



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:50 AM GMT

PDB ID : 2IZP
Title : BIPD - AN INVASION PRTEIN ASSOCIATED WITH THE TYPE-III SECRETION SYSTEM OF BURKHOLDERIA PSEUDOMALLEI.
Authors : Erskine, P.T.; Knight, M.J.; Ruaux, A.; Mikolajek, H.; Wong-Fat-Sang, N.; Withers, J.; Gill, R.; Wood, S.P.; Wood, M.; Fox, G.C.; Cooper, J.B.
Deposited on : 2006-07-25
Resolution : 2.10 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

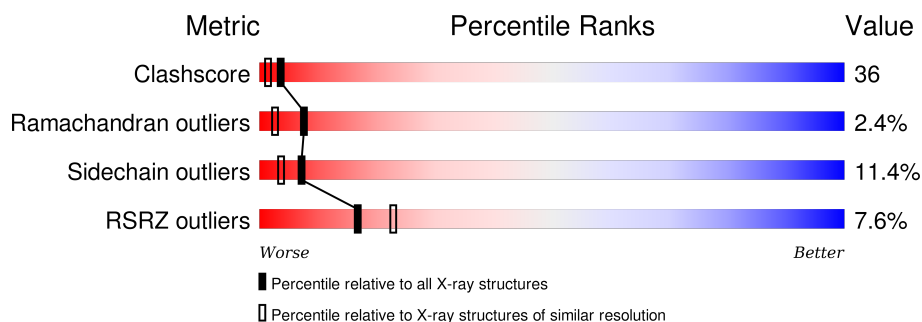
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	303	
1	B	303	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4845 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 PUTATIVE MEMBRANE ANTIGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2090	1296	376	413	5			
1	B	269	Total	C	N	O	S	0	0	0
			2074	1287	371	412	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1009	SER	ARG	CONFLICT	UNP Q63K37
B	2009	SER	ARG	CONFLICT	UNP Q63K37

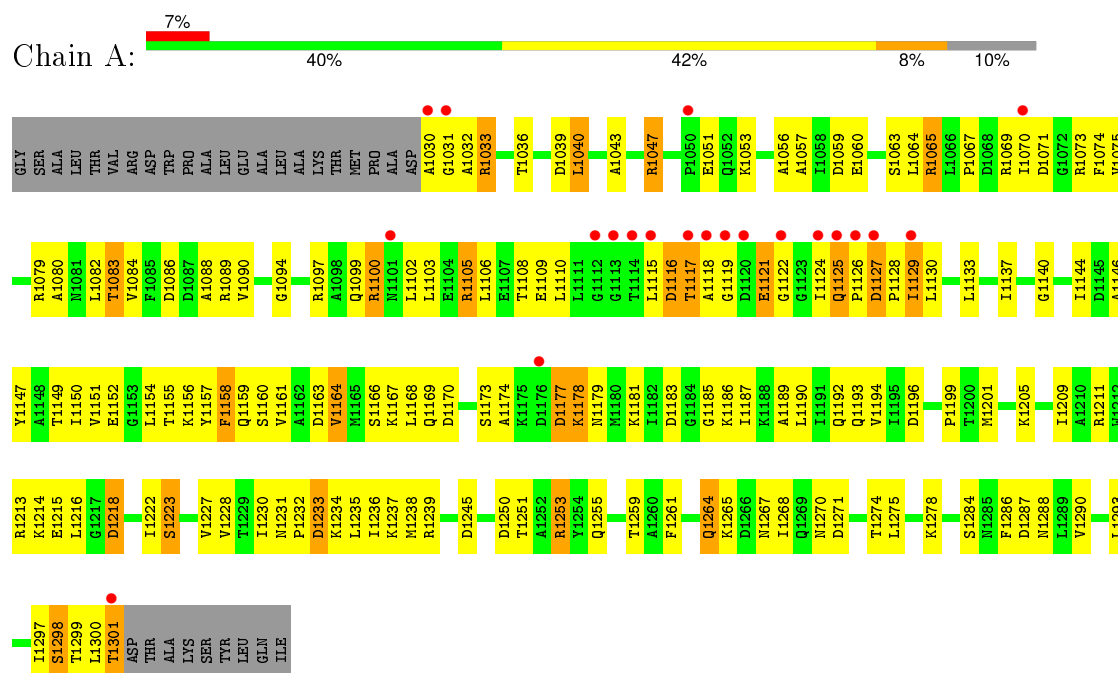
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	312	Total	O	0	0
			312	312		
2	B	369	Total	O	0	0
			369	369		

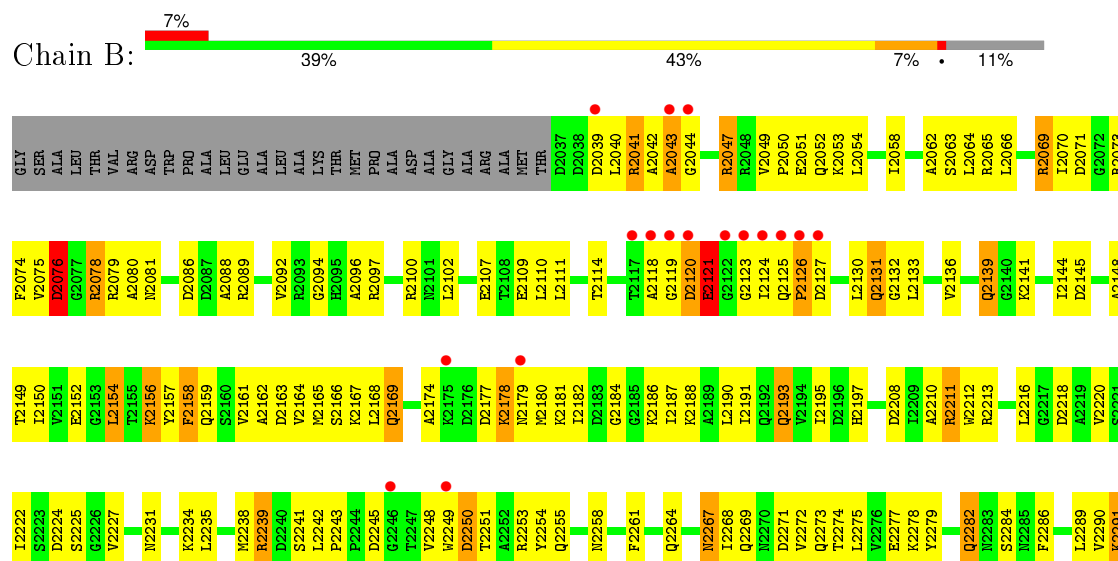
3 Residue-property plots

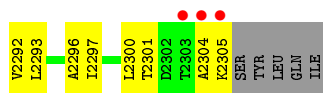
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PUTATIVE MEMBRANE ANTIGEN



• Molecule 1: PUTATIVE MEMBRANE ANTIGEN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.51Å 56.20Å 84.21Å 90.00° 94.47° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 9.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (10.00-2.10) 91.4 (9.50-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.11Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.226 , 0.299 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 111.8	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	3 of 26873 reflections (0.011%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4845	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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

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	0.28	0/2118	0.87	3/2865 (0.1%)
1	B	0.27	0/2102	0.80	0/2844
All	All	0.28	0/4220	0.84	3/5709 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1100	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	1239	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	A	1100	ARG	CD-NE-CZ	5.14	130.79	123.60

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	2090	0	2088	151	0
1	B	2074	0	2070	151	0
2	A	312	0	0	27	0
2	B	369	0	0	19	0
All	All	4845	0	4158	298	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 36.

All (298) 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:1070:ILE:HD12	1:A:1075:VAL:HG21	1.55	0.86
1:B:2154:LEU:HD11	1:B:2275:LEU:HD13	1.57	0.86
1:A:1235:LEU:HA	1:A:1238:MET:HE3	1.59	0.84
1:B:2168:LEU:HD22	1:B:2187:ILE:HG23	1.59	0.84
1:A:1065:ARG:HB2	1:A:1065:ARG:HH11	1.46	0.80
1:B:2058:ILE:HD13	1:B:2273:GLN:HG2	1.64	0.80
1:B:2047:ARG:HD3	1:B:2051:GLU:OE2	1.82	0.80
1:B:2286:PHE:O	1:B:2290:VAL:HG23	1.82	0.79
1:A:1154:LEU:HD13	1:A:1275:LEU:HD13	1.66	0.78
1:A:1067:PRO:HD3	1:A:1169:GLN:HG2	1.66	0.78
1:A:1146:ALA:O	1:A:1150:ILE:HG13	1.85	0.77
1:B:2100:ARG:HD3	1:B:2145:ASP:OD1	1.85	0.76
1:B:2078:ARG:HB2	1:B:2078:ARG:HH11	1.50	0.76
1:A:1125:GLN:HG3	2:A:2113:HOH:O	1.84	0.76
1:B:2047:ARG:O	1:B:2050:PRO:HD2	1.85	0.76
1:B:2066:LEU:HD12	1:B:2258:ASN:OD1	1.87	0.75
1:A:1100:ARG:HD3	2:A:2121:HOH:O	1.85	0.75
1:B:2216:LEU:HD23	1:B:2220:VAL:HG21	1.69	0.74
1:B:2064:LEU:HD21	1:B:2080:ALA:HB2	1.68	0.74
1:B:2164:VAL:O	1:B:2168:LEU:HG	1.87	0.74
1:A:1201:MET:HB2	1:A:1228:VAL:HB	1.70	0.74
1:B:2119:GLY:HA3	1:B:2125:GLN:OE1	1.88	0.74
1:A:1033:ARG:H	1:A:1033:ARG:HD2	1.52	0.73
1:B:2109:GLU:OE1	1:B:2297:ILE:HD13	1.88	0.73
1:B:2166:SER:O	1:B:2169:GLN:HG3	1.87	0.73
1:A:1213:ARG:HG2	1:A:1222:ILE:HD12	1.71	0.72
1:B:2300:LEU:HD13	2:B:3229:HOH:O	1.88	0.72
1:A:1293:LEU:O	1:A:1297:ILE:HG23	1.90	0.72
1:A:1234:LYS:HE2	1:A:1271:ASP:OD2	1.88	0.72
1:B:2110:LEU:HD12	2:B:3229:HOH:O	1.89	0.71
1:B:2178:LYS:HG2	1:B:2251:THR:HB	1.70	0.71
1:A:1251:THR:O	1:A:1255:GLN:HG2	1.91	0.71
1:A:1047:ARG:O	1:A:1051:GLU:HG3	1.90	0.71
1:B:2216:LEU:HD22	1:B:2222:ILE:HD11	1.73	0.71
1:A:1102:LEU:O	1:A:1106:LEU:HG	1.92	0.70
1:A:1108:THR:HG23	2:A:2100:HOH:O	1.90	0.70
1:B:2049:VAL:O	1:B:2053:LYS:HG2	1.89	0.70
1:A:1097:ARG:HB3	2:A:2091:HOH:O	1.91	0.70
1:B:2164:VAL:HG22	1:B:2168:LEU:HD21	1.72	0.69
1:B:2065:ARG:HD3	2:B:3184:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1147:TYR:O	1:A:1151:VAL:HG23	1.93	0.69
1:A:1140:GLY:O	1:A:1144:ILE:HG13	1.93	0.69
1:B:2096:ALA:HB1	1:B:2100:ARG:HH12	1.58	0.68
1:B:2179:ASN:HB3	1:B:2248:VAL:HG13	1.75	0.68
1:B:2125:GLN:HB2	1:B:2127:ASP:OD2	1.93	0.68
1:B:2193:GLN:HB3	2:B:3276:HOH:O	1.94	0.68
1:B:2145:ASP:O	1:B:2149:THR:HG23	1.94	0.68
1:B:2039:ASP:HB2	1:B:2041:ARG:NH1	2.10	0.67
1:B:2274:THR:HG23	2:B:3345:HOH:O	1.95	0.67
1:A:1117:THR:HG23	1:A:1118:ALA:H	1.59	0.67
1:A:1250:ASP:OD2	1:A:1253:ARG:HB2	1.94	0.67
1:B:2297:ILE:O	1:B:2301:THR:HG23	1.95	0.66
1:A:1071:ASP:HB2	1:A:1073:ARG:NH1	2.10	0.65
1:A:1032:ALA:HB1	1:A:1106:LEU:HD23	1.78	0.65
2:A:2233:HOH:O	1:B:2118:ALA:HB2	1.96	0.65
1:A:1056:ALA:O	1:A:1059:ASP:HB2	1.96	0.65
1:A:1186:LYS:O	1:A:1189:ALA:HB3	1.96	0.65
1:A:1116:ASP:HB2	2:A:2108:HOH:O	1.97	0.65
1:A:1064:LEU:HD21	1:A:1080:ALA:HA	1.79	0.64
1:A:1083:THR:HA	1:A:1086:ASP:OD2	1.96	0.64
1:B:2107:GLU:O	1:B:2111:LEU:HD13	1.98	0.64
1:A:1231:ASN:OD1	1:A:1233:ASP:HB3	1.97	0.64
1:B:2131:GLN:HG2	2:B:3241:HOH:O	1.98	0.64
1:B:2188:LYS:HG3	1:B:2239:ARG:HG2	1.80	0.63
1:A:1271:ASP:O	1:A:1275:LEU:HD12	1.98	0.63
1:A:1069:ARG:HD3	1:A:1073:ARG:O	1.98	0.62
1:B:2132:GLY:O	1:B:2136:VAL:HG23	1.99	0.62
1:B:2074:PHE:CD1	1:B:2174:ALA:HB2	2.33	0.62
1:A:1177:ASP:HB3	2:A:2067:HOH:O	2.00	0.61
1:B:2078:ARG:HD3	2:B:3183:HOH:O	2.01	0.61
1:B:2186:LYS:HG3	1:B:2245:ASP:OD1	2.00	0.61
1:A:1126:PRO:CG	1:B:2211:ARG:HG3	2.31	0.60
1:B:2191:ILE:HG23	1:B:2235:LEU:HD22	1.84	0.59
1:A:1126:PRO:HG2	1:B:2211:ARG:HG3	1.83	0.59
1:B:2168:LEU:HD23	1:B:2190:LEU:HD13	1.84	0.59
1:B:2273:GLN:O	1:B:2277:GLU:HG3	2.02	0.59
1:B:2235:LEU:HD23	1:B:2238:MET:HE3	1.84	0.59
1:B:2150:ILE:HD13	1:B:2216:LEU:HD21	1.85	0.59
1:A:1199:PRO:HG2	1:A:1230:ILE:HD12	1.83	0.59
1:A:1156:LYS:HD2	2:A:2124:HOH:O	2.03	0.59
1:B:2164:VAL:HG23	1:B:2190:LEU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:LEU:HD13	1:A:1297:ILE:HG22	1.84	0.59
1:B:2212:TRP:O	1:B:2216:LEU:HD13	2.02	0.58
1:A:1235:LEU:HD23	1:A:1238:MET:CE	2.33	0.58
1:B:2178:LYS:HG2	1:B:2251:THR:CB	2.34	0.58
1:B:2184:GLY:HA3	1:B:2243:PRO:O	2.04	0.58
1:B:2043:ALA:HA	2:B:3169:HOH:O	2.03	0.58
1:A:1047:ARG:HD2	2:A:2046:HOH:O	2.04	0.57
1:A:1235:LEU:HD23	1:A:1238:MET:HE1	1.87	0.57
1:A:1064:LEU:HB2	1:A:1265:LYS:NZ	2.19	0.57
1:A:1209:ILE:H	1:A:1209:ILE:HD12	1.71	0.56
1:A:1259:THR:HG21	2:A:2301:HOH:O	2.04	0.56
1:A:1168:LEU:HB2	1:A:1187:ILE:HG12	1.86	0.56
1:B:2124:ILE:HG13	1:B:2126:PRO:HD3	1.88	0.56
1:A:1234:LYS:HD3	1:A:1267:ASN:HB3	1.87	0.56
1:A:1129:ILE:O	1:A:1129:ILE:HG12	2.05	0.56
1:B:2064:LEU:HD21	1:B:2080:ALA:CB	2.37	0.55
1:A:1237:LYS:HE3	2:A:2201:HOH:O	2.07	0.55
1:B:2227:VAL:HG12	2:B:3315:HOH:O	2.05	0.55
1:B:2251:THR:O	1:B:2255:GLN:HG3	2.07	0.55
1:A:1215:GLU:O	1:A:1278:LYS:HE3	2.06	0.55
1:B:2234:LYS:O	1:B:2238:MET:HG3	2.07	0.55
1:B:2150:ILE:CD1	1:B:2216:LEU:HD21	2.38	0.54
1:B:2120:ASP:O	1:B:2125:GLN:HA	2.07	0.54
1:A:1183:ASP:HA	1:A:1245:ASP:HA	1.89	0.54
1:B:2235:LEU:HA	1:B:2238:MET:HE3	1.89	0.54
1:A:1083:THR:O	1:A:1086:ASP:HB2	2.08	0.54
1:B:2047:ARG:NH2	1:B:2284:SER:HB2	2.22	0.54
1:A:1053:LYS:O	1:A:1056:ALA:HB3	2.08	0.53
1:B:2181:LYS:HE3	2:B:3270:HOH:O	2.07	0.53
1:A:1218:ASP:HB3	2:A:2185:HOH:O	2.08	0.53
1:B:2208:ASP:OD2	1:B:2210:ALA:HB3	2.08	0.53
1:A:1301:THR:HG21	2:A:2249:HOH:O	2.09	0.53
1:B:2152:GLU:O	1:B:2156:LYS:HE3	2.09	0.53
1:B:2250:ASP:H	1:B:2253:ARG:HB3	1.74	0.53
1:B:2268:ILE:O	1:B:2271:ASP:HB2	2.08	0.53
1:A:1110:LEU:CD1	1:A:1297:ILE:HG22	2.38	0.53
1:B:2187:ILE:HG22	1:B:2242:LEU:HD13	1.91	0.53
1:B:2078:ARG:HH11	1:B:2078:ARG:CB	2.21	0.53
1:B:2079:ARG:NH2	1:B:2169:GLN:HB2	2.24	0.52
1:B:2041:ARG:HD3	1:B:2041:ARG:H	1.73	0.52
1:B:2069:ARG:HA	1:B:2073:ARG:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2039:ASP:HB2	1:B:2041:ARG:HH11	1.74	0.52
1:A:1069:ARG:HA	1:A:1073:ARG:O	2.10	0.52
1:A:1150:ILE:O	1:A:1154:LEU:HG	2.10	0.52
1:B:2249:TRP:HE3	1:B:2254:TYR:HA	1.74	0.52
1:B:2235:LEU:HD23	1:B:2238:MET:CE	2.40	0.52
1:A:1032:ALA:CB	1:A:1106:LEU:HD23	2.39	0.52
1:A:1133:LEU:O	1:A:1137:ILE:HG13	2.08	0.52
1:A:1154:LEU:CD1	1:A:1275:LEU:HD13	2.38	0.52
1:B:2063:SER:O	1:B:2078:ARG:HD2	2.09	0.52
1:B:2124:ILE:HA	1:B:2130:LEU:CD2	2.39	0.51
1:B:2227:VAL:HG12	1:B:2227:VAL:O	2.10	0.51
1:A:1073:ARG:HD2	2:A:2068:HOH:O	2.10	0.51
1:A:1071:ASP:HB2	1:A:1073:ARG:HH12	1.75	0.51
1:B:2102:LEU:HD21	1:B:2290:VAL:HG11	1.91	0.51
1:B:2154:LEU:O	1:B:2157:TYR:HB3	2.10	0.51
1:A:1163:ASP:OD1	1:A:1167:LYS:HE2	2.10	0.51
1:B:2216:LEU:CD2	1:B:2220:VAL:HG21	2.39	0.51
1:A:1157:TYR:HB2	1:A:1230:ILE:HD13	1.93	0.50
1:A:1199:PRO:HG2	1:A:1230:ILE:CD1	2.40	0.50
1:A:1161:VAL:HG22	1:A:1235:LEU:HD21	1.94	0.50
1:B:2248:VAL:O	1:B:2248:VAL:HG12	2.09	0.50
1:A:1103:LEU:HD22	1:A:1137:ILE:HG23	1.93	0.50
1:B:2124:ILE:HG23	1:B:2125:GLN:H	1.76	0.50
1:A:1059:ASP:HB3	2:A:2059:HOH:O	2.11	0.50
1:B:2070:ILE:HD13	1:B:2075:VAL:HG21	1.92	0.50
1:A:1234:LYS:O	1:A:1238:MET:HG3	2.12	0.50
1:B:2249:TRP:CE3	1:B:2253:ARG:HG3	2.47	0.50
1:B:2212:TRP:HE3	1:B:2216:LEU:HD11	1.75	0.50
1:A:1201:MET:CB	1:A:1228:VAL:HB	2.39	0.49
1:A:1119:GLY:HA3	1:A:1121:GLU:OE1	2.12	0.49
1:B:2047:ARG:HH22	1:B:2284:SER:HB2	1.76	0.49
1:B:2148:ALA:O	1:B:2152:GLU:OE2	2.30	0.49
1:A:1099:GLN:HG2	1:A:1286:PHE:CE2	2.47	0.49
1:A:1205:LYS:HD2	2:A:2164:HOH:O	2.13	0.49
1:B:2054:LEU:HD11	1:B:2092:VAL:CG2	2.43	0.49
1:A:1232:PRO:O	1:A:1236:ILE:HG12	2.12	0.49
1:B:2279:TYR:O	1:B:2282:GLN:HB3	2.13	0.49
1:A:1082:LEU:O	1:A:1086:ASP:OD2	2.30	0.49
1:B:2188:LYS:CG	1:B:2239:ARG:HG2	2.42	0.49
1:B:2168:LEU:HD23	1:B:2190:LEU:CD1	2.43	0.49
1:B:2096:ALA:HB1	1:B:2100:ARG:NH1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2064:LEU:HD21	1:B:2080:ALA:CA	2.43	0.48
1:A:1297:ILE:HG13	1:A:1298:SER:N	2.27	0.48
1:A:1125:GLN:HG2	1:A:1125:GLN:O	2.14	0.48
1:B:2304:ALA:O	1:B:2305:LYS:O	2.32	0.48
1:B:2159:GLN:O	1:B:2162:ALA:HB3	2.14	0.48
1:A:1149:THR:O	1:A:1152:GLU:HB2	2.14	0.47
1:B:2278:LYS:HG2	2:B:3350:HOH:O	2.13	0.47
1:B:2110:LEU:HG	1:B:2130:LEU:HD11	1.96	0.47
1:B:2293:LEU:O	1:B:2296:ALA:HB3	2.14	0.47
1:A:1121:GLU:HG3	2:A:2115:HOH:O	2.14	0.47
1:A:1067:PRO:CD	1:A:1169:GLN:HG2	2.41	0.47
1:A:1064:LEU:HD21	1:A:1080:ALA:CA	2.43	0.46
1:A:1159:GLN:HB3	2:A:2127:HOH:O	2.15	0.46
1:A:1124:ILE:HB	1:A:1125:GLN:NE2	2.30	0.46
1:A:1053:LYS:HB3	1:A:1088:ALA:HA	1.97	0.46
1:B:2249:TRP:CE3	1:B:2254:TYR:HA	2.50	0.46
1:B:2039:ASP:OD1	1:B:2291:LYS:HE2	2.16	0.46
1:A:1157:TYR:HE1	1:A:1235:LEU:HD11	1.80	0.46
1:A:1086:ASP:HA	2:A:2085:HOH:O	2.14	0.46
1:B:2042:ALA:O	1:B:2043:ALA:HB2	2.16	0.46
1:B:2154:LEU:HD11	1:B:2275:LEU:CD1	2.37	0.46
1:B:2182:ILE:HD12	1:B:2249:TRP:CG	2.50	0.46
1:A:1297:ILE:O	1:A:1301:THR:HB	2.16	0.46
1:A:1036:THR:OG1	1:A:1039:ASP:OD2	2.30	0.46
1:A:1040:LEU:O	1:A:1043:ALA:HB3	2.15	0.46
1:B:2157:TYR:O	1:B:2161:VAL:HG23	2.16	0.46
1:A:1161:VAL:HA	1:A:1164:VAL:HG23	1.97	0.46
1:B:2144:ILE:HD11	1:B:2286:PHE:CE1	2.50	0.45
1:A:1270:ASN:HA	2:A:2225:HOH:O	2.15	0.45
1:A:1073:ARG:HG3	1:A:1073:ARG:HH11	1.82	0.45
1:A:1089:ARG:HG2	1:A:1155:THR:CG2	2.46	0.45
1:B:2065:ARG:HG2	1:B:2065:ARG:HH11	1.81	0.45
1:A:1089:ARG:HG2	1:A:1155:THR:HG21	1.98	0.45
1:A:1213:ARG:NH1	1:A:1223:SER:O	2.50	0.45
1:B:2086:ASP:OD1	1:B:2089:ARG:NH1	2.50	0.45
1:A:1264:GLN:NE2	2:A:2216:HOH:O	2.50	0.45
1:A:1030:ALA:O	1:A:1032:ALA:N	2.50	0.45
1:A:1053:LYS:O	1:A:1056:ALA:N	2.50	0.45
1:B:2094:GLY:HA2	1:B:2097:ARG:NH1	2.31	0.45
1:A:1047:ARG:HH11	1:A:1047:ARG:HG2	1.81	0.45
1:A:1106:LEU:HD11	1:A:1290:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2179:ASN:HB3	1:B:2248:VAL:CG1	2.44	0.45
1:B:2079:ARG:HH21	1:B:2169:GLN:HB2	1.82	0.45
1:B:2131:GLN:NE2	2:B:3240:HOH:O	2.50	0.45
1:B:2081:ASN:ND2	2:B:3203:HOH:O	2.49	0.45
1:A:1209:ILE:O	1:A:1213:ARG:HG3	2.17	0.45
1:B:2218:ASP:O	1:B:2231:ASN:ND2	2.49	0.45
1:A:1284:SER:O	1:A:1287:ASP:OD2	2.33	0.45
1:A:1287:ASP:OD2	1:A:1288:ASN:N	2.49	0.45
1:B:2213:ARG:NH2	1:B:2222:ILE:O	2.50	0.45
1:B:2187:ILE:HG22	1:B:2242:LEU:CD1	2.47	0.45
1:A:1070:ILE:HD12	1:A:1075:VAL:CG2	2.37	0.44
1:B:2141:LYS:O	1:B:2145:ASP:OD2	2.35	0.44
1:B:2049:VAL:HB	1:B:2050:PRO:HD3	1.99	0.44
1:B:2121:GLU:HB3	1:B:2124:ILE:CG2	2.48	0.44
1:A:1185:GLY:N	1:A:1245:ASP:OD2	2.50	0.44
1:A:1083:THR:O	1:A:1086:ASP:N	2.50	0.44
1:A:1270:ASN:ND2	2:A:2227:HOH:O	2.50	0.44
1:A:1065:ARG:HH11	1:A:1065:ARG:CB	2.22	0.44
1:B:2258:ASN:ND2	2:B:3327:HOH:O	2.50	0.44
1:B:2124:ILE:HG23	1:B:2125:GLN:N	2.32	0.44
1:A:1178:LYS:HA	1:A:1178:LYS:HD2	1.51	0.44
1:A:1164:VAL:HG21	1:A:1194:VAL:HG21	2.00	0.44
1:A:1150:ILE:HD13	1:A:1216:LEU:HD11	2.00	0.44
1:A:1238:MET:HB3	1:A:1261:PHE:CE1	2.53	0.44
1:B:2110:LEU:HD21	1:B:2133:LEU:HB3	1.99	0.44
1:B:2124:ILE:HA	1:B:2130:LEU:HD22	2.00	0.44
1:B:2089:ARG:HG2	1:B:2152:GLU:HG2	2.00	0.44
1:B:2070:ILE:HD12	1:B:2070:ILE:N	2.33	0.44
1:A:1074:PHE:HZ	2:A:2137:HOH:O	2.01	0.44
1:A:1238:MET:CE	1:A:1268:ILE:HD11	2.47	0.43
1:A:1069:ARG:HH22	1:A:1174:ALA:HB1	1.83	0.43
1:A:1274:THR:O	1:A:1278:LYS:HG3	2.18	0.43
1:A:1064:LEU:HB2	1:A:1265:LYS:HZ3	1.83	0.43
1:B:2154:LEU:HA	1:B:2154:LEU:HD23	1.78	0.43
1:B:2253:ARG:NH2	2:B:3324:HOH:O	2.50	0.43
1:A:1057:ALA:O	1:A:1060:GLU:N	2.51	0.43
1:B:2039:ASP:HB3	1:B:2040:LEU:H	1.49	0.43
1:A:1129:ILE:HB	2:B:3355:HOH:O	2.17	0.43
1:B:2076:ASP:HB2	2:B:3196:HOH:O	2.18	0.43
1:B:2235:LEU:HA	1:B:2238:MET:CE	2.47	0.43
1:B:2180:MET:O	1:B:2182:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:SER:O	1:A:1301:THR:HB	2.18	0.43
1:B:2062:ALA:HB2	1:B:2269:GLN:OE1	2.19	0.43
1:A:1079:ARG:NH2	1:A:1170:ASP:OD2	2.51	0.43
1:A:1214:LYS:HD2	2:A:2176:HOH:O	2.19	0.43
1:A:1090:VAL:O	1:A:1094:GLY:N	2.49	0.43
1:A:1127:ASP:N	1:A:1128:PRO:HD2	2.34	0.43
1:A:1230:ILE:O	1:A:1232:PRO:HD3	2.18	0.43
1:A:1032:ALA:HB2	1:A:1105:ARG:HB3	2.00	0.43
1:A:1186:LYS:N	1:A:1245:ASP:OD2	2.50	0.43
1:B:2289:LEU:O	1:B:2293:LEU:HG	2.19	0.43
1:A:1115:LEU:HG	1:A:1116:ASP:H	1.83	0.42
1:B:2238:MET:O	1:B:2241:SER:OG	2.34	0.42
1:B:2054:LEU:HD23	1:B:2088:ALA:HB1	2.01	0.42
1:B:2191:ILE:HG22	1:B:2195:ILE:HD11	2.00	0.42
1:A:1154:LEU:O	1:A:1158:PHE:HB2	2.19	0.42
1:A:1178:LYS:O	1:A:1179:ASN:ND2	2.52	0.42
1:A:1060:GLU:OE2	1:A:1063:SER:OG	2.37	0.42
1:A:1130:LEU:CD2	1:A:1300:LEU:HD13	2.49	0.42
1:B:2164:VAL:CG2	1:B:2190:LEU:HB3	2.49	0.42
1:B:2150:ILE:O	1:B:2154:LEU:HB2	2.20	0.42
1:B:2157:TYR:OH	1:B:2268:ILE:HD13	2.20	0.42
1:A:1164:VAL:CG2	1:A:1194:VAL:HG21	2.49	0.42
1:B:2156:LYS:HE3	1:B:2156:LYS:HB2	1.22	0.42
1:A:1300:LEU:HD21	1:B:2292:VAL:CG2	2.50	0.42
1:B:2163:ASP:OD1	1:B:2167:LYS:HE3	2.19	0.42
1:A:1164:VAL:CG1	1:A:1190:LEU:HB3	2.49	0.42
1:A:1032:ALA:N	1:A:1109:GLU:OE2	2.52	0.42
1:B:2264:GLN:O	1:B:2267:ASN:HB2	2.20	0.42
1:A:1192:GLN:NE2	1:A:1192:GLN:O	2.51	0.42
1:A:1067:PRO:HD3	1:A:1169:GLN:CG	2.45	0.41
1:A:1160:SER:O	1:A:1164:VAL:HG23	2.20	0.41
1:B:2124:ILE:HA	1:B:2130:LEU:HD23	2.02	0.41
1:A:1047:ARG:NE	2:A:2051:HOH:O	2.50	0.41
1:B:2139:GLN:HB2	2:B:3243:HOH:O	2.19	0.41
1:B:2039:ASP:OD1	1:B:2291:LYS:HD3	2.20	0.41
1:A:1298:SER:OG	1:A:1299:THR:N	2.53	0.41
1:A:1223:SER:OG	1:A:1227:VAL:HB	2.21	0.41
1:A:1301:THR:O	1:A:1301:THR:HG22	2.19	0.41
1:B:2193:GLN:O	1:B:2197:HIS:HB2	2.20	0.41
1:A:1126:PRO:HG3	1:B:2211:ARG:HG3	2.00	0.41
1:B:2305:LYS:HE3	2:B:3369:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:GLN:NE2	1:A:1196:ASP:OD2	2.54	0.41
1:B:2065:ARG:HG2	1:B:2065:ARG:NH1	2.36	0.41
1:A:1286:PHE:HD2	2:A:2238:HOH:O	2.02	0.41
1:A:1234:LYS:CD	1:A:1267:ASN:HB3	2.51	0.40
1:B:2191:ILE:O	1:B:2191:ILE:HG22	2.20	0.40
1:B:2238:MET:HB3	1:B:2261:PHE:CE1	2.56	0.40
1:B:2158:PHE:HA	1:B:2158:PHE:HD1	1.75	0.40
1:B:2268:ILE:O	1:B:2272:VAL:HG23	2.22	0.40
1:A:1083:THR:HG23	1:A:1084:VAL:H	1.86	0.40
1:A:1147:TYR:HH	1:A:1215:GLU:CD	2.25	0.40
1:A:1128:PRO:HG3	2:A:2115:HOH:O	2.22	0.40
1:A:1186:LYS:HG2	1:A:1245:ASP:OD1	2.21	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	270/303 (89%)	246 (91%)	18 (7%)	6 (2%)	8	3
1	B	267/303 (88%)	238 (89%)	22 (8%)	7 (3%)	7	2
All	All	537/606 (89%)	484 (90%)	40 (7%)	13 (2%)	7	3

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1121	GLU
1	A	1127	ASP
1	A	1223	SER
1	B	2043	ALA
1	B	2076	ASP
1	B	2126	PRO

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Mol	Chain	Res	Type
1	A	1031	GLY
1	B	2123	GLY
1	A	1178	LYS
1	B	2177	ASP
1	B	2121	GLU
1	B	2044	GLY
1	A	1122	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	223/247 (90%)	199 (89%)	24 (11%)	8	4
1	B	223/247 (90%)	196 (88%)	27 (12%)	6	3
All	All	446/494 (90%)	395 (89%)	51 (11%)	7	4

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1033	ARG
1	A	1040	LEU
1	A	1047	ARG
1	A	1065	ARG
1	A	1083	THR
1	A	1105	ARG
1	A	1116	ASP
1	A	1117	THR
1	A	1125	GLN
1	A	1129	ILE
1	A	1158	PHE
1	A	1164	VAL
1	A	1166	SER
1	A	1173	SER
1	A	1177	ASP
1	A	1181	LYS

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Mol	Chain	Res	Type
1	A	1193	GLN
1	A	1211	ARG
1	A	1218	ASP
1	A	1233	ASP
1	A	1253	ARG
1	A	1264	GLN
1	A	1298	SER
1	A	1301	THR
1	B	2041	ARG
1	B	2047	ARG
1	B	2052	GLN
1	B	2069	ARG
1	B	2071	ASP
1	B	2076	ASP
1	B	2078	ARG
1	B	2114	THR
1	B	2120	ASP
1	B	2121	GLU
1	B	2131	GLN
1	B	2139	GLN
1	B	2154	LEU
1	B	2156	LYS
1	B	2158	PHE
1	B	2165	MET
1	B	2169	GLN
1	B	2178	LYS
1	B	2193	GLN
1	B	2211	ARG
1	B	2224	ASP
1	B	2225	SER
1	B	2239	ARG
1	B	2250	ASP
1	B	2267	ASN
1	B	2282	GLN
1	B	2291	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	1095	HIS
1	A	1125	GLN
1	A	1192	GLN

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Mol	Chain	Res	Type
1	A	1193	GLN
1	A	1267	ASN
1	A	1269	GLN
1	B	2052	GLN
1	B	2101	ASN
1	B	2125	GLN
1	B	2159	GLN
1	B	2169	GLN
1	B	2193	GLN
1	B	2264	GLN
1	B	2267	ASN
1	B	2282	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	272/303 (89%)	0.40	21 (7%) 16 22	15, 40, 91, 137	0
1	B	269/303 (88%)	0.36	20 (7%) 17 24	24, 45, 78, 100	0
All	All	541/606 (89%)	0.38	41 (7%) 17 23	15, 43, 81, 137	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1117	THR	8.5
1	A	1125	GLN	7.9
1	A	1119	GLY	7.7
1	A	1115	LEU	6.4
1	A	1124	ILE	5.8
1	B	2304	ALA	5.4
1	B	2124	ILE	4.7
1	A	1031	GLY	4.6
1	B	2117	THR	4.4
1	B	2123	GLY	4.3
1	B	2119	GLY	4.2
1	A	1301	THR	4.1
1	B	2179	ASN	4.1
1	B	2118	ALA	4.1
1	A	1126	PRO	4.0
1	A	1112	GLY	3.7
1	A	1127	ASP	3.6
1	A	1114	THR	3.6
1	B	2127	ASP	3.6
1	A	1122	GLY	3.4
1	B	2039	ASP	3.3
1	A	1120	ASP	3.3
1	B	2126	PRO	3.2
1	A	1030	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	2125	GLN	2.8
1	B	2303	THR	2.8
1	A	1118	ALA	2.7
1	B	2120	ASP	2.7
1	B	2043	ALA	2.6
1	A	1113	GLY	2.6
1	B	2044	GLY	2.5
1	B	2246	GLY	2.5
1	A	1050	PRO	2.3
1	A	1129	ILE	2.3
1	B	2122	GLY	2.3
1	B	2175	LYS	2.3
1	B	2305	LYS	2.2
1	A	1070	ILE	2.2
1	B	2249	TRP	2.2
1	A	1101	ASN	2.2
1	A	1176	ASP	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.