WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:43 PM GMT

|		
PDB ID	:	1Q9J
Title	:	Structure of polyketide synthase associated protein 5 from Mycobacterium tuberculosis
Authors	:	Buglino, J.; Onwueme, K.C.; Quadri, L.E.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2003-08-25
Resolution	:	2.75 Å(reported)

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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 2.75 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
Clashscore		27
Ramachandran outliers		2.7%
Sidechain outliers		5.2%
RSRZ outliers		5.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
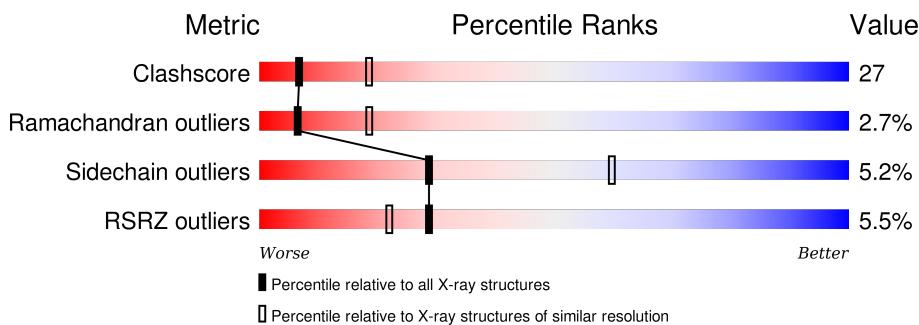
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	422	5% · 50% 38% · 8%
1	B	422	5% · 52% 39% · 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6225 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 Polyketide synthase associated protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total 2962	C 1893	N 495	O 560	S 14	0	0	0
1	B	399	Total 3037	C 1939	N 508	O 577	S 13	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total 90	O 90	0	0
2	B	136	Total 136	O 136	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: Polyketide synthase associated protein 5
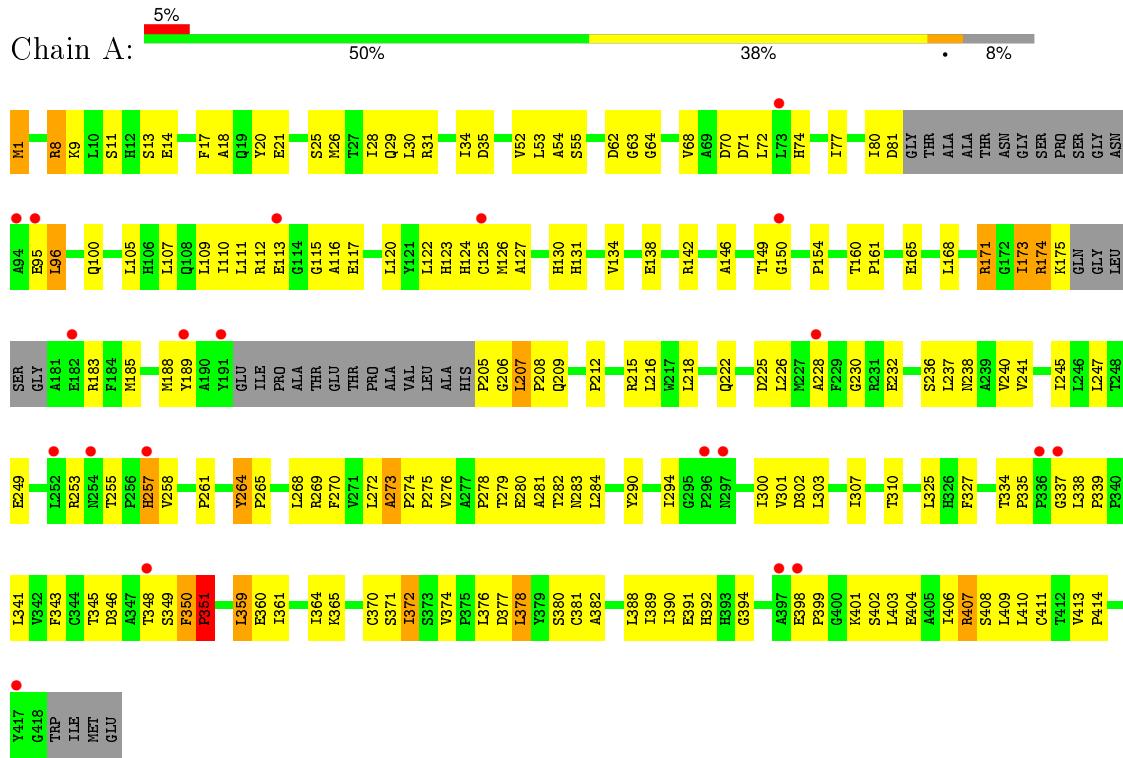
- Molecule 1: Polyketide synthase associated protein 5
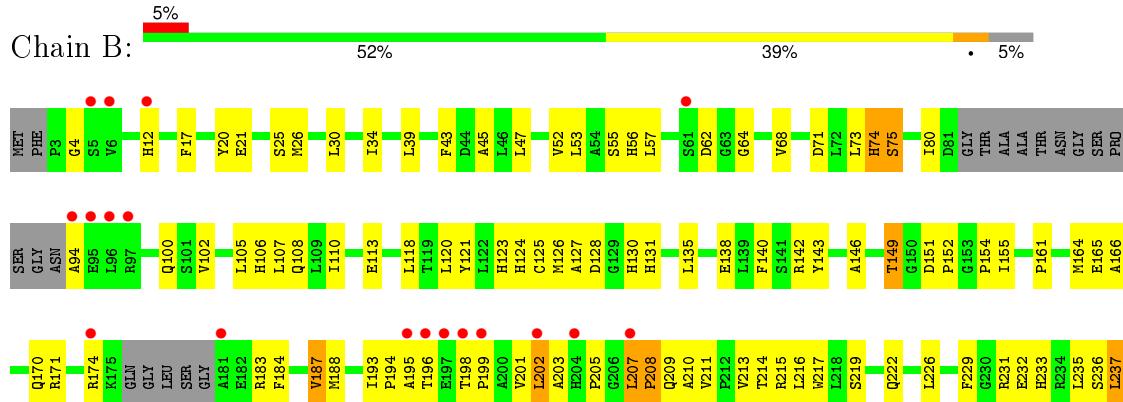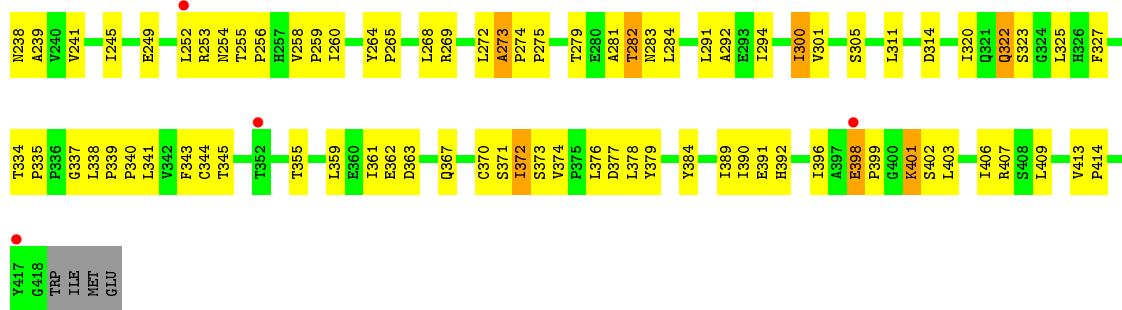
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	172.98Å 172.98Å 80.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.75 19.99 – 2.75	Depositor EDS
% Data completeness (in resolution range)	93.7 (20.00-2.75) 93.7 (19.99-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.295 0.231 , (Not available)	Depositor DCC
R_{free} test set	1172 reflections (3.46%)	DCC
Wilson B-factor (Å^2)	63.4	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.5	EDS
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	1 of 35078 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6225	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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	0.40	0/3032	0.63	0/4142
1	B	0.40	0/3110	0.62	0/4255
All	All	0.40	0/6142	0.62	0/8397

There are no bond length outliers.

There are no bond angle outliers.

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	2962	0	2938	171	0
1	B	3037	0	3011	152	0
2	A	90	0	0	7	0
2	B	136	0	0	7	12
All	All	6225	0	5949	323	12

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 27.

All (323) 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:348:THR:HG22	1:A:382:ALA:HA	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:HG23	2:A:423:HOH:O	1.70	0.91
1:A:273:ALA:CB	1:A:274:PRO:HD2	2.01	0.90
1:B:300:ILE:HD12	1:B:300:ILE:H	1.33	0.90
1:B:282:THR:HG22	1:B:283:ASN:ND2	1.88	0.89
1:A:371:SER:O	1:A:374:VAL:HG23	1.71	0.88
1:B:216:LEU:HD22	1:B:407:ARG:HH21	1.39	0.86
1:A:282:THR:HG22	1:A:283:ASN:ND2	1.93	0.83
1:A:392:HIS:HB2	1:A:403:LEU:HD13	1.60	0.82
1:A:52:VAL:HG21	1:A:161:PRO:HD2	1.61	0.81
1:A:34:ILE:HG21	1:A:109:LEU:HD21	1.63	0.81
1:B:273:ALA:HB3	1:B:274:PRO:HD3	1.63	0.80
1:A:216:LEU:HG	1:A:403:LEU:HD23	1.63	0.80
1:A:269:ARG:HE	1:A:278:PRO:HA	1.47	0.80
1:A:273:ALA:HB1	1:A:274:PRO:CD	2.13	0.79
1:B:210:ALA:HB1	1:B:367:GLN:NE2	1.98	0.78
1:B:199:PRO:HA	2:B:439:HOH:O	1.84	0.78
1:B:164:MET:HG3	1:B:284:LEU:HD12	1.68	0.76
1:A:55:SER:HB2	1:A:68:VAL:O	1.84	0.76
1:A:20:TYR:HD2	1:A:374:VAL:HG22	1.51	0.76
1:A:273:ALA:HB1	1:A:274:PRO:HD2	1.65	0.76
1:A:21:GLU:HA	1:A:100:GLN:OE1	1.85	0.76
1:B:273:ALA:CB	1:B:274:PRO:HD3	2.16	0.75
1:B:209:GLN:OE1	1:B:372:ILE:HG23	1.85	0.75
1:B:57:LEU:HD12	1:B:100:GLN:HB2	1.68	0.75
1:B:26:MET:HG2	2:B:424:HOH:O	1.86	0.74
1:A:273:ALA:CB	1:A:274:PRO:CD	2.65	0.74
1:A:218:LEU:HD11	1:A:407:ARG:HH22	1.52	0.74
1:A:370:CYS:HB2	1:A:374:VAL:HG21	1.67	0.74
1:B:107:LEU:HD11	1:B:118:LEU:HD11	1.70	0.72
1:A:226:LEU:HD21	1:A:410:LEU:HD22	1.71	0.72
1:B:273:ALA:HB3	1:B:274:PRO:CD	2.20	0.71
1:A:112:ARG:HB2	1:A:115:GLY:O	1.89	0.71
1:A:273:ALA:HB3	1:A:274:PRO:HD2	1.71	0.71
1:A:273:ALA:O	1:A:274:PRO:C	2.27	0.70
1:A:238:ASN:HB3	1:A:346:ASP:OD1	1.91	0.70
1:A:247:LEU:HD23	1:A:294:ILE:HD13	1.73	0.69
1:A:348:THR:CG2	1:A:382:ALA:HA	2.21	0.69
1:B:334:THR:HG23	1:B:341:LEU:CD1	2.23	0.69
1:B:127:ALA:HB1	1:B:131:HIS:HB3	1.74	0.68
1:A:26:MET:HE3	1:A:365:LYS:O	1.94	0.68
1:B:131:HIS:CE1	1:B:279:THR:HG22	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:TYR:HD2	1:B:374:VAL:HG22	1.59	0.68
1:B:171:ARG:NE	1:B:274:PRO:HD2	2.09	0.68
1:B:56:HIS:HB3	1:B:102:VAL:O	1.94	0.67
1:B:138:GLU:O	1:B:142:ARG:HG3	1.94	0.67
1:A:168:LEU:HD22	1:A:173:ILE:HD12	1.77	0.67
1:B:174:ARG:HG2	1:B:174:ARG:HH11	1.60	0.67
1:B:259:PRO:HB2	1:B:291:LEU:HD11	1.76	0.67
1:A:269:ARG:NE	1:A:278:PRO:HA	2.08	0.66
1:A:265:PRO:HG3	1:A:345:THR:HG23	1.77	0.66
1:B:335:PRO:HG2	1:B:338:LEU:HD12	1.75	0.66
1:A:390:ILE:HG22	1:A:403:LEU:HD11	1.78	0.66
1:A:215:ARG:HD2	1:A:391:GLU:OE1	1.96	0.66
1:A:334:THR:HG23	1:A:341:LEU:HD13	1.79	0.65
1:A:26:MET:HE2	1:A:364:ILE:HG23	1.76	0.65
1:A:272:LEU:O	1:A:273:ALA:O	2.13	0.65
1:B:52:VAL:HG21	1:B:161:PRO:CD	2.26	0.65
1:B:130:HIS:HD2	1:B:269:ARG:HD2	1.62	0.64
1:A:228:ALA:HA	2:A:427:HOH:O	1.95	0.64
1:B:273:ALA:CB	1:B:274:PRO:CD	2.75	0.64
1:A:138:GLU:O	1:A:142:ARG:HG3	1.98	0.64
1:B:201:VAL:HG11	1:B:372:ILE:HG22	1.80	0.63
1:B:207:LEU:HB2	1:B:208:PRO:HD3	1.80	0.63
1:A:189:TYR:HE2	2:A:463:HOH:O	1.82	0.63
1:A:183:ARG:HH12	1:A:310:THR:HG21	1.62	0.62
1:B:12:HIS:HB3	2:B:433:HOH:O	1.99	0.62
1:B:30:LEU:HD21	1:B:140:PHE:HE2	1.65	0.62
1:A:168:LEU:HB3	1:A:173:ILE:HB	1.82	0.62
1:A:335:PRO:HG2	1:A:338:LEU:HD12	1.82	0.62
1:A:338:LEU:HD23	1:A:339:PRO:HD2	1.81	0.62
1:B:146:ALA:HB2	1:B:152:PRO:HB3	1.81	0.62
1:B:20:TYR:CD2	1:B:374:VAL:HG22	2.35	0.62
1:A:398:GLU:HB3	1:A:401:LYS:HB2	1.82	0.62
1:A:218:LEU:HD21	1:A:407:ARG:NH2	2.16	0.61
1:A:53:LEU:HD23	1:A:126:MET:HE2	1.81	0.61
1:A:350:PHE:N	1:A:351:PRO:HD3	2.15	0.61
1:A:218:LEU:HD11	1:A:407:ARG:NH2	2.15	0.61
1:A:31:ARG:HA	1:A:115:GLY:HA3	1.81	0.60
1:B:231:ARG:C	1:B:233:HIS:H	2.04	0.60
1:B:193:ILE:HD12	1:B:339:PRO:HA	1.81	0.60
1:A:100:GLN:HG2	1:A:123:HIS:CE1	2.36	0.60
1:B:268:LEU:HB2	1:B:284:LEU:HG	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PRO:HA	1:A:371:SER:HA	1.81	0.60
1:A:95:GLU:O	1:A:96:LEU:HB2	2.00	0.60
1:A:174:ARG:HD3	1:A:174:ARG:N	2.17	0.60
1:A:377:ASP:OD1	1:A:392:HIS:HE1	1.85	0.59
1:B:43:PHE:CE2	1:B:47:LEU:HD11	2.37	0.59
1:A:168:LEU:HD22	1:A:173:ILE:CD1	2.32	0.59
1:A:300:ILE:HG22	1:A:301:VAL:N	2.16	0.59
1:B:52:VAL:HG21	1:B:161:PRO:HD2	1.84	0.59
1:A:237:LEU:O	1:A:241:VAL:HG23	2.02	0.59
1:B:55:SER:HB2	1:B:68:VAL:O	2.03	0.58
1:A:77:ILE:HG22	1:A:107:LEU:HD23	1.85	0.58
1:B:105:LEU:HD11	1:B:120:LEU:HD11	1.85	0.58
1:B:203:ALA:CB	1:B:209:GLN:HG3	2.33	0.58
1:B:45:ALA:HA	1:B:155:ILE:HD11	1.86	0.57
1:A:8:ARG:NH1	1:A:161:PRO:O	2.34	0.57
1:B:282:THR:HG22	1:B:283:ASN:HD22	1.65	0.57
1:A:215:ARG:HH12	1:A:365:LYS:HA	1.69	0.57
1:A:218:LEU:HD21	1:A:407:ARG:CZ	2.34	0.57
1:B:171:ARG:HG3	1:B:171:ARG:NH1	2.19	0.57
1:B:203:ALA:HB1	1:B:209:GLN:HG3	1.87	0.57
1:A:125:CYS:O	1:A:282:THR:HG21	2.05	0.56
1:B:396:ILE:HB	1:B:399:PRO:HG3	1.87	0.56
1:A:249:GLU:HB3	1:A:253:ARG:HE	1.69	0.56
1:A:290:TYR:CE2	1:A:307:ILE:HG12	2.40	0.56
1:A:398:GLU:N	1:A:399:PRO:HD3	2.20	0.56
1:A:409:LEU:O	1:A:413:VAL:HG23	2.06	0.56
1:A:21:GLU:HG3	1:A:205:PRO:HB2	1.86	0.56
1:A:282:THR:CG2	1:A:283:ASN:ND2	2.68	0.56
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.69	0.56
1:B:215:ARG:HD2	1:B:391:GLU:OE2	2.06	0.55
1:A:348:THR:HA	1:A:382:ALA:CB	2.35	0.55
1:B:21:GLU:HA	1:B:100:GLN:OE1	2.06	0.55
1:A:264:TYR:HB2	1:A:265:PRO:HD2	1.87	0.55
1:B:334:THR:HG23	1:B:341:LEU:HD12	1.88	0.55
1:B:392:HIS:HB2	1:B:403:LEU:HD13	1.88	0.55
1:A:174:ARG:HD3	1:A:174:ARG:H	1.71	0.55
1:A:349:SER:O	1:A:350:PHE:HB2	2.07	0.54
1:B:202:LEU:HG	2:B:506:HOH:O	2.06	0.54
1:A:34:ILE:HG21	1:A:109:LEU:CD2	2.35	0.54
1:B:171:ARG:HE	1:B:274:PRO:HD2	1.72	0.54
1:A:376:LEU:O	1:A:394:GLY:HA3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:VAL:HG21	1:B:161:PRO:HD3	1.88	0.54
1:A:404:GLU:HA	1:A:407:ARG:HB2	1.89	0.54
1:A:28:ILE:HG23	1:A:361:ILE:HG23	1.89	0.54
1:A:111:LEU:HA	1:A:116:ALA:HB2	1.91	0.53
1:B:236:SER:O	1:B:239:ALA:HB3	2.08	0.53
1:A:413:VAL:N	1:A:414:PRO:HD2	2.23	0.53
1:B:292:ALA:HB1	1:B:294:ILE:HD11	1.91	0.53
1:B:409:LEU:HD12	1:B:413:VAL:HG23	1.91	0.53
1:B:219:SER:OG	1:B:222:GLN:HG3	2.09	0.52
1:A:9:LYS:NZ	1:A:64:GLY:HA3	2.23	0.52
1:B:211:VAL:HG11	1:B:376:LEU:HD23	1.91	0.52
1:A:8:ARG:HH11	1:A:160:THR:HG22	1.74	0.52
1:A:80:ILE:HG22	1:A:81:ASP:N	2.25	0.52
1:A:171:ARG:NH1	1:A:274:PRO:O	2.33	0.52
1:A:123:HIS:HD2	1:A:125:CYS:H	1.58	0.52
1:B:43:PHE:CD1	1:B:107:LEU:HD22	2.45	0.52
1:B:105:LEU:HD12	1:B:106:HIS:H	1.75	0.52
1:A:72:LEU:HD12	1:A:72:LEU:N	2.24	0.52
1:A:282:THR:HG22	1:A:283:ASN:HD22	1.73	0.52
1:B:377:ASP:OD1	1:B:392:HIS:HE1	1.93	0.52
1:B:323:SER:OG	1:B:325:LEU:HG	2.10	0.52
1:A:276:VAL:HA	1:A:280:GLU:OE1	2.10	0.51
1:A:125:CYS:O	1:A:282:THR:CG2	2.58	0.51
1:A:131:HIS:HD2	1:A:281:ALA:O	1.93	0.51
1:A:110:ILE:O	1:A:116:ALA:HB1	2.11	0.51
1:A:343:PHE:HB3	1:A:378:LEU:HD12	1.91	0.51
1:B:413:VAL:N	1:B:414:PRO:HD2	2.26	0.51
1:B:80:ILE:HD13	1:B:94:ALA:N	2.25	0.51
1:A:183:ARG:NH1	1:A:310:THR:HG21	2.24	0.51
1:A:168:LEU:HB2	2:A:435:HOH:O	2.10	0.51
1:B:149:THR:C	1:B:151:ASP:H	2.14	0.51
1:A:218:LEU:HD12	1:A:388:LEU:HB3	1.93	0.50
1:A:402:SER:O	1:A:406:ILE:HG13	2.12	0.50
1:A:149:THR:HG22	1:A:150:GLY:H	1.77	0.50
1:A:268:LEU:HB2	1:A:284:LEU:HG	1.93	0.50
1:A:216:LEU:HD13	1:A:407:ARG:HG3	1.94	0.50
1:B:207:LEU:O	1:B:371:SER:HA	2.11	0.50
1:B:260:ILE:HD12	1:B:294:ILE:HD13	1.94	0.50
1:B:21:GLU:HG2	1:B:100:GLN:CD	2.32	0.50
1:A:74:HIS:HB2	2:A:483:HOH:O	2.12	0.50
1:A:247:LEU:HA	1:A:294:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:HG22	1:A:403:LEU:CD1	2.42	0.49
1:B:402:SER:O	1:B:406:ILE:HG13	2.12	0.49
1:A:348:THR:HG22	1:A:382:ALA:CA	2.28	0.49
1:A:218:LEU:HD12	1:A:388:LEU:HD23	1.93	0.49
1:A:13:SER:HB3	1:A:165:GLU:OE1	2.12	0.49
1:B:34:ILE:N	1:B:34:ILE:HD12	2.27	0.49
1:B:258:VAL:O	1:B:258:VAL:HG13	2.12	0.49
1:A:1:MET:HA	2:A:425:HOH:O	2.12	0.49
1:A:105:LEU:HD13	1:A:122:LEU:HD13	1.94	0.49
1:B:355:THR:HG21	1:B:361:ILE:HG13	1.94	0.49
1:B:265:PRO:HD3	1:B:327:PHE:CZ	2.47	0.49
1:A:127:ALA:HB1	1:A:131:HIS:HB3	1.95	0.48
1:A:149:THR:HG22	1:A:150:GLY:N	2.28	0.48
1:A:207:LEU:HA	1:A:208:PRO:HD3	1.67	0.48
1:B:207:LEU:CB	1:B:208:PRO:HD3	2.41	0.48
1:B:126:MET:O	1:B:282:THR:HG23	2.14	0.48
1:B:43:PHE:CE1	1:B:107:LEU:HB2	2.48	0.48
1:A:142:ARG:NH2	1:A:154:PRO:O	2.46	0.48
1:B:146:ALA:O	1:B:149:THR:O	2.32	0.48
1:B:174:ARG:HG2	1:B:174:ARG:NH1	2.28	0.48
1:A:218:LEU:HG	1:A:407:ARG:NH1	2.29	0.47
1:B:254:ASN:C	1:B:256:PRO:HD3	2.35	0.47
1:A:130:HIS:HD2	1:A:269:ARG:HD2	1.80	0.47
1:A:350:PHE:N	1:A:351:PRO:CD	2.77	0.47
1:A:381:CYS:HA	1:A:389:ILE:O	2.14	0.47
1:A:30:LEU:HB3	1:A:359:LEU:HD21	1.96	0.47
1:B:131:HIS:HD2	1:B:281:ALA:O	1.96	0.47
1:A:370:CYS:CB	1:A:374:VAL:HG21	2.41	0.47
1:B:131:HIS:CD2	1:B:279:THR:HA	2.49	0.47
1:A:257:HIS:HB2	2:A:454:HOH:O	2.14	0.47
1:B:106:HIS:HB2	1:B:121:TYR:HB2	1.96	0.47
1:B:107:LEU:CD1	1:B:118:LEU:HD11	2.44	0.47
1:B:25:SER:HA	1:B:120:LEU:O	2.14	0.47
1:B:398:GLU:HB2	1:B:401:LYS:HE3	1.97	0.47
1:B:213:VAL:HG12	1:B:214:THR:N	2.30	0.47
1:B:143:TYR:CE2	1:B:359:LEU:HD12	2.50	0.47
1:A:26:MET:CE	1:A:364:ILE:HG23	2.42	0.46
1:B:255:THR:O	1:B:258:VAL:HG12	2.15	0.46
1:A:274:PRO:HA	1:A:275:PRO:HD2	1.78	0.46
1:B:143:TYR:HE2	1:B:359:LEU:HD12	1.79	0.46
1:A:18:ALA:HA	1:A:100:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:HD11	1:A:410:LEU:HD12	1.98	0.46
1:A:34:ILE:N	1:A:34:ILE:HD12	2.30	0.46
1:A:161:PRO:HB3	1:A:279:THR:O	2.16	0.46
1:B:194:PRO:O	1:B:196:THR:N	2.46	0.46
1:B:164:MET:HB2	1:B:283:ASN:O	2.16	0.46
1:B:17:PHE:CD2	1:B:124:HIS:HB3	2.50	0.46
1:A:134:VAL:HG21	1:A:278:PRO:HB2	1.98	0.46
1:B:264:TYR:HB2	1:B:265:PRO:HD2	1.98	0.46
1:A:226:LEU:HD22	1:A:410:LEU:HB3	1.97	0.46
1:A:146:ALA:O	1:A:149:THR:O	2.33	0.46
1:B:235:LEU:HD11	1:B:301:VAL:HG13	1.98	0.46
1:B:282:THR:CG2	1:B:283:ASN:ND2	2.69	0.45
1:B:71:ASP:HB2	1:B:73:LEU:HD13	1.98	0.45
1:A:183:ARG:HH12	1:A:310:THR:CG2	2.27	0.45
1:A:265:PRO:HB3	1:A:327:PHE:CD2	2.51	0.45
1:A:236:SER:O	1:A:240:VAL:HG23	2.17	0.45
1:B:370:CYS:HB2	1:B:374:VAL:HG21	1.98	0.45
1:B:30:LEU:HD21	1:B:140:PHE:CE2	2.50	0.45
1:B:311:LEU:HD12	1:B:320:ILE:HD11	1.98	0.45
1:A:189:TYR:CD1	1:A:337:GLY:HA3	2.52	0.45
1:A:388:LEU:HD12	1:A:389:ILE:H	1.82	0.45
1:A:265:PRO:HD3	1:A:327:PHE:CZ	2.51	0.45
1:B:231:ARG:C	1:B:233:HIS:N	2.70	0.45
1:A:212:PRO:HG2	1:A:394:GLY:O	2.17	0.45
1:B:292:ALA:HB1	1:B:294:ILE:CD1	2.47	0.45
1:B:245:ILE:HG12	1:B:406:ILE:HD13	1.99	0.45
1:B:226:LEU:O	1:B:229:PHE:HB3	2.16	0.45
1:B:260:ILE:HB	1:B:292:ALA:HB3	2.00	0.44
1:B:238:ASN:HB3	2:B:499:HOH:O	2.17	0.44
1:A:261:PRO:HG2	1:A:341:LEU:HA	1.99	0.44
1:B:241:VAL:O	1:B:245:ILE:HG13	2.16	0.44
1:B:183:ARG:NH2	1:B:314:ASP:OD2	2.41	0.44
1:A:171:ARG:HG2	1:A:273:ALA:HB3	1.99	0.44
1:A:327:PHE:HE2	1:A:345:THR:HG1	1.65	0.44
1:B:334:THR:HA	1:B:341:LEU:HD13	1.99	0.44
1:A:209:GLN:HG3	1:A:372:ILE:HG12	1.98	0.44
1:A:29:GLN:OE1	1:A:117:GLU:HG2	2.17	0.44
1:B:73:LEU:H	1:B:73:LEU:HD12	1.82	0.43
1:A:17:PHE:CD2	1:A:124:HIS:HB3	2.53	0.43
1:B:300:ILE:H	1:B:300:ILE:CD1	2.08	0.43
1:B:56:HIS:CE1	1:B:68:VAL:HB	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:THR:O	1:A:258:VAL:HG22	2.18	0.43
1:B:108:GLN:OE1	1:B:110:ILE:HD11	2.18	0.43
1:B:184:PHE:O	1:B:187:VAL:HG23	2.18	0.43
1:A:222:GLN:NE2	1:A:411:CYS:SG	2.91	0.43
1:A:230:GLY:C	1:A:232:GLU:H	2.22	0.43
1:A:185:MET:HA	1:A:188:MET:HG2	2.01	0.43
1:A:268:LEU:HB3	1:A:272:LEU:HG	1.99	0.43
1:B:300:ILE:HD11	2:B:425:HOH:O	2.18	0.43
1:B:216:LEU:CD2	1:B:407:ARG:HH21	2.22	0.43
1:A:273:ALA:O	1:A:275:PRO:N	2.51	0.43
1:B:193:ILE:CD1	1:B:340:PRO:HD3	2.49	0.43
1:A:20:TYR:O	1:A:21:GLU:C	2.58	0.42
1:A:26:MET:HE3	1:A:365:LYS:C	2.39	0.42
1:B:53:LEU:HD13	1:B:105:LEU:HD22	2.01	0.42
1:B:258:VAL:CG1	1:B:258:VAL:O	2.67	0.42
1:B:135:LEU:HD23	1:B:135:LEU:HA	1.75	0.42
1:B:166:ALA:O	1:B:170:GLN:HB2	2.19	0.42
1:A:226:LEU:HD13	1:A:410:LEU:O	2.19	0.42
1:B:130:HIS:CD2	1:B:269:ARG:HD2	2.48	0.42
1:B:107:LEU:HD11	1:B:118:LEU:CD1	2.44	0.42
1:A:209:GLN:CG	1:A:372:ILE:HG12	2.50	0.42
1:B:74:HIS:O	1:B:75:SER:OG	2.33	0.42
1:A:11:SER:OG	1:A:14:GLU:HG3	2.19	0.42
1:A:212:PRO:HG2	1:A:394:GLY:C	2.39	0.42
1:B:252:LEU:HD11	1:B:402:SER:HB3	2.02	0.42
1:A:8:ARG:NH1	1:A:160:THR:HG22	2.35	0.42
1:A:31:ARG:CA	1:A:115:GLY:HA3	2.49	0.42
1:B:378:LEU:HD12	1:B:379:TYR:H	1.84	0.42
1:B:217:TRP:CZ3	1:B:389:ILE:HD11	2.54	0.42
1:A:35:ASP:OD2	1:A:35:ASP:O	2.37	0.42
1:B:142:ARG:NH2	1:B:154:PRO:O	2.53	0.42
1:A:54:ALA:O	1:A:70:ASP:HB2	2.20	0.42
1:B:322:GLN:HB3	1:B:322:GLN:HE21	1.58	0.42
1:A:206:GLY:O	1:A:207:LEU:C	2.58	0.42
1:A:407:ARG:NH2	1:A:410:LEU:HB2	2.35	0.42
1:B:45:ALA:HA	1:B:155:ILE:CD1	2.50	0.42
1:A:407:ARG:HG2	1:A:407:ARG:HH11	1.85	0.41
1:B:123:HIS:HD2	1:B:125:CYS:SG	2.43	0.41
1:A:174:ARG:CD	1:A:174:ARG:H	2.32	0.41
1:A:25:SER:HA	1:A:120:LEU:O	2.20	0.41
1:A:348:THR:O	1:A:349:SER:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ALA:HB1	1:B:274:PRO:HD3	1.99	0.41
1:A:134:VAL:HG21	1:A:278:PRO:CB	2.51	0.41
1:B:390:ILE:O	1:B:403:LEU:HD21	2.20	0.41
1:B:216:LEU:HG	1:B:403:LEU:HD23	2.03	0.41
1:B:210:ALA:HB1	1:B:367:GLN:HE21	1.82	0.41
1:B:105:LEU:CD1	1:B:120:LEU:HD11	2.51	0.41
1:A:359:LEU:O	1:A:360:GLU:HG3	2.20	0.41
1:B:373:SER:O	1:B:374:VAL:C	2.58	0.41
1:A:245:ILE:HG12	1:A:406:ILE:HD13	2.03	0.41
1:B:249:GLU:O	1:B:253:ARG:HG3	2.21	0.41
1:B:188:MET:HA	1:B:337:GLY:O	2.21	0.41
1:B:268:LEU:HB3	1:B:272:LEU:HG	2.03	0.41
1:A:255:THR:HB	1:A:258:VAL:HG21	2.03	0.41
1:B:237:LEU:HA	1:B:237:LEU:HD23	1.87	0.41
1:A:303:LEU:O	1:A:307:ILE:HG13	2.20	0.41
1:B:73:LEU:HD12	1:B:73:LEU:N	2.35	0.41
1:A:123:HIS:CD2	1:A:125:CYS:H	2.38	0.41
1:A:30:LEU:O	1:A:115:GLY:HA3	2.20	0.41
1:B:231:ARG:O	1:B:233:HIS:N	2.52	0.41
1:B:128:ASP:OD2	1:B:283:ASN:HA	2.20	0.41
1:A:31:ARG:HA	1:A:115:GLY:CA	2.49	0.41
1:A:276:VAL:HG13	1:A:280:GLU:CD	2.41	0.41
1:B:343:PHE:O	1:B:378:LEU:HD12	2.21	0.41
1:A:35:ASP:C	1:A:35:ASP:OD2	2.58	0.41
1:B:249:GLU:O	1:B:253:ARG:HD2	2.20	0.41
1:A:126:MET:O	1:A:127:ALA:HB2	2.21	0.40
1:A:185:MET:HA	1:A:188:MET:CG	2.51	0.40
1:B:384:TYR:HE1	2:B:449:HOH:O	2.03	0.40
1:B:274:PRO:HA	1:B:275:PRO:HD2	1.95	0.40
1:A:173:ILE:H	1:A:173:ILE:HG13	1.61	0.40
1:B:210:ALA:HB1	1:B:367:GLN:HE22	1.83	0.40
1:B:215:ARG:NH2	1:B:217:TRP:HZ2	2.20	0.40
1:B:110:ILE:HD12	1:B:110:ILE:N	2.37	0.40
1:B:362:GLU:O	1:B:363:ASP:HB2	2.21	0.40
1:B:344:CYS:HA	1:B:379:TYR:O	2.21	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:533:HOH:O	2:B:556:HOH:O[4_555]	1.31	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:538:HOH:O	2:B:545:HOH:O[4_555]	1.33	0.87
2:B:534:HOH:O	2:B:570:HOH:O[4_555]	1.37	0.83
2:B:532:HOH:O	2:B:554:HOH:O[4_555]	1.40	0.80
2:B:571:HOH:O	2:B:571:HOH:O[4_555]	1.48	0.72
2:B:557:HOH:O	2:B:567:HOH:O[4_555]	1.50	0.70
2:B:535:HOH:O	2:B:571:HOH:O[4_555]	1.69	0.51
2:B:530:HOH:O	2:B:558:HOH:O[4_555]	1.81	0.39
2:B:552:HOH:O	2:B:567:HOH:O[4_555]	1.88	0.32
2:B:558:HOH:O	2:B:566:HOH:O[4_555]	1.88	0.32
2:B:527:HOH:O	2:B:538:HOH:O[4_555]	2.06	0.14
2:B:559:HOH:O	2:B:559:HOH:O[4_555]	2.11	0.09

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	380/422 (90%)	336 (88%)	35 (9%)	9 (2%)	7	22
1	B	393/422 (93%)	339 (86%)	42 (11%)	12 (3%)	5	15
All	All	773/844 (92%)	675 (87%)	77 (10%)	21 (3%)	6	18

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	GLU
1	A	273	ALA
1	B	273	ALA
1	A	96	LEU
1	A	173	ILE
1	B	282	THR
1	A	372	ILE
1	B	205	PRO
1	B	207	LEU

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Mol	Chain	Res	Type
1	B	232	GLU
1	A	257	HIS
1	A	351	PRO
1	B	75	SER
1	B	113	GLU
1	B	195	ALA
1	B	208	PRO
1	B	401	LYS
1	A	350	PHE
1	B	4	GLY
1	A	63	GLY
1	B	64	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	324/348 (93%)	305 (94%)	19 (6%)	24	53
1	B	332/348 (95%)	317 (96%)	15 (4%)	34	66
All	All	656/696 (94%)	622 (95%)	34 (5%)	29	60

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	ARG
1	A	62	ASP
1	A	71	ASP
1	A	171	ARG
1	A	174	ARG
1	A	175	LYS
1	A	207	LEU
1	A	225	ASP
1	A	264	TYR
1	A	270	PHE

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Mol	Chain	Res	Type
1	A	302	ASP
1	A	325	LEU
1	A	351	PRO
1	A	359	LEU
1	A	378	LEU
1	A	380	SER
1	A	407	ARG
1	A	408	SER
1	B	39	LEU
1	B	62	ASP
1	B	74	HIS
1	B	149	THR
1	B	165	GLU
1	B	187	VAL
1	B	198	THR
1	B	202	LEU
1	B	237	LEU
1	B	300	ILE
1	B	305	SER
1	B	322	GLN
1	B	345	THR
1	B	372	ILE
1	B	398	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	130	HIS
1	A	131	HIS
1	A	209	GLN
1	A	222	GLN
1	A	233	HIS
1	A	317	ASN
1	A	322	GLN
1	A	367	GLN
1	A	392	HIS
1	B	56	HIS
1	B	123	HIS
1	B	130	HIS
1	B	131	HIS
1	B	170	GLN

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Mol	Chain	Res	Type
1	B	317	ASN
1	B	322	GLN
1	B	367	GLN
1	B	392	HIS

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	388/422 (91%)	0.09	21 (5%)	29	22	33, 68, 113, 136	0
1	B	399/422 (94%)	-0.04	22 (5%)	29	22	34, 62, 104, 147	0
All	All	787/844 (93%)	0.02	43 (5%)	29	22	33, 65, 111, 147	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	THR	5.4
1	B	174	ARG	4.5
1	B	207	LEU	4.4
1	A	191	TYR	4.1
1	A	189	TYR	4.1
1	B	197	GLU	4.0
1	A	254	ASN	3.9
1	A	297	ASN	3.6
1	B	12	HIS	3.5
1	A	397	ALA	3.4
1	B	398	GLU	3.2
1	B	95	GLU	3.2
1	A	94	ALA	3.1
1	B	195	ALA	3.0
1	B	96	LEU	3.0
1	A	150	GLY	3.0
1	B	6	VAL	2.9
1	A	398	GLU	2.8
1	B	97	ARG	2.8
1	A	417	TYR	2.8
1	B	199	PRO	2.7
1	A	113	GLU	2.6
1	A	257	HIS	2.6
1	A	348	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	252	LEU	2.5
1	A	296	PRO	2.5
1	A	182	GLU	2.5
1	B	252	LEU	2.4
1	A	336	PRO	2.4
1	B	181	ALA	2.3
1	B	61	SER	2.3
1	A	337	GLY	2.3
1	B	5	SER	2.2
1	A	228	ALA	2.2
1	B	204	HIS	2.2
1	A	73	LEU	2.2
1	A	95	GLU	2.2
1	B	202	LEU	2.1
1	B	352	THR	2.2
1	B	417	TYR	2.1
1	B	198	THR	2.1
1	B	94	ALA	2.1
1	A	125	CYS	2.1

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.