W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:35 PM GMT

PDB ID	:	1L0W
Title	:	Aspartyl-tRNA synthetase-1 from space-grown crystals
Authors	:	Ng, J.D.; Sauter, C.; Lorber, B.; Kirkland, N.; Arnez, J.; Giege, R.
Deposited on	:	2002-02-14
Resolution	:	2.01 Å(reported)

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)	:	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 (i)

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

The reported resolution of this entry is 2.01 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		17
Ramachandran outliers		1.0%
Sidechain outliers		5.5%
RSRZ outliers		11.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
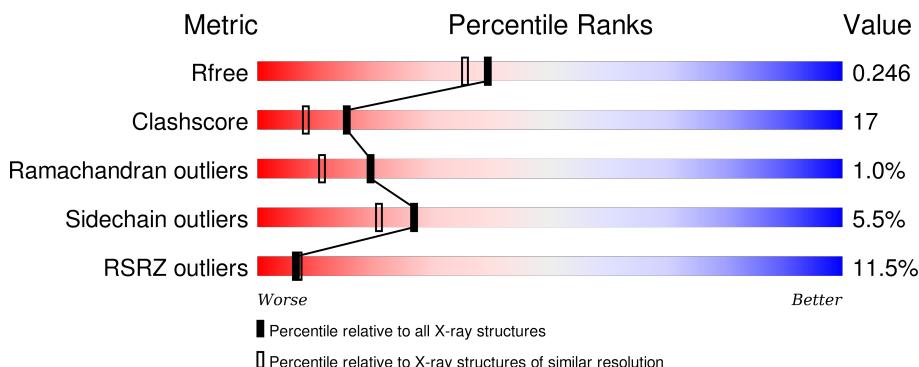
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	580	13% — 68% / 28% / •
1	B	580	10% — 70% / 26% / •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9521 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 Aspartyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	0	0
			4667	2980	840	836	11			
1	B	580	Total	C	N	O	S	0	0	0
			4667	2980	840	836	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	109	Total	O	0	0
			109	109		

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: Aspartyl-tRNA synthetase
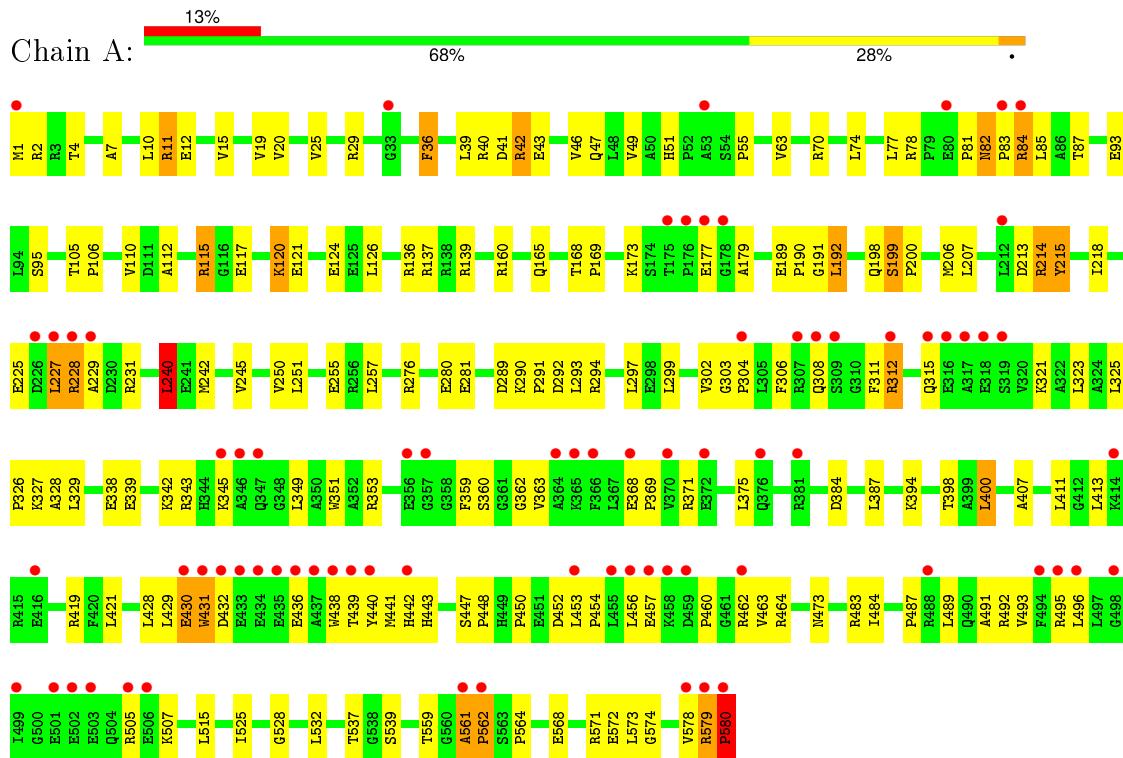
- Molecule 1: Aspartyl-tRNA synthetase
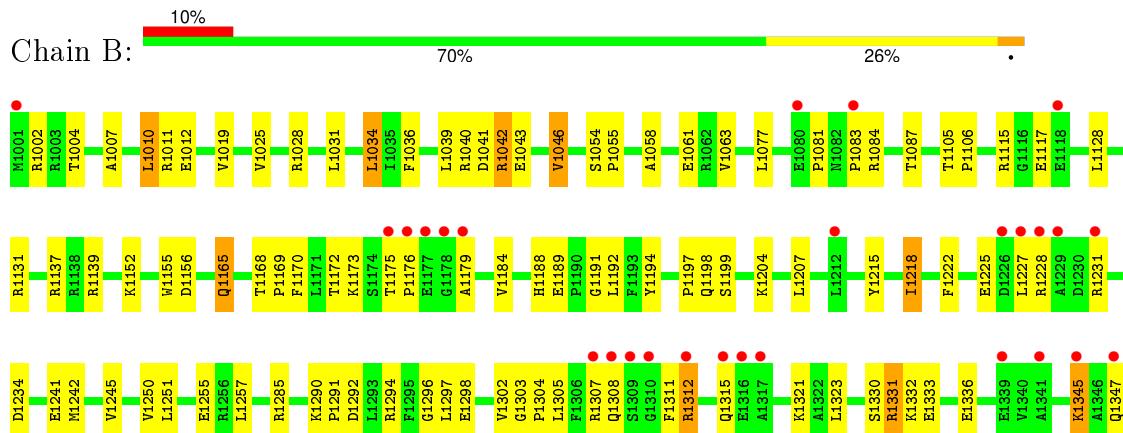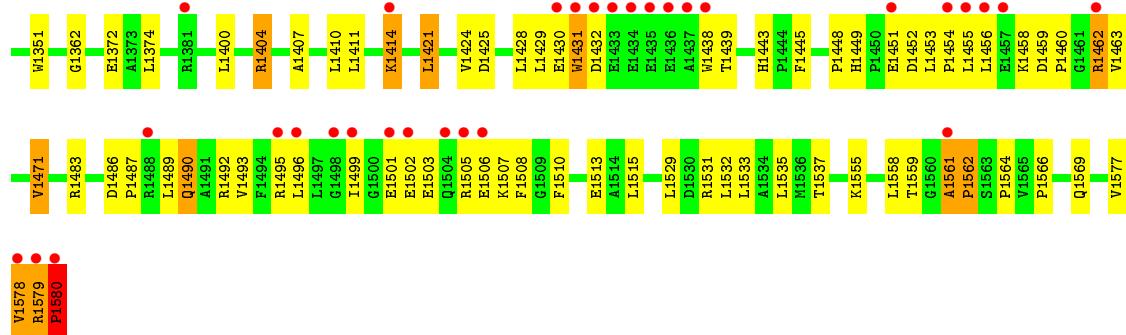
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.02Å 156.10Å 177.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.98 – 2.01 11.97 – 2.01	Depositor EDS
% Data completeness (in resolution range)	70.7 (11.98-2.01) 70.8 (11.97-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.246 0.217 , 0.246	Depositor DCC
R_{free} test set	2437 reflections (2.98%)	DCC
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 74.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 81861 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9521	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.41	0/4779	0.74	9/6467 (0.1%)
1	B	0.43	0/4779	0.79	6/6467 (0.1%)
All	All	0.42	0/9558	0.76	15/12934 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1561	ALA	C-N-CD	-21.54	73.21	120.60
1	B	1561	ALA	C-N-CA	13.73	179.67	122.00
1	A	579	ARG	C-N-CD	-11.48	95.35	120.60
1	A	561	ALA	C-N-CD	-9.71	99.25	120.60
1	A	580	PRO	N-CA-C	7.55	131.74	112.10
1	A	561	ALA	C-N-CA	7.46	153.34	122.00
1	A	580	PRO	CA-N-CD	-6.93	101.80	111.50
1	B	1579	ARG	C-N-CD	-6.62	106.03	120.60
1	B	1404	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	A	218	ILE	N-CA-C	-5.91	95.04	111.00
1	A	580	PRO	CA-CB-CG	-5.52	93.51	104.00
1	B	1580	PRO	CA-CB-CG	-5.50	93.55	104.00
1	B	1218	ILE	N-CA-C	-5.24	96.85	111.00
1	A	240	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	528	GLY	N-CA-C	-5.20	100.10	113.10

There are no chirality outliers.

There are no planarity outliers.

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	4667	0	4679	186	0
1	B	4667	0	4676	167	0
2	A	78	0	0	1	0
2	B	109	0	0	3	0
All	All	9521	0	9355	326	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 17.

All (326) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1307:ARG:HD3	1:B:1315:GLN:HG2	1.27	1.15
1:A:579:ARG:HB3	1:A:580:PRO:HD2	1.31	1.13
1:A:574:GLY:HA3	1:B:1580:PRO:HG3	1.30	1.13
1:A:306:PHE:HB3	1:A:315:GLN:HE22	1.19	1.04
1:A:160:ARG:HH11	1:A:160:ARG:HB3	1.23	1.03
1:B:1428:LEU:HD22	1:B:1448:PRO:HB3	1.47	0.96
1:B:1302:VAL:HG23	1:B:1305:LEU:HD12	1.48	0.95
1:B:1296:GLY:O	1:B:1404:ARG:NH1	1.99	0.95
1:A:574:GLY:CA	1:B:1580:PRO:HG3	1.96	0.94
1:B:1430:GLU:HG2	1:B:1431:TRP:H	1.38	0.88
1:A:120:LYS:HD3	1:A:120:LYS:H	1.36	0.87
1:B:1579:ARG:O	1:B:1580:PRO:HB3	1.75	0.86
1:B:1218:ILE:HG13	1:B:1218:ILE:O	1.74	0.85
1:B:1172:THR:HG22	1:B:1173:LYS:H	1.41	0.84
1:A:2:ARG:NH2	1:B:1245:VAL:HG12	1.93	0.84
1:B:1424:VAL:HG12	1:B:1425:ASP:H	1.43	0.84
1:A:115:ARG:HB2	1:A:115:ARG:HH11	1.42	0.83
1:B:1424:VAL:HG12	1:B:1425:ASP:N	1.94	0.83
1:A:292:ASP:OD1	1:A:294:ARG:HD3	1.80	0.80
1:A:242:MET:HE3	1:A:250:VAL:HG22	1.62	0.79
1:A:179:ALA:HB3	1:A:198:GLN:OE1	1.83	0.79
1:A:579:ARG:CB	1:A:580:PRO:HD2	2.01	0.78
1:A:428:LEU:HD22	1:A:448:PRO:HB3	1.66	0.78
1:A:110:VAL:HG13	1:A:137:ARG:HG2	1.65	0.78
1:B:1297:LEU:HB2	1:B:1404:ARG:NH1	1.99	0.78
1:A:306:PHE:HB3	1:A:315:GLN:NE2	1.99	0.77
1:A:411:LEU:HB2	1:A:413:LEU:HD13	1.67	0.76

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PRO:HD3	1:B:1580:PRO:HD2	1.68	0.76
1:B:1242:MET:CE	1:B:1250:VAL:HG22	2.16	0.76
1:A:84:ARG:HA	1:A:84:ARG:HE	1.50	0.75
1:A:227:LEU:HD12	1:A:231:ARG:CB	2.17	0.74
1:A:173:LYS:HB2	1:B:1561:ALA:HB2	1.70	0.74
1:A:227:LEU:HD12	1:A:231:ARG:HB3	1.69	0.73
1:B:1179:ALA:HB3	1:B:1198:GLN:OE1	1.88	0.73
1:A:120:LYS:HD3	1:A:120:LYS:N	2.03	0.73
1:A:4:THR:OG1	1:A:19:VAL:HG23	1.87	0.73
1:B:1137:ARG:HH22	1:B:1139:ARG:NH2	1.87	0.72
1:A:561:ALA:HB2	1:B:1173:LYS:HB2	1.71	0.72
1:B:1566:PRO:HG2	1:B:1569:GLN:HB2	1.72	0.71
1:B:1297:LEU:HB2	1:B:1404:ARG:HH11	1.54	0.71
1:A:251:LEU:O	1:A:255:GLU:HG3	1.89	0.71
1:B:1307:ARG:HD3	1:B:1315:GLN:CG	2.16	0.71
1:B:1011:ARG:HG3	1:B:1011:ARG:HH11	1.57	0.70
1:A:579:ARG:O	1:A:580:PRO:HB2	1.90	0.70
1:A:306:PHE:CB	1:A:315:GLN:HE22	2.01	0.69
1:B:1455:LEU:HD23	1:B:1458:LYS:HE3	1.72	0.69
1:A:190:PRO:HB3	1:B:1580:PRO:CD	2.23	0.69
1:A:574:GLY:HA3	1:B:1580:PRO:CG	2.18	0.69
1:B:1430:GLU:HG2	1:B:1431:TRP:N	2.08	0.69
1:A:448:PRO:HD2	1:A:484:ILE:HD11	1.73	0.69
1:B:1307:ARG:HB2	1:B:1315:GLN:OE1	1.93	0.69
1:A:160:ARG:NH1	1:A:160:ARG:HB3	2.04	0.68
1:A:55:PRO:HG2	1:A:95:SER:O	1.94	0.68
1:A:572:GLU:O	1:B:1580:PRO:HB2	1.94	0.67
1:B:1449:HIS:ND1	1:B:1451:GLU:HG2	2.09	0.67
1:A:190:PRO:HB3	1:B:1580:PRO:HD3	1.76	0.67
1:B:1242:MET:HE2	1:B:1250:VAL:HG22	1.75	0.67
1:A:432:ASP:HB3	1:A:438:TRP:HA	1.77	0.67
1:B:1155:TRP:CH2	1:B:1165:GLN:HG3	2.30	0.67
1:A:303:GLY:N	1:A:304:PRO:HD2	2.09	0.66
1:B:1225:GLU:HG3	1:B:1227:LEU:HB2	1.77	0.66
1:B:1012:GLU:HG3	1:B:1077:LEU:HD21	1.77	0.66
1:A:110:VAL:O	1:A:110:VAL:HG12	1.95	0.65
1:B:1430:GLU:CG	1:B:1431:TRP:H	2.09	0.65
1:A:110:VAL:HG13	1:A:137:ARG:CG	2.27	0.65
1:A:82:ASN:C	1:A:82:ASN:HD22	2.00	0.64
1:A:487:PRO:HG3	1:A:515:LEU:HB3	1.80	0.64
1:B:1058:ALA:O	1:B:1061:GLU:HG2	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ALA:HA	1:A:115:ARG:NH1	2.13	0.64
1:A:25:VAL:HG21	1:A:63:VAL:HG11	1.80	0.64
1:A:110:VAL:HG11	1:A:136:ARG:HB2	1.79	0.64
1:B:1155:TRP:CZ2	1:B:1165:GLN:HG3	2.31	0.64
1:A:229:ALA:HB3	1:A:231:ARG:NH1	2.13	0.64
1:B:1115:ARG:HB3	1:B:1117:GLU:HG3	1.79	0.64
1:B:1424:VAL:CG1	1:B:1425:ASP:H	2.10	0.64
1:A:447:SER:HA	1:A:484:ILE:HD11	1.79	0.63
1:B:1004:THR:OG1	1:B:1019:VAL:HG23	1.98	0.62
1:B:1292:ASP:OD2	1:B:1294:ARG:HD3	1.99	0.62
1:B:1168:THR:HG23	1:B:1169:PRO:HD2	1.81	0.62
1:A:112:ALA:HA	1:A:115:ARG:HH12	1.65	0.62
1:B:1432:ASP:CB	1:B:1438:TRP:HA	2.30	0.62
1:A:489:LEU:HD23	1:A:489:LEU:O	2.00	0.62
1:B:1449:HIS:CE1	1:B:1451:GLU:HG2	2.35	0.62
1:A:299:LEU:HD22	1:A:400:LEU:HD13	1.81	0.62
1:A:574:GLY:N	1:B:1580:PRO:HG3	2.14	0.61
1:A:456:LEU:O	1:A:496:LEU:HD21	2.00	0.61
1:B:1331:ARG:HH11	1:B:1331:ARG:HG2	1.64	0.61
1:A:228:ARG:H	1:A:228:ARG:HD3	1.64	0.61
1:B:1302:VAL:CG2	1:B:1305:LEU:HD12	2.26	0.61
1:B:1432:ASP:CG	1:B:1438:TRP:HA	2.20	0.61
1:B:1025:VAL:HG21	1:B:1063:VAL:HG11	1.83	0.61
1:B:1231:ARG:HH11	1:B:1531:ARG:HH21	1.48	0.61
1:A:368:GLU:N	1:A:369:PRO:HD2	2.16	0.61
1:A:432:ASP:CB	1:A:438:TRP:HA	2.31	0.60
1:B:1578:VAL:HG12	1:B:1579:ARG:N	2.17	0.60
1:A:505:ARG:O	1:A:505:ARG:HG2	2.01	0.60
1:A:84:ARG:HA	1:A:84:ARG:NE	2.16	0.60
1:A:225:GLU:O	1:A:227:LEU:HD22	2.00	0.60
1:A:562:PRO:HD3	1:B:1194:TYR:CE1	2.37	0.60
1:B:1031:LEU:HD22	1:B:1036:PHE:CE1	2.37	0.59
1:A:4:THR:HG1	1:A:19:VAL:HG23	1.66	0.59
1:B:1489:LEU:O	1:B:1489:LEU:HD23	2.02	0.59
1:A:484:ILE:HD12	1:A:489:LEU:HD22	1.83	0.59
1:B:1137:ARG:HH22	1:B:1139:ARG:HH21	1.49	0.59
1:B:1529:LEU:O	1:B:1533:LEU:HD23	2.02	0.59
1:B:1499:ILE:HG23	1:B:1503:GLU:OE1	2.03	0.59
1:B:1432:ASP:HB3	1:B:1438:TRP:HA	1.84	0.59
1:A:228:ARG:N	1:A:228:ARG:HD3	2.18	0.59
1:A:206:MET:HE1	1:B:1558:LEU:HD11	1.82	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1579:ARG:O	1:B:1580:PRO:CB	2.44	0.58
1:B:1456:LEU:O	1:B:1460:PRO:HG3	2.03	0.58
1:A:343:ARG:HE	1:A:343:ARG:HA	1.68	0.58
1:A:115:ARG:CB	1:A:115:ARG:HH11	2.15	0.58
1:A:25:VAL:HG21	1:A:63:VAL:CG1	2.33	0.58
1:B:1034:LEU:HD12	1:B:1036:PHE:CE1	2.39	0.58
1:B:1336:GLU:OE2	1:B:1410:LEU:HD21	2.04	0.58
1:A:371:ARG:O	1:A:375:LEU:HD13	2.03	0.58
1:A:462:ARG:HG3	1:A:462:ARG:O	2.02	0.58
1:A:7:ALA:O	1:A:46:VAL:HG22	2.04	0.58
1:B:1430:GLU:HB3	1:B:1439:THR:HG23	1.86	0.58
1:B:1007:ALA:HB1	1:B:1046:VAL:HG22	1.86	0.58
1:A:7:ALA:O	1:A:46:VAL:CG2	2.52	0.57
1:A:463:VAL:O	1:A:463:VAL:HG23	2.04	0.57
1:A:173:LYS:HB2	1:B:1559:THR:CG2	2.35	0.57
1:A:7:ALA:HB1	1:A:46:VAL:HG23	1.86	0.57
1:A:579:ARG:O	1:A:580:PRO:CB	2.52	0.57
1:B:1555:LYS:HG2	1:B:1562:PRO:HG3	1.86	0.57
1:A:430:GLU:HG2	1:A:441:MET:HB2	1.86	0.57
1:B:1455:LEU:HD13	1:B:1462:ARG:HE	1.70	0.57
1:A:81:PRO:O	1:A:83:PRO:HD3	2.05	0.57
1:A:173:LYS:HB2	1:B:1559:THR:HG22	1.86	0.56
1:B:1204:LYS:HD2	1:B:1241:GLU:HB2	1.87	0.56
1:B:1007:ALA:O	1:B:1046:VAL:HG13	2.06	0.56
1:B:1251:LEU:O	1:B:1255:GLU:HG3	2.05	0.56
1:B:1225:GLU:HB2	1:B:1227:LEU:HD23	1.88	0.56
1:B:1443:HIS:HE1	1:B:1445:PHE:CD1	2.24	0.56
1:A:29:ARG:HH11	1:A:29:ARG:HG3	1.70	0.55
1:A:12:GLU:HG3	1:A:77:LEU:HD21	1.88	0.55
1:A:339:GLU:O	1:A:343:ARG:HG2	2.06	0.55
1:B:1566:PRO:HG2	1:B:1569:GLN:CB	2.36	0.55
1:A:431:TRP:HD1	1:A:431:TRP:O	1.90	0.54
1:B:1503:GLU:O	1:B:1507:LYS:HG2	2.07	0.54
1:B:1345:LYS:NZ	1:B:1345:LYS:HB2	2.21	0.54
1:A:276:ARG:HG3	1:A:276:ARG:HH11	1.73	0.54
1:A:160:ARG:CB	1:A:160:ARG:HH11	2.08	0.54
1:A:177:GLU:HB2	1:A:507:LYS:NZ	2.23	0.54
1:B:1004:THR:HG1	1:B:1019:VAL:HG23	1.72	0.54
1:A:431:TRP:O	1:A:431:TRP:CD1	2.61	0.54
1:A:537:THR:HG23	1:A:539:SER:OG	2.07	0.54
1:A:2:ARG:HH22	1:B:1245:VAL:HG12	1.69	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1455:LEU:HD13	1:B:1462:ARG:NE	2.23	0.54
1:B:1039:LEU:HD13	1:B:1040:ARG:N	2.23	0.53
1:A:39:LEU:HD13	1:A:40:ARG:N	2.23	0.53
1:A:12:GLU:O	1:A:15:VAL:HG23	2.08	0.53
1:A:349:LEU:HD11	1:A:387:LEU:HD12	1.90	0.53
1:B:1421:LEU:HG	1:B:1471:VAL:HG13	1.90	0.53
1:A:49:VAL:HG13	1:A:93:GLU:HA	1.90	0.53
1:A:227:LEU:HD12	1:A:231:ARG:HB2	1.88	0.53
1:A:359:PHE:CE1	1:A:371:ARG:HG3	2.43	0.53
1:A:439:THR:HG22	1:A:440:TYR:N	2.23	0.53
1:A:189:GLU:HB3	1:A:192:LEU:HD22	1.91	0.53
1:A:430:GLU:HG2	1:A:441:MET:CB	2.39	0.53
1:A:290:LYS:N	1:A:291:PRO:HD3	2.23	0.53
1:B:1507:LYS:HG3	1:B:1508:PHE:CD2	2.44	0.52
1:A:564:PRO:HA	1:B:1191:GLY:O	2.09	0.52
1:B:1152:LYS:HE2	1:B:1156:ASP:OD1	2.08	0.52
1:A:343:ARG:HA	1:A:343:ARG:NE	2.25	0.52
1:A:492:ARG:HA	1:A:495:ARG:HD2	1.92	0.52
1:A:453:LEU:N	1:A:454:PRO:HD2	2.24	0.52
1:A:363:VAL:O	1:A:363:VAL:HG22	2.10	0.52
1:A:559:THR:HG23	1:B:1510:PHE:CE2	2.45	0.51
1:B:1424:VAL:CG1	1:B:1425:ASP:N	2.64	0.51
1:B:1456:LEU:O	1:B:1496:LEU:HD11	2.11	0.51
1:A:10:LEU:HD22	1:A:46:VAL:HG11	1.93	0.51
1:A:492:ARG:HA	1:A:495:ARG:CD	2.39	0.51
1:A:456:LEU:HG	1:A:496:LEU:HD21	1.93	0.51
1:B:1492:ARG:O	1:B:1495:ARG:HB2	2.11	0.51
1:A:191:GLY:O	1:B:1564:PRO:HA	2.10	0.51
1:B:1302:VAL:HG22	1:B:1302:VAL:O	2.10	0.50
1:B:1459:ASP:OD1	1:B:1462:ARG:HD2	2.11	0.50
1:A:227:LEU:CD2	1:A:227:LEU:H	2.25	0.50
1:B:1042:ARG:HD3	1:B:1043:GLU:OE1	2.10	0.50
1:A:568:GLU:N	1:A:568:GLU:OE2	2.44	0.50
1:B:1025:VAL:HG21	1:B:1063:VAL:CG1	2.40	0.50
1:A:110:VAL:HG11	1:A:136:ARG:CB	2.42	0.50
1:B:1081:PRO:O	1:B:1083:PRO:HD3	2.10	0.50
1:B:1218:ILE:HG12	2:B:19:HOH:O	2.12	0.50
1:B:1010:LEU:HD23	1:B:1046:VAL:HG11	1.93	0.50
1:B:1010:LEU:O	1:B:1087:THR:HG22	2.12	0.50
1:B:1189:GLU:HB2	1:B:1192:LEU:HD22	1.94	0.50
1:A:447:SER:HA	1:A:484:ILE:CD1	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:ALA:O	1:B:1046:VAL:CG1	2.60	0.50
1:B:1321:LYS:CB	1:B:1400:LEU:HD12	2.41	0.50
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.77	0.49
1:A:245:VAL:HG12	1:B:1002:ARG:NH2	2.26	0.49
1:B:1332:LYS:HD3	1:B:1332:LYS:O	2.12	0.49
1:B:1537:THR:O	1:B:1537:THR:CG2	2.61	0.49
1:A:190:PRO:CD	1:B:1580:PRO:HD2	2.40	0.49
1:B:1011:ARG:HH11	1:B:1011:ARG:CG	2.20	0.49
1:A:82:ASN:C	1:A:82:ASN:ND2	2.66	0.49
1:A:115:ARG:NH1	1:A:117:GLU:CD	2.67	0.48
1:A:579:ARG:HB2	1:A:579:ARG:NH1	2.28	0.48
1:B:1285:ARG:HD2	1:B:1298:GLU:OE1	2.14	0.48
1:A:227:LEU:HD23	1:A:227:LEU:O	2.14	0.48
1:A:11:ARG:HH21	1:A:87:THR:HG22	1.78	0.48
1:A:120:LYS:H	1:A:120:LYS:CD	2.10	0.48
1:B:1222:PHE:CD2	1:B:1234:ASP:HB3	2.49	0.48
1:B:1290:LYS:N	1:B:1291:PRO:HD3	2.28	0.47
1:B:1297:LEU:HB3	1:B:1323:LEU:HD11	1.95	0.47
1:A:407:ALA:O	1:A:411:LEU:HG	2.14	0.47
1:B:1531:ARG:O	1:B:1535:LEU:HD23	2.14	0.47
1:B:1040:ARG:HG2	1:B:1041:ASP:N	2.29	0.47
1:A:215:TYR:C	1:A:215:TYR:CD2	2.87	0.47
1:A:297:LEU:HB3	1:A:323:LEU:HD11	1.97	0.47
1:A:561:ALA:HB2	1:B:1173:LYS:CB	2.43	0.47
1:B:1225:GLU:CG	1:B:1227:LEU:HD23	2.45	0.47
1:B:1002:ARG:HA	2:B:31:HOH:O	2.13	0.47
1:B:1489:LEU:HD23	1:B:1493:VAL:HG23	1.97	0.47
1:B:1492:ARG:HA	1:B:1495:ARG:HD2	1.96	0.47
1:A:338:GLU:HG2	1:A:342:LYS:HE2	1.97	0.47
1:A:325:LEU:HD12	1:A:329:LEU:HD11	1.95	0.46
1:A:168:THR:HG23	1:A:169:PRO:HD2	1.97	0.46
1:A:49:VAL:HG22	1:A:51:HIS:CD2	2.50	0.46
1:B:1537:THR:O	1:B:1537:THR:HG22	2.14	0.46
1:A:326:PRO:HA	1:A:384:ASP:OD1	2.15	0.46
1:B:1414:LYS:HE3	1:B:1414:LYS:H	1.79	0.46
1:A:438:TRP:CH2	1:A:460:PRO:HG2	2.50	0.46
1:A:302:VAL:C	1:A:304:PRO:HD2	2.35	0.46
1:A:115:ARG:NH1	1:A:115:ARG:HB2	2.22	0.46
1:B:1453:LEU:N	1:B:1454:PRO:HD2	2.30	0.46
1:B:1311:PHE:O	1:B:1312:ARG:C	2.54	0.46
1:A:240:LEU:HD22	1:A:525:ILE:HG22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HG3	1:A:43:GLU:N	2.31	0.46
1:B:1292:ASP:OD2	1:B:1294:ARG:CD	2.64	0.45
1:A:1:MET:SD	1:A:70:ARG:NH1	2.89	0.45
1:A:573:LEU:C	1:B:1580:PRO:HG3	2.36	0.45
1:A:351:TRP:O	1:A:362:GLY:HA3	2.17	0.45
1:B:1011:ARG:NH1	1:B:1011:ARG:CG	2.77	0.45
1:B:1184:VAL:HB	1:B:1194:TYR:HB2	1.99	0.45
1:A:489:LEU:HD23	1:A:489:LEU:C	2.35	0.45
1:A:303:GLY:N	1:A:304:PRO:CD	2.78	0.45
1:A:432:ASP:CG	1:A:438:TRP:HA	2.38	0.45
1:A:311:PHE:O	1:A:312:ARG:C	2.55	0.45
1:A:110:VAL:O	1:A:110:VAL:CG1	2.65	0.45
1:A:83:PRO:O	1:A:84:ARG:HB2	2.17	0.45
1:A:19:VAL:HG22	1:A:20:VAL:N	2.32	0.45
1:A:537:THR:CG2	1:A:539:SER:OG	2.65	0.45
1:A:559:THR:O	1:B:1173:LYS:HD2	2.17	0.44
1:A:190:PRO:HB2	1:B:1577:VAL:CG1	2.48	0.44
1:A:559:THR:HG22	1:B:1173:LYS:HD2	2.00	0.44
1:A:7:ALA:HB2	1:A:39:LEU:HD12	2.00	0.44
1:B:1502:GLU:O	1:B:1506:GLU:HG3	2.17	0.44
1:A:177:GLU:HB2	1:A:507:LYS:HZ2	1.82	0.44
1:B:1421:LEU:HG	1:B:1471:VAL:CG1	2.47	0.44
1:A:492:ARG:O	1:A:495:ARG:HB2	2.17	0.44
1:B:1321:LYS:HB2	1:B:1400:LEU:HD12	1.98	0.44
1:A:2:ARG:HA	2:A:617:HOH:O	2.16	0.44
1:B:1505:ARG:HH11	1:B:1505:ARG:HG2	1.81	0.44
1:B:1330:SER:OG	1:B:1333:GLU:HG3	2.17	0.44
1:A:213:ASP:OD1	1:A:214:ARG:HD3	2.17	0.44
1:A:450:PRO:O	1:A:453:LEU:HB2	2.18	0.44
1:A:429:LEU:HD13	1:A:438:TRP:CB	2.47	0.43
1:B:1486:ASP:HA	1:B:1487:PRO:HD3	1.89	0.43
1:A:84:ARG:C	1:A:85:LEU:HD22	2.37	0.43
1:A:321:LYS:HB2	1:A:400:LEU:HD12	2.00	0.43
1:A:489:LEU:HD23	1:A:493:VAL:HG23	2.00	0.43
1:B:1489:LEU:C	1:B:1489:LEU:HD23	2.39	0.43
1:B:1555:LYS:HG2	1:B:1562:PRO:CG	2.47	0.43
1:B:1168:THR:HG23	1:B:1169:PRO:CD	2.48	0.43
1:A:387:LEU:HD22	1:A:387:LEU:N	2.34	0.43
1:A:229:ALA:HB3	1:A:231:ARG:HH12	1.79	0.43
1:B:1501:GLU:O	1:B:1505:ARG:HG3	2.19	0.43
1:A:173:LYS:CB	1:B:1559:THR:CG2	2.97	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:HG2	1:A:41:ASP:N	2.34	0.43
1:B:1175:THR:HG23	1:B:1176:PRO:HD2	2.00	0.43
1:B:1307:ARG:HD2	1:B:1307:ARG:HA	1.73	0.42
1:B:1172:THR:HG22	1:B:1173:LYS:N	2.21	0.42
1:B:1227:LEU:HB3	1:B:1231:ARG:HB2	2.00	0.42
1:A:189:GLU:CB	1:A:192:LEU:HD22	2.48	0.42
1:A:36:PHE:N	1:A:36:PHE:CD1	2.87	0.42
1:A:227:LEU:HB2	1:A:231:ARG:HB2	2.01	0.42
1:A:457:GLU:OE1	1:A:492:ARG:NH2	2.52	0.42
1:B:1452:ASP:HB3	1:B:1463:VAL:HG13	2.01	0.42
1:B:1002:ARG:HD3	2:B:31:HOH:O	2.19	0.42
1:B:1170:PHE:O	1:B:1197:PRO:HD3	2.19	0.42
1:A:280:GLU:HG3	1:A:281:GLU:N	2.34	0.42
1:A:368:GLU:N	1:A:369:PRO:CD	2.82	0.42
1:B:1042:ARG:CD	1:B:1043:GLU:OE1	2.68	0.42
1:B:1487:PRO:HG3	1:B:1515:LEU:HB3	2.02	0.42
1:A:47:GLN:NE2	1:A:78:ARG:NH2	2.66	0.42
1:B:1028:ARG:NH1	1:B:1061:GLU:O	2.49	0.42
1:A:491:ALA:O	1:A:495:ARG:HG3	2.20	0.42
1:B:1407:ALA:O	1:B:1411:LEU:HG	2.19	0.42
1:B:1296:GLY:C	1:B:1404:ARG:HH12	2.17	0.42
1:A:327:LYS:HG2	1:A:328:ALA:N	2.35	0.42
1:A:137:ARG:HH22	1:A:139:ARG:NH2	2.18	0.41
1:A:7:ALA:CB	1:A:39:LEU:HD12	2.49	0.41
1:B:1105:THR:HA	1:B:1106:PRO:HD3	1.82	0.41
1:A:293:LEU:O	1:A:419:ARG:NH1	2.53	0.41
1:B:1428:LEU:CD2	1:B:1448:PRO:HB3	2.35	0.41
1:A:121:GLU:OE2	1:A:139:ARG:NH2	2.53	0.41
1:B:1456:LEU:HG	1:B:1496:LEU:HD11	2.01	0.41
1:B:1004:THR:OG1	1:B:1019:VAL:CG2	2.66	0.41
1:A:394:LYS:O	1:A:398:THR:HG23	2.20	0.41
1:B:1490:GLN:OE1	1:B:1490:GLN:O	2.38	0.41
1:A:448:PRO:CD	1:A:484:ILE:HD11	2.46	0.41
1:B:1430:GLU:CG	1:B:1431:TRP:N	2.74	0.41
1:A:353:ARG:HB2	1:A:360:SER:OG	2.20	0.41
1:B:1351:TRP:O	1:B:1362:GLY:HA3	2.20	0.41
1:A:487:PRO:HG3	1:A:515:LEU:CB	2.50	0.41
1:B:1429:LEU:HD13	1:B:1438:TRP:HB2	2.03	0.41
1:A:105:THR:HA	1:A:106:PRO:HD3	1.91	0.41
1:B:1347:GLN:HA	1:B:1347:GLN:OE1	2.21	0.41
1:A:289:ASP:C	1:A:291:PRO:HD3	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1188:HIS:O	1:B:1189:GLU:HG3	2.21	0.41
1:B:1303:GLY:N	1:B:1304:PRO:CD	2.84	0.41
1:A:579:ARG:HB2	1:A:579:ARG:CZ	2.50	0.40
1:B:1331:ARG:HH11	1:B:1331:ARG:CG	2.33	0.40
1:A:442:HIS:HB2	1:A:443:HIS:H	1.71	0.40
1:B:1054:SER:HA	1:B:1055:PRO:HD3	1.92	0.40
1:A:443:HIS:HE2	1:A:483:ARG:HH11	1.70	0.40
1:A:39:LEU:C	1:A:39:LEU:HD13	2.42	0.40
1:A:571:ARG:HD2	1:A:571:ARG:HA	1.87	0.40
1:A:294:ARG:HD2	1:A:473:ASN:CG	2.42	0.40
1:B:1189:GLU:CB	1:B:1192:LEU:HD22	2.51	0.40
1:A:199:SER:HA	1:A:200:PRO:HD3	1.89	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	578/580 (100%)	537 (93%)	35 (6%)	6 (1%)	19	11
1	B	578/580 (100%)	538 (93%)	34 (6%)	6 (1%)	19	11
All	All	1156/1160 (100%)	1075 (93%)	69 (6%)	12 (1%)	19	11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	312	ARG
1	B	1084	ARG
1	B	1312	ARG
1	B	1562	PRO
1	A	308	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1308	GLN
1	A	345	LYS
1	A	562	PRO
1	B	1345	LYS
1	B	1578	VAL
1	A	578	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	483/483 (100%)	455 (94%)	28 (6%)	25	19
1	B	483/483 (100%)	458 (95%)	25 (5%)	29	23
All	All	966/966 (100%)	913 (94%)	53 (6%)	27	21

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	36	PHE
1	A	42	ARG
1	A	74	LEU
1	A	82	ASN
1	A	115	ARG
1	A	120	LYS
1	A	124	GLU
1	A	126	LEU
1	A	165	GLN
1	A	192	LEU
1	A	199	SER
1	A	207	LEU
1	A	214	ARG
1	A	215	TYR
1	A	227	LEU
1	A	228	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	240	LEU
1	A	257	LEU
1	A	400	LEU
1	A	421	LEU
1	A	430	GLU
1	A	431	TRP
1	A	436	GLU
1	A	452	ASP
1	A	464	ARG
1	A	532	LEU
1	A	580	PRO
1	B	1010	LEU
1	B	1034	LEU
1	B	1042	ARG
1	B	1046	VAL
1	B	1128	LEU
1	B	1131	ARG
1	B	1165	GLN
1	B	1199	SER
1	B	1207	LEU
1	B	1215	TYR
1	B	1228	ARG
1	B	1257	LEU
1	B	1331	ARG
1	B	1372	GLU
1	B	1374	LEU
1	B	1414	LYS
1	B	1421	LEU
1	B	1431	TRP
1	B	1462	ARG
1	B	1471	VAL
1	B	1483	ARG
1	B	1490	GLN
1	B	1513	GLU
1	B	1532	LEU
1	B	1580	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	82	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	143	ASN
1	A	165	GLN
1	A	201	GLN
1	A	205	GLN
1	A	260	HIS
1	A	315	GLN
1	B	1143	ASN
1	B	1205	GLN
1	B	1376	GLN
1	B	1504	GLN
1	B	1569	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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	580/580 (100%)	0.45	75 (12%)	5	5	15, 38, 91, 139	0
1	B	580/580 (100%)	0.27	58 (10%)	9	10	14, 33, 90, 136	0
All	All	1160/1160 (100%)	0.36	133 (11%)	6	7	14, 35, 91, 139	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	TRP	18.3
1	B	1437	ALA	15.2
1	B	1434	GLU	13.4
1	B	1580	PRO	11.7
1	A	435	GLU	11.3
1	B	1431	TRP	11.2
1	A	580	PRO	11.0
1	B	1433	GLU	10.2
1	A	437	ALA	10.1
1	A	436	GLU	9.1
1	B	1227	LEU	8.8
1	B	1176	PRO	8.7
1	B	1436	GLU	8.4
1	A	178	GLY	8.3
1	A	308	GLN	8.1
1	B	1435	GLU	7.9
1	A	227	LEU	7.4
1	A	307	ARG	7.4
1	B	1228	ARG	7.0
1	A	495	ARG	6.4
1	A	434	GLU	6.3
1	B	1307	ARG	6.3
1	A	316	GLU	6.0
1	A	309	SER	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	433	GLU	6.0
1	B	1432	ASP	5.9
1	A	432	ASP	5.8
1	B	1316	GLU	5.7
1	A	462	ARG	5.3
1	B	1178	GLY	5.3
1	A	312	ARG	5.2
1	A	499	ILE	4.9
1	A	176	PRO	4.9
1	A	84	ARG	4.8
1	A	177	GLU	4.7
1	B	1309	SER	4.7
1	B	1177	GLU	4.7
1	B	1505	ARG	4.7
1	B	1317	ALA	4.6
1	A	579	ARG	4.6
1	A	228	ARG	4.6
1	B	1495	ARG	4.5
1	B	1438	TRP	4.2
1	B	1312	ARG	4.2
1	B	1488	ARG	4.1
1	A	53	ALA	4.1
1	A	345	LYS	4.0
1	B	1315	GLN	3.9
1	A	438	TRP	3.9
1	B	1578	VAL	3.9
1	B	1414	LYS	3.8
1	B	1229	ALA	3.8
1	A	357	GLY	3.8
1	A	365	LYS	3.8
1	B	1504	GLN	3.7
1	B	1083	PRO	3.7
1	A	458	LYS	3.6
1	A	505	ARG	3.6
1	A	372	GLU	3.6
1	A	455	LEU	3.6
1	A	381	ARG	3.6
1	B	1455	LEU	3.5
1	B	1345	LYS	3.5
1	B	1579	ARG	3.5
1	B	1001	MET	3.5
1	A	1	MET	3.4

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1381	ARG	3.4
1	A	315	GLN	3.4
1	B	1080	GLU	3.4
1	A	578	VAL	3.3
1	A	488	ARG	3.2
1	A	356	GLU	3.2
1	A	229	ALA	3.1
1	B	1502	GLU	3.1
1	B	1506	GLU	3.1
1	A	561	ALA	3.1
1	A	304	PRO	3.1
1	A	494	PHE	3.0
1	B	1430	GLU	3.0
1	B	1456	LEU	3.0
1	A	346	ALA	3.0
1	A	414	LYS	3.0
1	A	318	GLU	3.0
1	B	1308	GLN	3.0
1	A	317	ALA	2.9
1	A	80	GLU	2.9
1	A	347	GLN	2.8
1	B	1175	THR	2.8
1	B	1561	ALA	2.8
1	A	502	GLU	2.8
1	A	506	GLU	2.8
1	B	1454	PRO	2.7
1	A	440	TYR	2.7
1	A	439	THR	2.7
1	B	1226	ASP	2.7
1	A	456	LEU	2.7
1	A	562	PRO	2.7
1	A	175	THR	2.6
1	A	83	PRO	2.6
1	A	501	GLU	2.6
1	A	370	VAL	2.6
1	A	366	PHE	2.6
1	A	368	GLU	2.6
1	B	1451	GLU	2.6
1	B	1501	GLU	2.5
1	A	430	GLU	2.5
1	B	1118	GLU	2.5
1	B	1462	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1499	ILE	2.5
1	A	442	HIS	2.4
1	A	226	ASP	2.4
1	A	416	GLU	2.4
1	A	503	GLU	2.3
1	B	1231	ARG	2.3
1	B	1347	GLN	2.3
1	B	1310	GLY	2.3
1	B	1498	GLY	2.3
1	A	457	GLU	2.3
1	A	376	GLN	2.2
1	B	1179	ALA	2.2
1	A	498	GLY	2.1
1	B	1212	LEU	2.1
1	B	1457	GLU	2.1
1	A	33	GLY	2.1
1	A	453	LEU	2.1
1	B	1339	GLU	2.1
1	A	319	SER	2.1
1	A	459	ASP	2.1
1	A	212	LEU	2.1
1	A	496	LEU	2.0
1	B	1496	LEU	2.0
1	A	364	ALA	2.0
1	B	1341	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.