	LYS
1	A	1107	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1113	LYS
1	A	1120	ARG
1	A	1137	ASN
1	A	1143	GLU
1	A	1145	ILE
1	A	1172	LEU
1	A	1181	CYS
1	A	1210	ARG
1	A	1219	SER
1	A	1220	ASP
1	A	1221	GLU
1	A	1225	ASP
1	A	1226	GLU
1	A	1228	GLU
1	A	1229	LEU
1	A	1237	LYS
1	A	1241	LYS
1	A	1243	LYS
1	A	1258	ARG
1	A	1259	SER
1	A	1272	ARG
1	A	1280	LYS
1	A	1283	SER
1	A	1285	LYS
1	A	1288	LEU
1	A	1293	SER
1	A	1318	LEU
1	A	1324	TYR
1	A	1329	GLN
1	A	1334	SER
1	A	1344	ARG
1	A	1364	LEU
1	A	1417	SER
1	A	1419	GLN
1	A	1420	SER
1	A	1421	SER
1	A	1443	ARG
1	A	1444	SER
1	A	1453	VAL
1	A	1465	ARG
1	A	1476	LEU
1	A	1484	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1500	ARG
1	A	1502	ASN
1	A	1512	GLN
1	A	1516	LYS
1	A	1567	LYS
1	A	1587	ARG
1	A	1630	LYS
1	A	1633	LEU
1	A	1636	SER
1	A	1637	GLU
1	A	1639	LYS
1	A	1644	ASN
1	A	1673	ASN
1	A	1678	SER
1	A	1679	THR
1	A	1687	GLU
1	A	1691	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1023	GLN
1	A	1047	GLN
1	A	1105	GLN
1	A	1107	ASN
1	A	1168	ASN
1	A	1269	ASN
1	A	1418	GLN
1	A	1419	GLN
1	A	1479	GLN
1	A	1502	ASN
1	A	1512	GLN
1	A	1538	ASN
1	A	1611	GLN
1	A	1623	ASN
1	A	1673	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	691/691 (100%)	0.08	28 (4%) 41 42	27, 46, 85, 158	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1001	GLY	12.8
1	A	1002	ARG	10.1
1	A	1420	SER	7.8
1	A	1417	SER	5.8
1	A	1141	PRO	5.1
1	A	1220	ASP	5.0
1	A	1003	ARG	4.3
1	A	1418	GLN	4.2
1	A	1419	GLN	3.8
1	A	1691	LYS	3.5
1	A	1004	ARG	3.4
1	A	1638	THR	3.4
1	A	1219	SER	3.3
1	A	1221	GLU	3.2
1	A	1030	ARG	3.1
1	A	1637	GLU	3.0
1	A	1286	PHE	2.9
1	A	1101	GLY	2.8
1	A	1142	PRO	2.8
1	A	1222	ALA	2.8
1	A	1292	PRO	2.6
1	A	1102	GLY	2.5
1	A	1086	ARG	2.5
1	A	1215	PHE	2.4
1	A	1230	LEU	2.3
1	A	1103	SER	2.3
1	A	1214	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1500	ARG	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CL	A	1701	1/1	0.91	0.14	0.78	64,64,64,64	0
2	CL	A	1702	1/1	0.99	0.06	-2.70	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.