W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Jul 5, 2016 – 12:35 PM EDT

PDB ID	:	5DXF
Title	:	Structure of Candida albicans trehalose-6-phosphate phosphatase N-terminal domain
Authors	:	Miao, Y.; Brennan, R.G.
Deposited on	:	2015-09-23
Resolution	:	2.56 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
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)	:	rb-20027790

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 2.56 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		0.315
Clashscore		18
Ramachandran outliers		0.9%
Sidechain outliers		6.0%
RSRZ outliers		14.4%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
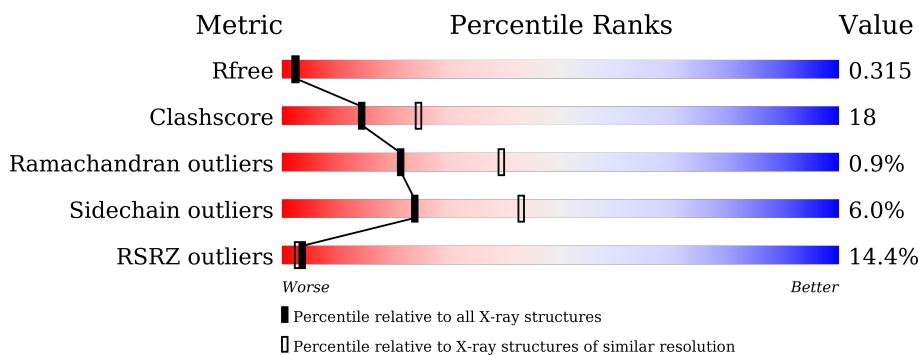
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

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	534	17% / 56% / 27% / • / 14%
1	B	534	8% / 65% / 19% / • / 12%
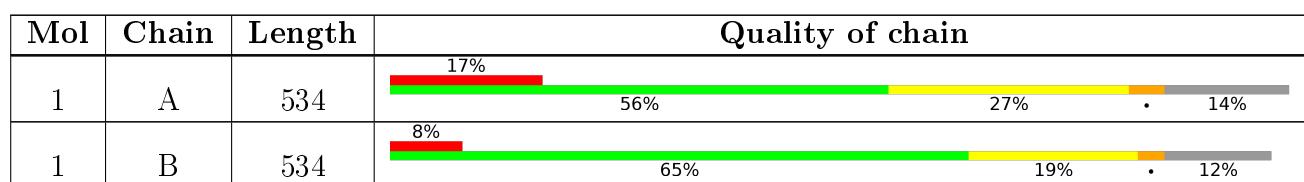
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7549 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 trehalose-6-phosphate phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total 3687	C 2366	N 620	O 686	S 15	0	0	0
1	B	468	Total 3764	C 2414	N 636	O 699	S 15	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	27	Total 27	O 27	0	0
2	B	71	Total 71	O 71	0	0

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: trehalose-6-phosphate phosphatase
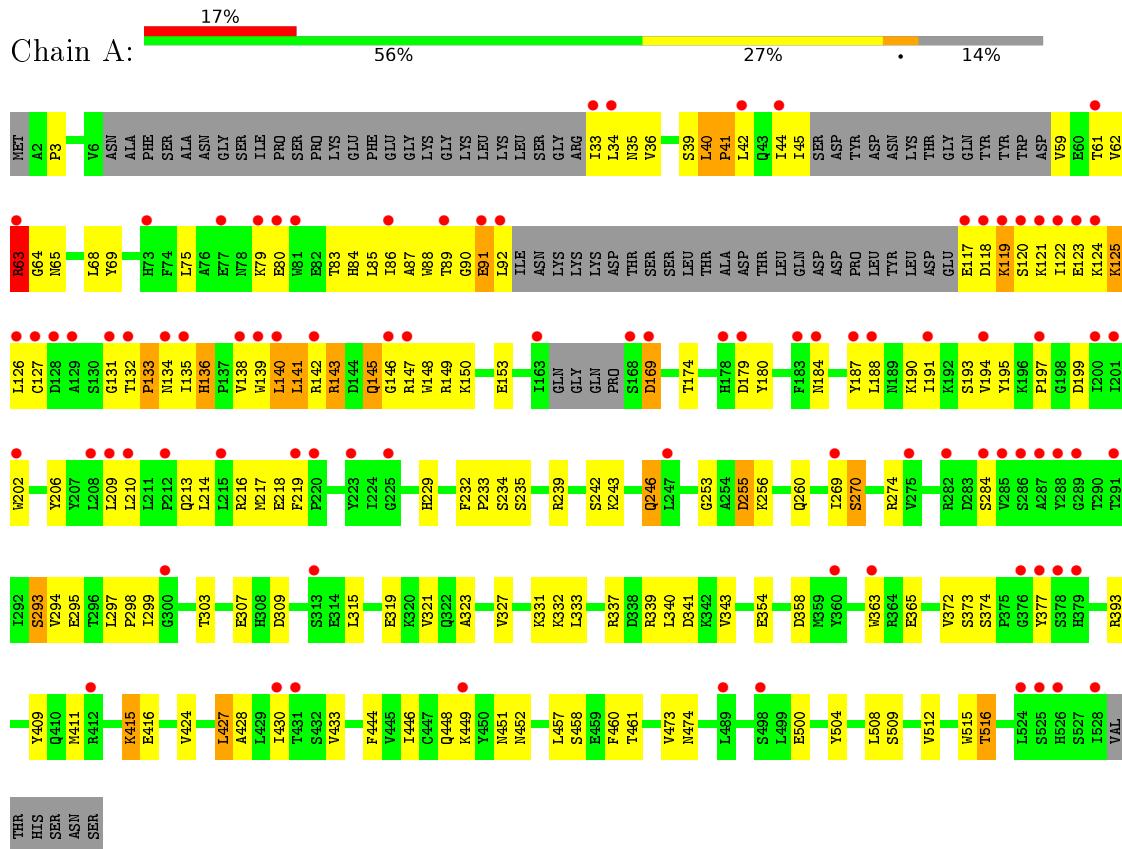
- Molecule 1: trehalose-6-phosphate phosphatase
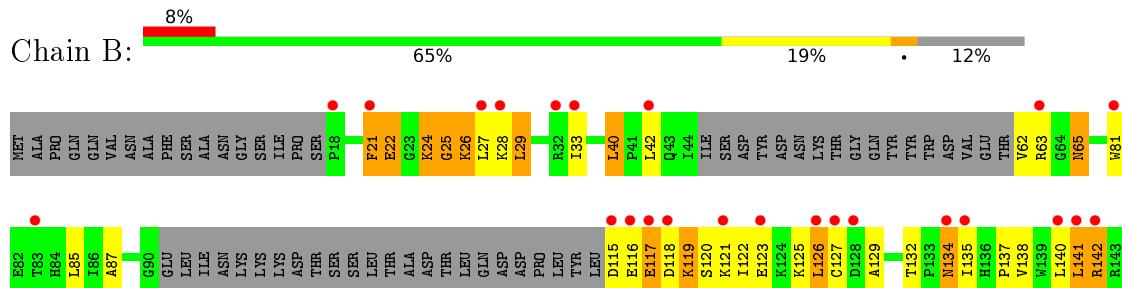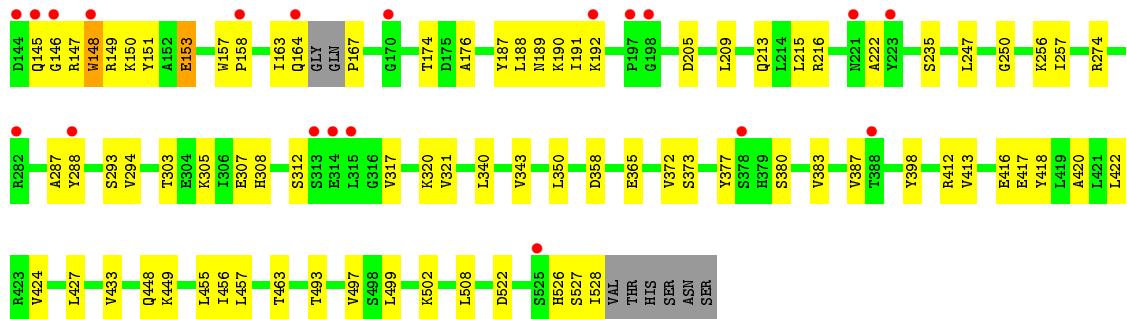
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.31Å 98.31Å 452.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.87 – 2.56 49.16 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.87-2.56) 93.8 (49.16-2.56)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.66 (at 2.58Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.266 , 0.298 0.279 , 0.315	Depositor DCC
R_{free} test set	1921 reflections (4.76%)	DCC
Wilson B-factor (Å^2)	49.2	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.8	EDS
L-test for twinning[2]	$<|L|>$ = 0.47, $<L^2>$ = 0.30	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7549	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.43	3/3766 (0.1%)	0.57	5/5102 (0.1%)
1	B	0.29	0/3847	0.52	2/5204 (0.0%)
All	All	0.37	3/7613 (0.0%)	0.54	7/10306 (0.1%)

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	2
1	B	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	PRO	N-CD	5.33	1.55	1.47
1	A	41	PRO	N-CD	5.13	1.55	1.47
1	A	298	PRO	N-CD	5.08	1.54	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	25	GLY	N-CA-C	5.96	127.99	113.10
1	A	136	HIS	C-N-CD	5.91	140.80	128.40
1	A	3	PRO	N-CA-CB	5.84	110.31	103.30
1	A	297	LEU	C-N-CD	5.76	140.50	128.40
1	A	40	LEU	C-N-CD	5.56	140.07	128.40
1	A	232	PHE	C-N-CD	5.46	139.87	128.40
1	B	63	ARG	NE-CZ-NH1	5.23	122.92	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	CYS	Peptide
1	A	63	ARG	Peptide
1	B	24	LYS	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	3687	0	3675	181	0
1	B	3764	0	3770	88	0
2	A	27	0	0	3	0
2	B	71	0	0	1	0
All	All	7549	0	7445	269	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 18.

All (269) 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:256:LYS:NZ	1:A:295:GLU:OE2	1.74	1.21
1:A:147:ARG:CG	1:A:179:ASP:OD2	1.88	1.20
1:B:122:ILE:O	1:B:126:LEU:HD21	1.40	1.19
1:A:62:VAL:O	1:A:64:GLY:N	1.82	1.12
1:A:44:ILE:HB	1:A:91:GLU:HG3	1.24	1.07
1:A:40:LEU:HD12	1:A:87:ALA:HB3	1.26	1.07
1:B:126:LEU:H	1:B:126:LEU:HD23	1.19	1.06
1:A:61:THR:CG2	1:A:63:ARG:HB2	1.88	1.04
1:A:147:ARG:HG3	1:A:179:ASP:OD2	1.55	1.02
1:A:134:ASN:O	1:A:136:HIS:CD2	2.15	0.98
1:A:415:LYS:H	1:A:415:LYS:HD2	1.28	0.97
1:B:118:ASP:HA	1:B:121:LYS:HG2	1.48	0.95
1:A:213:GLN:HE21	1:A:217:MET:HG2	1.32	0.94
1:A:142:ARG:HH22	1:A:143:ARG:HH21	1.15	0.93
1:A:85:LEU:HB3	1:A:135:ILE:HG23	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD12	1:A:87:ALA:CB	1.98	0.92
1:A:142:ARG:HH11	1:A:142:ARG:HG3	1.35	0.90
1:A:44:ILE:CB	1:A:91:GLU:HG3	2.02	0.90
1:B:40:LEU:HD13	1:B:87:ALA:HB3	1.55	0.89
1:A:40:LEU:CD1	1:A:87:ALA:HB3	2.02	0.89
1:B:122:ILE:O	1:B:126:LEU:CD2	2.22	0.88
1:B:42:LEU:HD12	1:B:62:VAL:HG11	1.54	0.88
1:B:116:GLU:HA	1:B:121:LYS:HE2	1.56	0.85
1:A:246:GLN:OE1	1:A:246:GLN:N	2.08	0.85
1:B:21:PHE:HD1	1:B:81:TRP:CD1	1.94	0.84
1:A:86:ILE:HD13	1:A:191:ILE:HG12	1.59	0.83
1:B:120:SER:HA	1:B:123:GLU:HG2	1.60	0.83
1:B:85:LEU:HB3	1:B:135:ILE:HG22	1.61	0.83
1:A:142:ARG:HG2	1:A:143:ARG:N	1.95	0.81
1:A:149:ARG:HG3	1:A:149:ARG:HH11	1.44	0.81
1:A:147:ARG:CD	1:A:179:ASP:OD2	2.28	0.81
1:A:44:ILE:HB	1:A:91:GLU:CG	2.07	0.80
1:A:62:VAL:C	1:A:64:GLY:H	1.86	0.79
1:A:125:LYS:NZ	1:A:125:LYS:HB2	1.98	0.79
1:A:415:LYS:CD	1:A:415:LYS:H	1.94	0.79
1:A:147:ARG:HG2	1:A:179:ASP:OD2	1.83	0.78
1:A:235:SER:OG	1:A:274:ARG:NH1	2.15	0.78
1:A:120:SER:HA	1:A:123:GLU:HG3	1.66	0.78
1:A:136:HIS:HD1	1:A:194:VAL:HG21	1.49	0.78
1:A:61:THR:HG22	1:A:63:ARG:HB2	1.65	0.77
1:A:187:TYR:O	1:A:191:ILE:HG13	1.86	0.76
1:A:512:VAL:O	1:A:516:THR:HG22	1.85	0.76
1:B:146:GLY:O	1:B:150:LYS:N	2.16	0.75
1:A:452:ASN:HA	1:A:500:GLU:HG3	1.67	0.75
1:A:41:PRO:O	1:A:61:THR:HB	1.88	0.74
1:B:21:PHE:CD1	1:B:81:TRP:CD1	2.75	0.74
1:A:141:LEU:N	1:A:141:LEU:HD23	2.03	0.73
1:A:147:ARG:HG3	1:A:179:ASP:CG	2.10	0.72
1:B:358:ASP:OD1	1:B:398:TYR:OH	2.08	0.72
1:A:169:ASP:OD1	1:A:169:ASP:N	2.23	0.71
1:A:141:LEU:HD23	1:A:141:LEU:H	1.53	0.71
1:A:142:ARG:NH1	1:A:142:ARG:HG3	1.97	0.71
1:B:149:ARG:NH1	1:B:377:TYR:OH	2.24	0.71
1:A:33:ILE:C	1:A:34:LEU:HD23	2.12	0.70
1:A:145:GLN:O	1:A:147:ARG:N	2.26	0.69
1:A:142:ARG:HH12	1:A:143:ARG:NH2	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HB2	1:A:89:THR:HG22	1.73	0.68
1:A:122:ILE:HA	1:A:125:LYS:HG2	1.74	0.68
1:A:136:HIS:ND1	1:A:194:VAL:HG21	2.09	0.68
1:A:36:VAL:HG23	1:A:202:TRP:O	1.96	0.66
1:B:158:PRO:HB3	1:B:163:ILE:HB	1.78	0.65
1:B:126:LEU:CD2	1:B:126:LEU:H	1.93	0.65
1:A:415:LYS:N	1:A:415:LYS:HD2	2.09	0.65
1:A:339:ARG:HG2	1:A:374:SER:HB2	1.79	0.64
1:A:134:ASN:O	1:A:136:HIS:HD2	1.75	0.64
1:A:218:GLU:C	1:A:219:PHE:HD1	2.01	0.64
1:A:65:ASN:HB2	1:A:69:TYR:CE2	2.33	0.63
1:A:84:HIS:HD2	1:A:136:HIS:NE2	1.97	0.63
1:B:321:VAL:HG13	1:B:424:VAL:HG22	1.81	0.62
1:A:61:THR:HG23	1:A:63:ARG:HB2	1.75	0.62
1:A:147:ARG:HD2	1:A:179:ASP:OD2	1.99	0.62
1:A:303:THR:HG23	1:A:446:ILE:HD11	1.82	0.62
1:B:118:ASP:O	1:B:121:LYS:HB2	1.98	0.62
1:A:40:LEU:HB2	1:A:89:THR:CG2	2.28	0.62
1:A:134:ASN:O	1:A:136:HIS:NE2	2.33	0.62
1:A:512:VAL:O	1:A:516:THR:CG2	2.49	0.61
1:A:195:TYR:CE1	1:A:199:ASP:HB2	2.36	0.61
1:A:303:THR:HG23	1:A:446:ILE:CD1	2.31	0.61
1:A:142:ARG:HH22	1:A:143:ARG:NH2	1.91	0.60
1:A:331:LYS:NZ	1:A:365:GLU:O	2.33	0.60
1:B:118:ASP:HA	1:B:121:LYS:CG	2.28	0.60
1:A:427:LEU:HD22	1:A:428:ALA:N	2.16	0.60
1:A:117:GLU:O	1:A:120:SER:HB2	2.02	0.60
1:A:122:ILE:HG23	1:A:125:LYS:HG2	1.84	0.59
1:A:243:LYS:HB3	1:A:246:GLN:HG2	1.84	0.59
1:A:45:ILE:O	1:A:45:ILE:HG22	2.02	0.59
1:B:320:LYS:HE2	1:B:417:GLU:HG3	1.84	0.59
1:A:44:ILE:O	1:A:44:ILE:HG22	2.02	0.59
1:A:142:ARG:NH2	1:A:143:ARG:HH21	1.94	0.59
1:A:321:VAL:HG13	1:A:424:VAL:HG22	1.85	0.58
1:A:451:ASN:ND2	2:A:607:HOH:O	2.35	0.58
1:A:61:THR:HG22	1:A:63:ARG:H	1.68	0.58
1:A:243:LYS:O	1:A:246:GLN:HG2	2.03	0.58
1:B:65:ASN:N	1:B:65:ASN:OD1	2.37	0.58
1:A:88:TRP:CZ2	1:A:90:GLY:HA3	2.39	0.58
1:B:164:GLN:HG2	1:B:167:PRO:HG3	1.84	0.58
1:A:149:ARG:HH11	1:A:149:ARG:CG	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ALA:O	1:A:138:VAL:HG23	2.04	0.58
1:A:136:HIS:CD2	1:A:136:HIS:N	2.72	0.58
1:A:34:LEU:HD22	1:A:84:HIS:HB2	1.85	0.57
1:A:180:TYR:OH	1:A:206:TYR:O	2.20	0.57
1:A:39:SER:HA	1:A:88:TRP:O	2.04	0.57
1:B:151:TYR:HB2	1:B:176:ALA:HB1	1.87	0.56
1:A:68:LEU:HD13	1:A:229:HIS:CE1	2.40	0.56
1:B:26:LYS:HG2	1:B:27:LEU:HG	1.86	0.56
1:B:380:SER:O	1:B:383:VAL:HB	2.06	0.56
1:A:255:ASP:OD2	1:A:255:ASP:N	2.38	0.56
1:A:140:LEU:HD23	1:A:148:TRP:CD2	2.41	0.56
1:A:147:ARG:HA	1:A:150:LYS:HG3	1.88	0.56
1:B:21:PHE:HD1	1:B:81:TRP:HD1	1.51	0.56
1:B:132:THR:HG21	1:B:135:ILE:HG23	1.87	0.56
1:A:132:THR:N	1:A:133:PRO:HA	2.21	0.55
1:A:332:LYS:HG3	1:A:363:TRP:HZ3	1.71	0.55
1:B:141:LEU:O	1:B:142:ARG:CB	2.54	0.55
1:A:142:ARG:NH2	1:A:143:ARG:HE	2.04	0.55
1:A:216:ARG:O	1:A:219:PHE:O	2.25	0.55
1:A:92:LEU:HD23	1:A:92:LEU:C	2.26	0.55
1:A:145:GLN:C	1:A:147:ARG:H	2.09	0.55
1:A:125:LYS:HZ2	1:A:125:LYS:HB2	1.70	0.55
1:A:354:GLU:OE1	1:A:393:ARG:NH1	2.41	0.54
1:A:44:ILE:CG2	1:A:91:GLU:HG3	2.37	0.54
1:B:502:LYS:NZ	2:B:605:HOH:O	2.41	0.54
1:B:120:SER:HA	1:B:123:GLU:CG	2.36	0.54
1:A:117:GLU:O	1:A:120:SER:N	2.37	0.54
1:B:40:LEU:CD1	1:B:87:ALA:HB3	2.34	0.54
1:A:149:ARG:HG3	1:A:149:ARG:NH1	2.19	0.54
1:A:44:ILE:HA	1:A:45:ILE:HD12	1.89	0.54
1:B:457:LEU:HD21	1:B:463:THR:HG23	1.89	0.54
1:B:412:ARG:NH1	1:B:413:VAL:O	2.42	0.53
1:A:218:GLU:HG3	1:A:219:PHE:CE1	2.43	0.53
1:B:256:LYS:HE2	1:B:522:ASP:HB3	1.90	0.53
1:B:118:ASP:O	1:B:122:ILE:HD12	2.07	0.53
1:A:140:LEU:HB3	1:A:148:TRP:CZ2	2.44	0.53
1:B:21:PHE:CD1	1:B:81:TRP:HD1	2.24	0.52
1:B:216:ARG:NH2	1:B:222:ALA:O	2.43	0.52
1:B:141:LEU:O	1:B:142:ARG:HB3	2.10	0.52
1:A:147:ARG:CG	1:A:179:ASP:CG	2.72	0.52
1:A:427:LEU:CD2	1:A:428:ALA:N	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PHE:CD1	1:A:219:PHE:N	2.77	0.52
1:B:213:GLN:HB2	1:B:250:GLY:HA2	1.91	0.51
1:A:141:LEU:H	1:A:141:LEU:CD2	2.16	0.51
1:A:75:LEU:HB3	1:A:83:THR:OG1	2.11	0.51
1:B:188:LEU:HD12	1:B:215:LEU:HD23	1.92	0.51
1:A:343:VAL:O	1:A:433:VAL:N	2.42	0.51
1:A:430:ILE:HB	1:A:457:LEU:HD12	1.93	0.51
1:A:145:GLN:C	1:A:147:ARG:N	2.62	0.51
1:B:140:LEU:HB3	1:B:148:TRP:CZ2	2.45	0.51
1:A:123:GLU:O	1:A:126:LEU:HB3	2.11	0.50
1:A:33:ILE:O	1:A:34:LEU:HD23	2.11	0.50
1:A:34:LEU:HD23	1:A:34:LEU:N	2.26	0.50
1:A:427:LEU:CD2	1:A:428:ALA:H	2.25	0.50
1:A:149:ARG:NH1	1:A:149:ARG:CG	2.74	0.50
1:B:129:ALA:HB1	1:B:134:ASN:OD1	2.11	0.50
1:B:125:LYS:HD3	1:B:137:PRO:HD2	1.94	0.50
1:B:153:GLU:O	1:B:157:TRP:HB3	2.12	0.49
1:B:493:THR:O	1:B:497:VAL:HG12	2.12	0.49
1:A:88:TRP:CZ2	1:A:90:GLY:CA	2.96	0.49
1:A:218:GLU:O	1:A:219:PHE:HD1	1.94	0.49
1:B:21:PHE:CD2	1:B:21:PHE:N	2.73	0.49
1:B:117:GLU:OE1	1:B:117:GLU:N	2.46	0.48
1:B:420:ALA:O	1:B:424:VAL:HG23	2.13	0.48
1:B:116:GLU:HG2	1:B:141:LEU:HD11	1.95	0.48
1:A:120:SER:HA	1:A:123:GLU:CG	2.40	0.48
1:A:337:ARG:NH2	2:A:610:HOH:O	2.47	0.48
1:A:119:LYS:HD3	1:A:122:ILE:HD12	1.94	0.48
1:A:142:ARG:NH1	1:A:143:ARG:NH2	2.60	0.48
1:A:256:LYS:HD3	1:A:293:SER:HB3	1.96	0.48
1:A:427:LEU:HD22	1:A:428:ALA:O	2.13	0.48
1:A:309:ASP:HA	1:A:315:LEU:HD12	1.96	0.48
1:A:65:ASN:HB2	1:A:69:TYR:CZ	2.49	0.48
1:B:427:LEU:HD11	1:B:456:ILE:HG13	1.96	0.48
1:A:125:LYS:NZ	1:A:125:LYS:CB	2.73	0.47
1:B:307:GLU:OE1	1:B:449:LYS:NZ	2.42	0.47
1:A:218:GLU:HA	1:A:218:GLU:OE2	2.13	0.47
1:B:189:ASN:HA	1:B:192:LYS:HE2	1.96	0.47
1:B:209:LEU:HD12	1:B:247:LEU:HD22	1.96	0.47
1:B:138:VAL:HG22	1:B:190:LYS:HG3	1.97	0.47
1:B:422:LEU:O	1:B:448:GLN:NE2	2.48	0.47
1:A:139:TRP:C	1:A:140:LEU:HD13	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ILE:HB	1:B:294:VAL:HG12	1.96	0.47
1:A:229:HIS:HA	1:A:260:GLN:HE21	1.80	0.47
1:B:122:ILE:HG22	1:B:122:ILE:O	2.16	0.46
1:A:142:ARG:HH11	1:A:142:ARG:CG	2.15	0.46
1:A:184:ASN:OD1	1:A:210:LEU:HB2	2.15	0.46
1:A:142:ARG:CG	1:A:143:ARG:N	2.73	0.46
1:B:118:ASP:CA	1:B:121:LYS:HG2	2.32	0.46
1:A:119:LYS:O	1:A:122:ILE:HB	2.16	0.46
1:B:119:LYS:HA	1:B:119:LYS:HD3	1.56	0.46
1:B:343:VAL:O	1:B:433:VAL:N	2.42	0.46
1:B:365:GLU:OE1	1:B:365:GLU:N	2.48	0.46
1:A:139:TRP:N	1:A:139:TRP:CD1	2.85	0.46
1:A:88:TRP:CG	1:A:89:THR:N	2.84	0.46
1:A:188:LEU:HD22	1:A:214:LEU:HB3	1.98	0.45
1:A:145:GLN:HG2	1:A:145:GLN:H	1.46	0.45
1:A:61:THR:HG22	1:A:63:ARG:CB	2.41	0.45
1:B:340:LEU:HG	1:B:373:SER:HB3	1.97	0.45
1:A:428:ALA:HB2	1:A:444:PHE:CE1	2.50	0.45
1:A:235:SER:O	1:A:239:ARG:HG3	2.17	0.45
1:A:340:LEU:HG	1:A:373:SER:HB2	1.98	0.45
1:A:142:ARG:NH2	1:A:143:ARG:NH2	2.60	0.45
1:A:218:GLU:C	1:A:219:PHE:CD1	2.85	0.45
1:B:416:GLU:H	1:B:416:GLU:CD	2.20	0.45
1:A:92:LEU:CD2	1:A:92:LEU:C	2.86	0.45
1:B:146:GLY:O	1:B:149:ARG:HB2	2.17	0.45
1:A:125:LYS:HZ3	1:A:125:LYS:HB2	1.75	0.45
1:A:140:LEU:HD13	1:A:140:LEU:N	2.33	0.45
1:A:269:ILE:HD11	1:A:294:VAL:HG21	1.99	0.44
1:B:412:ARG:CZ	1:B:413:VAL:O	2.65	0.44
1:A:458:SER:O	1:A:461:THR:HG22	2.16	0.44
1:B:418:TYR:CZ	1:B:422:LEU:HD11	2.52	0.44
1:A:307:GLU:OE1	1:A:449:LYS:NZ	2.35	0.44
1:A:195:TYR:CE2	1:A:197:PRO:HA	2.52	0.44
1:B:126:LEU:HG	1:B:127:CYS:H	1.82	0.44
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.53	0.44
1:B:235:SER:OG	1:B:274:ARG:NH1	2.49	0.44
1:A:299:ILE:HA	1:A:515:TRP:CD1	2.53	0.44
1:B:287:ALA:O	1:B:288:TYR:HB2	2.18	0.44
1:B:455:LEU:HD21	1:B:457:LEU:HD13	1.99	0.44
1:A:246:GLN:H	1:A:246:GLN:CD	2.06	0.43
1:A:323:ALA:O	1:A:327:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ASP:O	1:A:121:LYS:HE2	2.18	0.43
1:A:140:LEU:CD1	1:A:140:LEU:N	2.82	0.43
1:A:120:SER:O	1:A:123:GLU:HB2	2.18	0.43
1:B:527:SER:O	1:B:528:ILE:HG13	2.18	0.43
1:A:409:TYR:OH	2:A:601:HOH:O	2.20	0.43
1:A:125:LYS:HG3	1:A:126:LEU:N	2.32	0.43
1:A:416:GLU:CD	1:A:416:GLU:H	2.22	0.43
1:A:190:LYS:O	1:A:193:SER:HB3	2.19	0.43
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.77	0.42
1:B:157:TRP:HB3	1:B:158:PRO:HD3	2.00	0.42
1:B:29:LEU:HA	1:B:29:LEU:HD12	1.83	0.42
1:B:308:HIS:O	1:B:312:SER:HB2	2.19	0.42
1:A:216:ARG:NE	1:A:253:GLY:O	2.46	0.42
1:B:119:LYS:HD3	1:B:122:ILE:HD13	2.02	0.42
1:B:187:TYR:O	1:B:191:ILE:HG12	2.20	0.42
1:A:62:VAL:C	1:A:64:GLY:N	2.51	0.42
1:A:65:ASN:O	1:A:69:TYR:N	2.43	0.42
1:B:350:LEU:HD11	1:B:387:VAL:HG13	2.02	0.42
1:A:61:THR:HG22	1:A:63:ARG:N	2.34	0.42
1:A:139:TRP:O	1:A:140:LEU:HD12	2.20	0.41
1:A:206:TYR:HA	1:A:209:LEU:HG	2.01	0.41
1:A:216:ARG:HA	1:A:219:PHE:O	2.20	0.41
1:B:33:ILE:HG13	1:B:81:TRP:HB3	2.02	0.41
1:A:340:LEU:HA	1:A:340:LEU:HD23	1.80	0.41
1:B:293:SER:HB2	1:B:526:HIS:CD2	2.56	0.41
1:A:256:LYS:NZ	1:A:295:GLU:CD	2.63	0.41
1:A:448:GLN:OE1	1:A:451:ASN:HB3	2.20	0.41
1:B:116:GLU:HA	1:B:121:LYS:CE	2.39	0.41
1:B:150:LYS:HD3	1:B:150:LYS:HA	1.84	0.41
1:A:35:ASN:O	1:A:85:LEU:HD12	2.20	0.41
1:B:115:ASP:O	1:B:116:GLU:HB2	2.21	0.41
1:B:22:GLU:OE1	1:B:24:LYS:NZ	2.51	0.41
1:B:303:THR:HG21	1:B:508:LEU:HG	2.02	0.41
1:A:270:SER:O	1:A:274:ARG:HG3	2.21	0.41
1:A:86:ILE:HA	1:A:136:HIS:O	2.21	0.41
1:A:88:TRP:CH2	1:A:90:GLY:HA3	2.55	0.41
1:B:118:ASP:O	1:B:121:LYS:CB	2.68	0.41
1:A:139:TRP:C	1:A:140:LEU:CD1	2.89	0.40
1:A:142:ARG:NH1	1:A:143:ARG:CZ	2.83	0.40
1:A:142:ARG:NH2	1:A:143:ARG:NE	2.69	0.40
1:A:124:LYS:HA	1:A:124:LYS:HD3	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LYS:CD	1:A:415:LYS:N	2.73	0.40
1:A:44:ILE:O	1:A:45:ILE:C	2.59	0.40
1:A:460:PHE:HE2	1:A:474:ASN:OD1	2.04	0.40
1:A:149:ARG:O	1:A:153:GLU:HG2	2.21	0.40
1:A:149:ARG:HD3	1:A:377:TYR:HE2	1.86	0.40
1:B:499:LEU:HA	1:B:502:LYS:HE2	2.02	0.40
1:B:305:LYS:HE3	1:B:305:LYS:HB3	1.63	0.40
1:B:163:ILE:HD11	1:B:343:VAL:HG13	2.03	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	450/534 (84%)	427 (95%)	19 (4%)	4 (1%)	21	39
1	B	460/534 (86%)	434 (94%)	22 (5%)	4 (1%)	21	39
All	All	910/1068 (85%)	861 (95%)	41 (4%)	8 (1%)	21	39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	133	PRO
1	B	147	ARG
1	A	146	GLY
1	B	142	ARG
1	B	153	GLU
1	A	131	GLY
1	B	25	GLY

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	409/478 (86%)	377 (92%)	32 (8%)	16	28
1	B	419/478 (88%)	401 (96%)	18 (4%)	35	60
All	All	828/956 (87%)	778 (94%)	50 (6%)	24	43

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	59	VAL
1	A	63	ARG
1	A	79	LYS
1	A	80	GLU
1	A	91	GLU
1	A	119	LYS
1	A	125	LYS
1	A	140	LEU
1	A	141	LEU
1	A	143	ARG
1	A	145	GLN
1	A	169	ASP
1	A	174	THR
1	A	234	SER
1	A	242	SER
1	A	246	GLN
1	A	255	ASP
1	A	270	SER
1	A	284	SER
1	A	293	SER
1	A	319	GLU
1	A	333	LEU
1	A	341	ASP
1	A	358	ASP
1	A	372	VAL
1	A	411	MET

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Mol	Chain	Res	Type
1	A	415	LYS
1	A	427	LEU
1	A	473	VAL
1	A	509	SER
1	A	516	THR
1	B	21	PHE
1	B	22	GLU
1	B	26	LYS
1	B	28	LYS
1	B	29	LEU
1	B	40	LEU
1	B	65	ASN
1	B	117	GLU
1	B	119	LYS
1	B	126	LEU
1	B	134	ASN
1	B	141	LEU
1	B	145	GLN
1	B	148	TRP
1	B	174	THR
1	B	205	ASP
1	B	317	VAL
1	B	372	VAL

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	84	HIS
1	A	451	ASN
1	A	526	HIS
1	B	213	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(Å^2)	Q<0.9
1	A	460/534 (86%)	1.17	90 (19%)	1	1	33, 63, 108, 134	0
1	B	468/534 (87%)	0.74	44 (9%)	11	9	24, 43, 98, 130	0
All	All	928/1068 (86%)	0.96	134 (14%)	3	3	24, 56, 105, 134	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	THR	8.7
1	A	33	ILE	6.5
1	A	288	TYR	6.0
1	B	28	LYS	5.6
1	A	126	LEU	5.6
1	A	121	LYS	5.5
1	B	123	GLU	5.5
1	B	116	GLU	5.3
1	B	21	PHE	5.2
1	A	215	LEU	5.1
1	A	183	PHE	5.1
1	B	192	LYS	4.9
1	A	194	VAL	4.9
1	A	168	SER	4.8
1	A	201	ILE	4.7
1	A	191	ILE	4.7
1	A	524	LEU	4.6
1	B	42	LEU	4.5
1	A	489	LEU	4.4
1	B	221	ASN	4.3
1	A	147	ARG	4.3
1	B	126	LEU	4.3
1	A	289	GLY	4.2
1	B	145	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	135	ILE	4.2
1	A	200	ILE	4.1
1	A	139	TRP	4.0
1	A	127	CYS	4.0
1	A	81	TRP	4.0
1	B	314	GLU	4.0
1	A	44	ILE	4.0
1	B	146	GLY	3.9
1	B	121	LYS	3.8
1	B	81	TRP	3.8
1	A	135	ILE	3.7
1	A	118	ASP	3.7
1	A	131	GLY	3.6
1	A	138	VAL	3.6
1	A	120	SER	3.5
1	A	363	TRP	3.5
1	B	144	ASP	3.5
1	A	525	SER	3.5
1	A	123	GLU	3.5
1	A	89	THR	3.4
1	A	197	PRO	3.4
1	A	80	GLU	3.4
1	B	525	SER	3.4
1	A	34	LEU	3.4
1	A	122	ILE	3.3
1	B	83	THR	3.3
1	A	220	PRO	3.3
1	A	528	ILE	3.3
1	A	223	TYR	3.3
1	A	146	GLY	3.3
1	A	282	ARG	3.2
1	A	124	LYS	3.2
1	A	63	ARG	3.2
1	A	313	SER	3.2
1	A	291	THR	3.2
1	B	148	TRP	3.2
1	A	378	SER	3.1
1	B	140	LEU	3.1
1	B	141	LEU	3.1
1	A	61	THR	3.0
1	B	127	CYS	3.0
1	A	275	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	187	TYR	3.0
1	A	128	ASP	2.9
1	A	42	LEU	2.9
1	A	184	ASN	2.9
1	A	202	TRP	2.9
1	A	284	SER	2.9
1	A	79	LYS	2.9
1	A	169	ASP	2.8
1	A	77	GLU	2.8
1	A	287	ALA	2.8
1	B	313	SER	2.8
1	A	134	ASN	2.8
1	A	188	LEU	2.8
1	A	219	PHE	2.7
1	A	286	SER	2.7
1	A	269	ILE	2.7
1	A	117	GLU	2.7
1	B	32	ARG	2.7
1	B	198	GLY	2.6
1	B	117	GLU	2.6
1	A	225	GLY	2.6
1	B	282	ARG	2.6
1	B	63	ARG	2.6
1	A	119	LYS	2.5
1	B	197	PRO	2.5
1	A	376	GLY	2.5
1	A	212	PRO	2.5
1	A	377	TYR	2.5
1	B	388	THR	2.5
1	A	285	VAL	2.5
1	B	128	ASP	2.4
1	B	27	LEU	2.4
1	A	209	LEU	2.4
1	A	178	HIS	2.4
1	B	170	GLY	2.4
1	A	163	ILE	2.3
1	B	33	ILE	2.3
1	A	498	SER	2.3
1	A	140	LEU	2.3
1	B	18	PRO	2.3
1	A	431	THR	2.3
1	A	73	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	210	LEU	2.3
1	A	449	LYS	2.2
1	B	118	ASP	2.2
1	A	91	GLU	2.2
1	A	129	ALA	2.2
1	A	379	HIS	2.2
1	A	208	LEU	2.2
1	A	300	GLY	2.2
1	B	142	ARG	2.2
1	B	223	TYR	2.2
1	A	142	ARG	2.2
1	A	526	HIS	2.1
1	B	115	ASP	2.1
1	B	158	PRO	2.1
1	B	134	ASN	2.1
1	B	288	TYR	2.1
1	A	247	LEU	2.1
1	A	92	LEU	2.1
1	B	315	LEU	2.1
1	B	164	GLN	2.1
1	A	430	ILE	2.1
1	A	179	ASP	2.0
1	A	412	ARG	2.0
1	B	378	SER	2.0
1	A	86	ILE	2.0
1	A	360	TYR	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.