Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 09:36 am GMT

PDB ID	:	2BMF
Title	:	Dengue virus RNA helicase at 2.4A
Authors	:	Xu, T.; Sampath, A.; Chao, A.; Wen, D.; Nanao, M.; Chene, P.; Vasudevan, S.G.; Lescar, J.
Deposited on	:	2005-03-14
Resolution	:	2.41 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

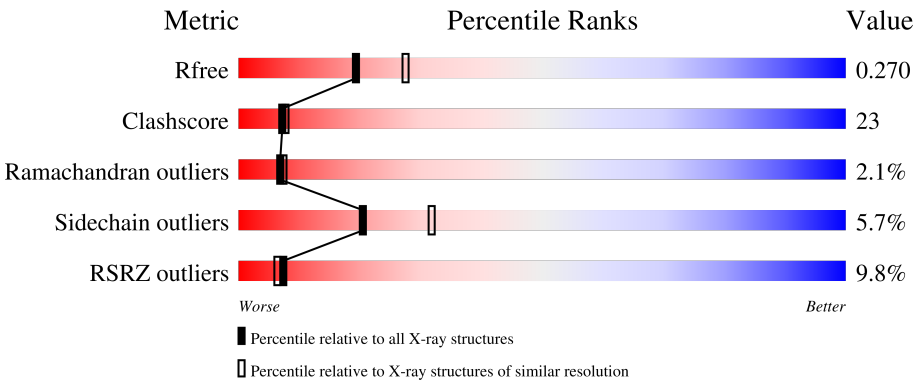
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	451	15% 54% 39%
1	B	451	4% 65% 30%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7360 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 RNA HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3531	2224	629	657	21	0	0	0
1	B	443	3556	2237	639	659	21	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	ALA	-	expression tag	UNP Q91H74
A	169	MET	-	expression tag	UNP Q91H74
A	170	ALA	-	expression tag	UNP Q91H74
B	168	ALA	-	expression tag	UNP Q91H74
B	169	MET	-	expression tag	UNP Q91H74
B	170	ALA	-	expression tag	UNP Q91H74

- Molecule 2 is water.

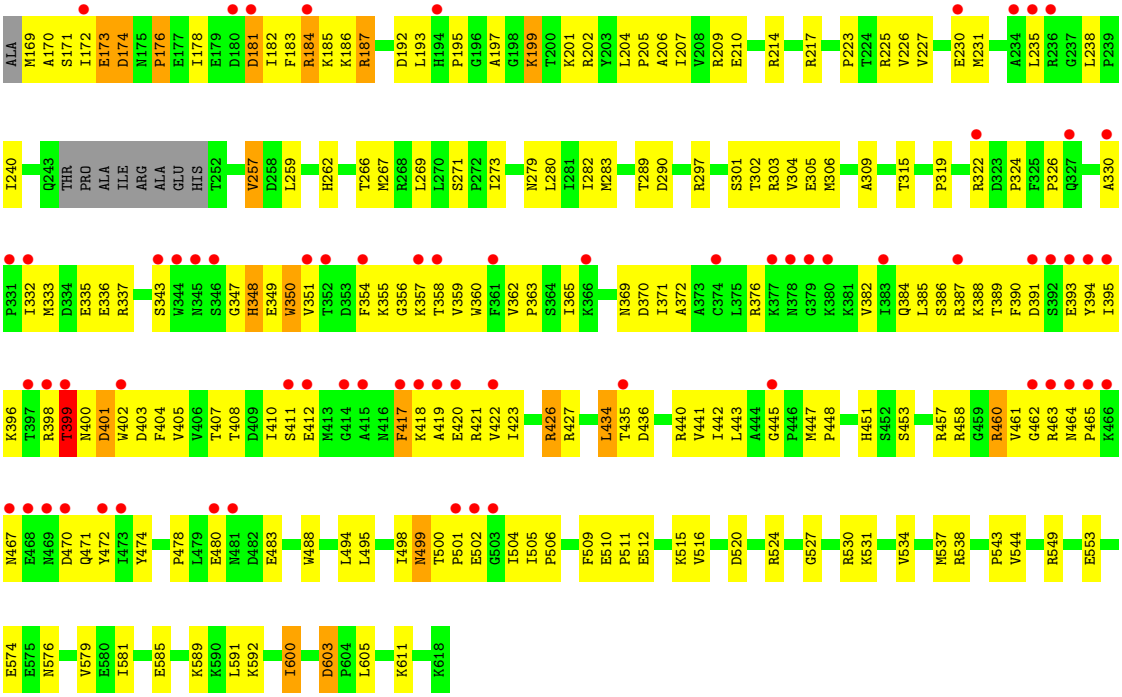
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	121	121	121	0	0
2	B	152	152	152	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

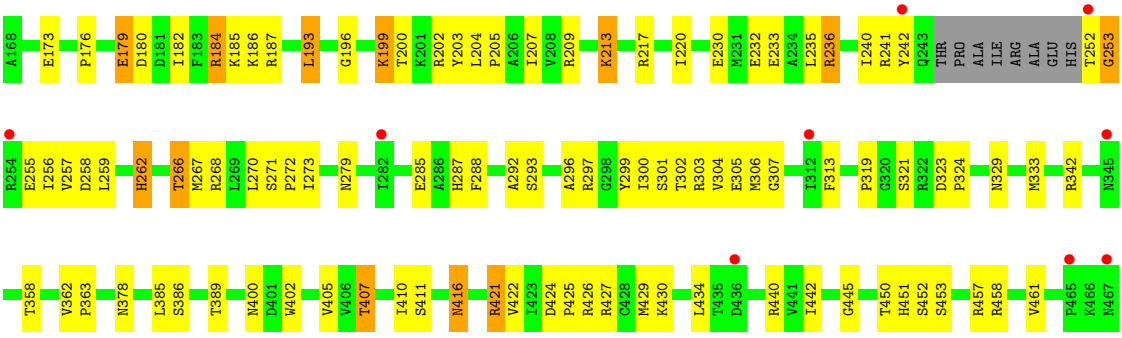
• Molecule 1: RNA HELICASE

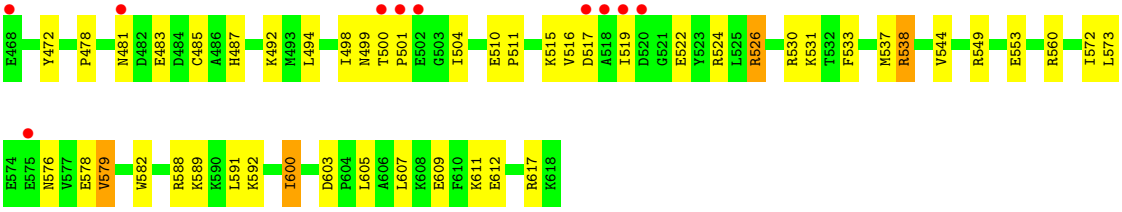
Chain A:



• Molecule 1: RNA HELICASE

Chain B:




E468
Y472
P478
N481
D482
E483
D484
C485
A486
H487
K492
M493
L494
I498
N499
T500
P501
E502
G503
I504
E510
P511
K515
V516
D517
A518
I519
D520
G521
E522
Y523
R524
L525
R526
R530
K531
T532
F533
M537
R538
V544
R549
E553
R560
I572
L573
E574
E575
N576
V577
E578
V579
W582
R588
K589
K590
L591
K592
I600
D603
P604
L605
A606
L607
K608
E609
F610
K611
E612
R617
K618

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.90Å 178.10Å 55.40Å 90.00° 101.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.41 27.50 – 2.41	Depositor EDS
% Data completeness (in resolution range)	93.8 (20.00-2.41) 94.1 (27.50-2.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.40 (at 2.42Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.270 0.222 , 0.270	Depositor DCC
R_{free} test set	1885 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.039 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7360	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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, 0.333 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	0.34	0/3606	0.59	0/4873
1	B	0.38	0/3631	0.63	0/4904
All	All	0.36	0/7237	0.61	0/9777

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	3531	0	3499	198	0
1	B	3556	0	3542	121	0
2	A	121	0	0	31	0
2	B	152	0	0	21	0
All	All	7360	0	7041	319	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 23.

All (319) 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:388:LYS:HD2	1:A:605:LEU:HD12	1.37	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:LEU:HB2	1:B:407:THR:HG23	1.35	1.05
1:A:382:VAL:HG11	1:A:404:PHE:HB2	1.52	0.92
1:A:458:ARG:HH11	1:A:458:ARG:HB3	1.38	0.89
1:B:537:MET:HE3	1:B:544:VAL:HG22	1.57	0.84
1:A:324:PRO:HB2	2:A:2059:HOH:O	1.77	0.84
1:B:510:GLU:HB3	1:B:511:PRO:HD3	1.61	0.83
1:A:333:MET:HB3	1:A:471:GLN:HB3	1.61	0.81
1:A:407:THR:HG22	1:A:408:THR:H	1.46	0.80
1:B:572:ILE:O	1:B:579:VAL:HG12	1.82	0.80
1:A:537:MET:HE1	1:A:544:VAL:HG22	1.64	0.80
1:A:515:LYS:HD2	2:A:2072:HOH:O	1.82	0.79
1:A:390:PHE:HB2	1:A:410:ILE:HD12	1.66	0.77
1:A:537:MET:CE	1:A:544:VAL:HG22	2.14	0.76
1:A:365:ILE:HD11	1:A:387:ARG:HB2	1.66	0.76
1:A:359:VAL:HG13	1:A:405:VAL:HB	1.66	0.76
1:B:407:THR:HG21	1:B:411:SER:OG	1.85	0.76
1:A:357:LYS:HB3	1:A:419:ALA:HA	1.69	0.74
1:A:421:ARG:HG3	1:A:471:GLN:HG3	1.69	0.74
1:B:230:GLU:HB2	2:B:2020:HOH:O	1.88	0.73
1:A:204:LEU:HB3	1:A:205:PRO:HD3	1.69	0.73
1:A:335:GLU:HB3	2:A:2037:HOH:O	1.89	0.73
1:A:420:GLU:O	1:A:470:ASP:HA	1.88	0.73
1:A:358:THR:HG21	1:A:421:ARG:NH1	2.04	0.73
1:A:333:MET:HB3	1:A:471:GLN:CB	2.20	0.71
1:B:266:THR:HG21	1:B:292:ALA:O	1.90	0.71
1:A:358:THR:HA	1:A:421:ARG:O	1.92	0.70
1:A:458:ARG:HB3	1:A:458:ARG:NH1	2.07	0.69
1:B:217:ARG:H	1:B:279:ASN:HD22	1.41	0.69
1:A:524:ARG:CZ	1:A:530:ARG:HH22	2.06	0.69
1:B:306:MET:SD	1:B:504:ILE:HD11	2.32	0.69
1:A:407:THR:HG21	1:A:411:SER:OG	1.92	0.68
1:A:322:ARG:HD3	1:A:480:GLU:HG3	1.75	0.68
1:A:356:GLY:O	1:A:403:ASP:HA	1.93	0.67
1:A:210:GLU:HG3	1:A:214:ARG:NH1	2.10	0.67
1:A:182:ILE:HG23	1:A:183:PHE:CD1	2.30	0.67
1:B:430:LYS:HD2	1:B:485:CYS:HB2	1.78	0.66
1:B:510:GLU:HG2	2:B:2110:HOH:O	1.95	0.66
1:B:494:LEU:HD21	1:B:537:MET:HE1	1.77	0.66
1:A:385:LEU:HB2	1:A:407:THR:HG23	1.77	0.66
1:A:376:ARG:HE	1:A:382:VAL:H	1.44	0.65
1:A:426:ARG:NH2	2:A:2059:HOH:O	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ARG:HD2	1:B:306:MET:CE	2.26	0.64
1:A:426:ARG:NE	1:A:474:TYR:HB2	2.13	0.64
1:B:213:LYS:HE3	1:B:213:LYS:N	2.12	0.64
1:B:362:VAL:HG22	1:B:363:PRO:HD2	1.78	0.64
1:A:538:ARG:HB3	2:A:2088:HOH:O	1.97	0.64
1:B:302:THR:O	1:B:306:MET:HG3	1.97	0.64
1:A:510:GLU:HB3	1:A:511:PRO:HD3	1.79	0.63
1:B:217:ARG:HA	1:B:256:ILE:HG12	1.81	0.63
1:A:172:ILE:C	1:A:174:ASP:H	2.02	0.63
1:A:210:GLU:HG3	1:A:214:ARG:HH11	1.63	0.62
1:B:235:LEU:HD23	1:B:240:ILE:HD13	1.81	0.62
1:B:416:ASN:HB3	2:B:2101:HOH:O	1.99	0.62
1:B:268:ARG:HG2	2:B:2037:HOH:O	1.98	0.62
1:A:495:LEU:HA	1:A:498:ILE:HG12	1.82	0.61
1:A:483:GLU:HA	2:A:2072:HOH:O	1.98	0.61
1:A:358:THR:HB	1:A:404:PHE:CE2	2.35	0.61
1:A:187:ARG:HA	1:A:187:ARG:HE	1.65	0.61
1:B:209:ARG:O	1:B:213:LYS:HD2	2.01	0.60
1:A:297:ARG:HD2	1:A:512:GLU:OE2	2.00	0.60
1:B:185:LYS:O	1:B:186:LYS:HB2	2.01	0.60
1:A:332:ILE:HA	1:A:470:ASP:O	2.01	0.60
1:A:407:THR:HG22	1:A:408:THR:N	2.16	0.60
1:B:607:LEU:HG	1:B:611:LYS:HD2	1.84	0.60
1:A:585:GLU:HG3	2:A:2121:HOH:O	2.03	0.59
1:A:279:ASN:HB2	2:A:2022:HOH:O	2.03	0.59
1:B:271:SER:HB2	2:B:2033:HOH:O	2.02	0.59
1:A:434:LEU:HD22	1:A:442:ILE:HD13	1.85	0.59
1:B:199:LYS:HD2	1:B:200:THR:N	2.18	0.59
1:A:369:ASN:HA	1:A:384:GLN:HE22	1.68	0.58
1:A:549:ARG:HD2	2:A:2096:HOH:O	2.03	0.58
1:A:209:ARG:HD3	1:A:238:LEU:HD21	1.84	0.58
1:A:399:THR:HA	1:A:418:LYS:HE2	1.84	0.58
1:B:179:GLU:HB3	1:B:182:ILE:HG12	1.84	0.58
1:A:223:PRO:HA	1:A:262:HIS:CD2	2.39	0.58
1:A:382:VAL:CG1	1:A:404:PHE:HB2	2.28	0.58
1:B:204:LEU:HB3	1:B:205:PRO:HD3	1.84	0.58
1:B:217:ARG:H	1:B:279:ASN:ND2	2.02	0.58
1:A:330:ALA:HB3	1:A:462:GLY:HA2	1.86	0.57
1:A:470:ASP:HB2	2:A:2035:HOH:O	2.03	0.57
1:B:272:PRO:HG2	1:B:531:LYS:HE2	1.87	0.57
1:A:266:THR:HA	1:A:269:LEU:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:MET:CE	1:B:544:VAL:HG22	2.33	0.57
1:B:301:SER:O	1:B:304:VAL:HG22	2.05	0.57
1:A:231:MET:O	1:A:235:LEU:HB2	2.04	0.57
1:B:196:GLY:HA3	1:B:329:ASN:HD21	1.68	0.57
1:B:524:ARG:CZ	1:B:530:ARG:HH22	2.17	0.57
1:A:440:ARG:NE	1:A:442:ILE:HD11	2.20	0.57
1:A:458:ARG:HH11	1:A:458:ARG:CB	2.14	0.56
1:B:617:ARG:HG2	1:B:617:ARG:HH11	1.70	0.56
1:A:240:ILE:HG23	1:A:257:VAL:HG22	1.87	0.56
1:A:297:ARG:NH1	2:A:2026:HOH:O	2.34	0.56
1:A:396:LYS:HB3	2:A:2050:HOH:O	2.05	0.56
1:A:359:VAL:O	1:A:422:VAL:HG13	2.05	0.56
1:B:573:LEU:HD22	2:B:2137:HOH:O	2.06	0.56
1:B:573:LEU:HD13	2:B:2137:HOH:O	2.06	0.55
1:A:173:GLU:HA	1:A:173:GLU:OE2	2.05	0.55
1:A:225:ARG:HG3	1:A:225:ARG:HH11	1.71	0.55
1:A:592:LYS:HD3	2:A:2109:HOH:O	2.06	0.55
1:A:421:ARG:HH12	1:A:423:ILE:HD11	1.70	0.55
1:A:386:SER:HB2	1:A:389:THR:OG1	2.06	0.55
1:A:304:VAL:HA	1:A:309:ALA:O	2.06	0.55
1:B:266:THR:HG22	1:B:296:ALA:HB2	1.88	0.55
1:A:435:THR:O	1:A:435:THR:HG22	2.07	0.55
1:B:426:ARG:NH1	1:B:478:PRO:HD3	2.22	0.54
1:B:358:THR:OG1	1:B:421:ARG:HD2	2.08	0.54
1:B:362:VAL:CG2	1:B:363:PRO:HD2	2.36	0.54
1:B:576:ASN:HA	2:B:2137:HOH:O	2.07	0.54
1:A:488:TRP:HB3	1:A:516:VAL:HG13	1.89	0.54
1:A:195:PRO:HB2	1:A:463:ARG:HD2	1.90	0.54
1:A:280:LEU:HD23	1:A:280:LEU:C	2.28	0.54
1:B:573:LEU:HD21	1:B:578:GLU:HG2	1.89	0.54
1:A:182:ILE:HG12	1:A:182:ILE:O	2.08	0.54
1:A:387:ARG:HG3	1:A:387:ARG:HH11	1.73	0.54
1:A:411:SER:HG	1:A:417:PHE:HZ	1.55	0.54
1:A:343:SER:HB2	1:A:370:ASP:OD2	2.07	0.53
1:A:230:GLU:N	1:A:230:GLU:OE2	2.41	0.53
1:A:399:THR:C	1:A:401:ASP:H	2.12	0.53
1:A:330:ALA:HB2	1:A:464:ASN:O	2.09	0.53
1:A:336:GLU:HG3	1:A:474:TYR:O	2.08	0.53
1:A:358:THR:HG21	1:A:421:ARG:HH11	1.71	0.53
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.74	0.53
1:A:210:GLU:CG	1:A:214:ARG:NH1	2.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:GLU:HA	1:A:574:GLU:OE1	2.09	0.53
1:A:460:ARG:HE	1:A:460:ARG:N	2.06	0.53
1:A:527:GLY:O	1:A:531:LYS:HG3	2.09	0.53
1:A:178:ILE:HD13	1:A:207:ILE:HA	1.90	0.53
1:A:217:ARG:N	2:A:2022:HOH:O	2.34	0.53
1:A:458:ARG:HG3	1:A:472:TYR:CG	2.44	0.53
1:A:376:ARG:NH2	1:A:382:VAL:O	2.41	0.52
1:A:442:ILE:CG2	1:A:443:LEU:N	2.73	0.52
1:A:193:LEU:HD13	1:A:199:LYS:HA	1.91	0.52
1:B:273:ILE:HD13	2:B:2033:HOH:O	2.09	0.52
1:B:196:GLY:HA3	1:B:329:ASN:ND2	2.25	0.52
1:A:396:LYS:HD3	2:A:2050:HOH:O	2.09	0.51
1:A:358:THR:HB	1:A:404:PHE:HE2	1.75	0.51
1:A:440:ARG:CZ	1:A:442:ILE:HD11	2.40	0.51
1:B:592:LYS:O	1:B:592:LYS:HG3	2.10	0.51
1:B:236:ARG:HD3	1:B:236:ARG:O	2.09	0.51
1:B:241:ARG:HD3	1:B:258:ASP:OD1	2.09	0.51
1:B:262:HIS:HB2	2:B:2028:HOH:O	2.10	0.51
1:B:453:SER:O	1:B:457:ARG:HG3	2.10	0.51
1:B:451:HIS:CD2	1:B:478:PRO:HB2	2.45	0.51
1:A:227:VAL:O	1:A:231:MET:HG3	2.11	0.51
1:A:280:LEU:HD21	1:A:282:ILE:CG1	2.41	0.51
1:B:299:TYR:HE1	1:B:500:THR:HG22	1.76	0.51
1:B:492:LYS:NZ	2:B:2113:HOH:O	2.43	0.51
1:A:355:LYS:HG3	2:A:2042:HOH:O	2.10	0.51
1:A:185:LYS:O	1:A:186:LYS:HB2	2.11	0.51
1:B:573:LEU:CD2	1:B:578:GLU:HG2	2.41	0.50
1:A:494:LEU:HD21	1:A:537:MET:HE1	1.93	0.50
1:B:184:ARG:O	1:B:187:ARG:HB2	2.11	0.50
1:B:193:LEU:CD2	1:B:199:LYS:HB3	2.42	0.50
1:B:422:VAL:HG23	1:B:461:VAL:HG13	1.93	0.50
1:B:450:THR:HG22	1:B:452:SER:H	1.76	0.50
1:A:524:ARG:CZ	1:A:530:ARG:NH2	2.73	0.50
1:A:421:ARG:NH1	1:A:423:ILE:HD11	2.27	0.50
1:B:522:GLU:HB3	2:B:2113:HOH:O	2.11	0.50
1:A:354:PHE:HA	2:A:2040:HOH:O	2.12	0.50
1:A:510:GLU:CB	1:A:511:PRO:HD3	2.42	0.50
1:A:192:ASP:HA	1:A:315:THR:O	2.12	0.50
1:A:348:HIS:HB2	2:A:2039:HOH:O	2.12	0.49
1:A:451:HIS:CE1	1:A:478:PRO:HB2	2.46	0.49
1:B:424:ASP:C	1:B:426:ARG:H	2.15	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:PHE:N	1:A:417:PHE:CD1	2.80	0.49
1:A:499:ASN:HD22	1:A:500:THR:N	2.10	0.49
1:A:510:GLU:HG3	2:A:2079:HOH:O	2.12	0.49
1:B:515:LYS:NZ	2:B:2111:HOH:O	2.45	0.49
1:B:499:ASN:OD1	1:B:524:ARG:NH2	2.43	0.49
1:A:382:VAL:HG12	1:A:404:PHE:H	1.77	0.49
1:A:387:ARG:HG3	1:A:387:ARG:NH1	2.28	0.48
1:B:285:GLU:OE2	1:B:287:HIS:HE1	1.96	0.48
1:B:363:PRO:O	1:B:429:MET:HG2	2.14	0.48
1:B:434:LEU:HD23	1:B:440:ARG:NH2	2.28	0.48
1:A:297:ARG:NH2	2:A:2026:HOH:O	2.42	0.48
1:A:357:LYS:CB	1:A:419:ALA:HA	2.42	0.48
1:A:382:VAL:HB	1:A:404:PHE:O	2.13	0.48
1:A:385:LEU:HD23	1:A:393:GLU:HB2	1.96	0.48
1:A:501:PRO:HB2	1:A:502:GLU:OE2	2.14	0.48
1:A:365:ILE:HD11	1:A:387:ARG:CB	2.39	0.48
1:B:176:PRO:HG3	1:B:202:ARG:NH2	2.28	0.48
1:A:421:ARG:NE	2:A:2058:HOH:O	2.46	0.48
1:B:519:ILE:HB	2:B:2113:HOH:O	2.13	0.48
1:A:181:ASP:HA	1:A:184:ARG:HB2	1.96	0.48
1:A:280:LEU:HD21	1:A:282:ILE:HG13	1.95	0.48
1:B:481:ASN:C	1:B:483:GLU:H	2.17	0.47
1:A:451:HIS:ND1	1:A:478:PRO:HB2	2.29	0.47
1:A:605:LEU:HD13	1:A:605:LEU:O	2.14	0.47
1:A:369:ASN:HA	1:A:384:GLN:NE2	2.30	0.47
1:B:526:ARG:HG2	1:B:526:ARG:HH11	1.79	0.47
1:A:209:ARG:HG2	1:A:238:LEU:HD22	1.97	0.47
1:A:271:SER:HB2	2:A:2018:HOH:O	2.14	0.47
1:A:579:VAL:HG23	1:A:591:LEU:HB3	1.97	0.47
1:A:376:ARG:HG3	1:A:376:ARG:HH11	1.80	0.47
1:B:297:ARG:HG2	1:B:313:PHE:CE1	2.50	0.47
1:B:524:ARG:NH2	1:B:530:ARG:HH22	2.13	0.47
1:A:262:HIS:CE1	1:A:283:MET:HG3	2.50	0.47
1:A:326:PRO:HD2	2:A:2065:HOH:O	2.14	0.47
1:A:385:LEU:CB	1:A:407:THR:HG23	2.42	0.47
1:B:203:TYR:O	1:B:207:ILE:HG13	2.14	0.46
1:B:402:TRP:CZ3	1:B:405:VAL:HG23	2.50	0.46
1:B:252:THR:HG22	1:B:253:GLY:N	2.30	0.46
1:B:579:VAL:HG13	1:B:591:LEU:HB3	1.97	0.46
1:A:358:THR:O	1:A:404:PHE:HA	2.14	0.46
1:B:516:VAL:HG22	1:B:517:ASP:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLU:HB2	1:A:504:ILE:HG22	1.97	0.46
1:A:226:VAL:HG23	1:A:391:ASP:OD1	2.16	0.46
1:A:304:VAL:CG2	1:A:305:GLU:N	2.79	0.46
1:A:358:THR:HB	1:A:404:PHE:CD2	2.51	0.46
1:A:171:SER:C	1:A:173:GLU:H	2.19	0.46
1:A:581:ILE:N	1:A:589:LYS:O	2.41	0.46
1:A:301:SER:O	1:A:305:GLU:HG3	2.15	0.45
1:B:573:LEU:HD23	1:B:578:GLU:HA	1.98	0.45
1:A:332:ILE:HD11	1:A:462:GLY:HA3	1.98	0.45
1:A:337:ARG:NE	2:A:2037:HOH:O	2.50	0.45
1:A:499:ASN:C	1:A:499:ASN:ND2	2.69	0.45
1:A:553:GLU:HG3	1:A:553:GLU:O	2.16	0.45
1:A:603:ASP:OD1	1:A:605:LEU:HB3	2.16	0.45
1:B:400:ASN:N	1:B:400:ASN:HD22	2.12	0.45
1:B:220:ILE:HB	1:B:259:LEU:HG	1.99	0.45
1:A:172:ILE:C	1:A:174:ASP:N	2.67	0.45
1:A:354:PHE:CG	1:A:421:ARG:NH2	2.83	0.45
1:B:241:ARG:HG3	1:B:255:GLU:HB2	1.99	0.45
1:A:176:PRO:HG2	1:A:206:ALA:HB2	1.97	0.45
1:A:421:ARG:HH11	1:A:423:ILE:HG13	1.82	0.45
1:B:179:GLU:OE1	1:B:180:ASP:N	2.49	0.45
1:B:262:HIS:HD2	1:B:293:SER:OG	1.99	0.45
1:A:302:THR:O	1:A:306:MET:HG3	2.17	0.45
1:A:372:ALA:O	1:A:376:ARG:HG2	2.16	0.45
1:B:589:LYS:NZ	2:B:2143:HOH:O	2.49	0.45
1:A:358:THR:HG23	1:A:422:VAL:HA	1.99	0.45
1:A:505:ILE:HG12	2:A:2075:HOH:O	2.17	0.45
1:B:296:ALA:O	1:B:300:ILE:HG13	2.17	0.45
1:B:434:LEU:HD22	1:B:442:ILE:HD12	1.99	0.45
1:A:269:LEU:HB3	1:A:498:ILE:HD12	1.99	0.44
1:A:441:VAL:C	1:A:442:ILE:HD12	2.37	0.44
1:A:225:ARG:HG3	1:A:225:ARG:NH1	2.31	0.44
1:A:262:HIS:HE1	1:A:283:MET:HG3	1.82	0.44
1:A:362:VAL:HB	1:A:363:PRO:HD2	1.99	0.44
1:A:434:LEU:HD22	1:A:442:ILE:CD1	2.47	0.44
1:B:487:HIS:HE1	2:B:2147:HOH:O	2.00	0.44
1:A:201:LYS:HG3	2:A:2010:HOH:O	2.18	0.44
1:A:289:THR:HA	2:A:2026:HOH:O	2.17	0.44
1:B:186:LYS:HA	1:B:304:VAL:O	2.18	0.44
1:B:272:PRO:HD2	2:B:2033:HOH:O	2.16	0.44
1:B:530:ARG:O	1:B:533:PHE:HB3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:VAL:HA	2:A:2069:HOH:O	2.16	0.44
1:A:267:MET:HE2	1:A:267:MET:HA	1.98	0.44
1:A:442:ILE:HG22	1:A:443:LEU:N	2.31	0.44
1:B:440:ARG:HG2	1:B:440:ARG:HH11	1.82	0.44
1:B:560:ARG:HA	1:B:560:ARG:HD3	1.89	0.44
1:B:232:GLU:HG3	1:B:242:TYR:CZ	2.53	0.44
1:A:472:TYR:CE2	1:A:474:TYR:HB3	2.53	0.43
1:B:524:ARG:CZ	1:B:530:ARG:NH2	2.80	0.43
1:A:304:VAL:HG23	1:A:305:GLU:N	2.33	0.43
1:B:402:TRP:CE3	1:B:405:VAL:HG23	2.53	0.43
1:B:240:ILE:HG12	1:B:257:VAL:HG13	2.01	0.43
1:B:385:LEU:CB	1:B:407:THR:HG23	2.25	0.43
1:B:442:ILE:HG12	2:B:2097:HOH:O	2.18	0.43
1:A:178:ILE:HD11	1:A:206:ALA:C	2.39	0.43
1:A:209:ARG:HG2	1:A:238:LEU:CD2	2.48	0.43
1:A:319:PRO:HG2	1:A:509:PHE:HE1	1.84	0.43
1:A:360:TRP:CE3	1:A:423:ILE:HD12	2.53	0.43
1:B:321:SER:HB2	1:B:452:SER:OG	2.19	0.43
1:B:510:GLU:HB3	1:B:511:PRO:CD	2.42	0.43
1:B:609:GLU:O	1:B:612:GLU:HB3	2.17	0.43
1:A:448:PRO:HG3	2:A:2060:HOH:O	2.18	0.43
1:B:271:SER:CB	2:B:2033:HOH:O	2.64	0.43
1:A:354:PHE:CG	1:A:355:LYS:N	2.86	0.43
1:A:509:PHE:CD1	1:A:511:PRO:HD2	2.54	0.43
1:B:299:TYR:CE1	1:B:500:THR:HG22	2.54	0.43
1:B:205:PRO:O	1:B:209:ARG:HG3	2.18	0.43
1:B:553:GLU:O	1:B:553:GLU:HG3	2.19	0.43
1:B:582:TRP:CZ3	1:B:588:ARG:HB2	2.54	0.43
1:B:425:PRO:O	1:B:427:ARG:HG2	2.19	0.42
1:B:500:THR:HB	1:B:501:PRO:HD2	2.01	0.42
1:B:450:THR:HG22	1:B:451:HIS:N	2.34	0.42
1:B:458:ARG:HD2	1:B:472:TYR:CD2	2.55	0.42
1:A:347:GLY:O	1:A:348:HIS:O	2.37	0.42
1:A:460:ARG:HE	1:A:460:ARG:CA	2.32	0.42
1:B:458:ARG:NH1	2:B:2100:HOH:O	2.47	0.42
1:A:442:ILE:HD12	1:A:442:ILE:N	2.33	0.42
1:A:356:GLY:HA2	1:A:403:ASP:HB3	2.01	0.42
1:A:534:VAL:HG12	1:A:538:ARG:HD3	2.01	0.42
1:B:267:MET:HG3	1:B:538:ARG:HG2	2.01	0.42
1:B:270:LEU:HD12	1:B:498:ILE:CG1	2.50	0.42
1:A:169:MET:HG3	1:A:170:ALA:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PRO:HG2	1:A:206:ALA:CB	2.50	0.42
1:A:447:MET:HB2	1:A:448:PRO:CD	2.50	0.42
1:B:617:ARG:HG2	1:B:617:ARG:NH1	2.35	0.41
1:B:522:GLU:CB	2:B:2113:HOH:O	2.68	0.41
1:A:350:TRP:HZ3	1:A:423:ILE:HG12	1.84	0.41
1:A:453:SER:O	1:A:457:ARG:HG3	2.20	0.41
1:A:543:PRO:HD2	1:A:600:ILE:CD1	2.51	0.41
1:B:303:ARG:HA	1:B:306:MET:HE2	2.03	0.41
1:A:448:PRO:HD3	2:A:2060:HOH:O	2.20	0.41
1:B:538:ARG:HA	1:B:538:ARG:HD3	1.84	0.41
1:B:600:ILE:HD12	1:B:600:ILE:HA	1.84	0.41
1:A:357:LYS:HB3	1:A:419:ALA:CA	2.45	0.41
1:A:402:TRP:HH2	1:A:418:LYS:H	1.67	0.41
1:A:360:TRP:CZ2	1:A:371:ILE:HD13	2.56	0.41
1:B:193:LEU:HD21	1:B:199:LYS:HB3	2.02	0.41
1:B:305:GLU:C	1:B:307:GLY:N	2.74	0.41
1:B:323:ASP:HA	1:B:324:PRO:HD3	1.70	0.41
1:A:226:VAL:HG11	1:A:394:TYR:CD2	2.55	0.41
1:A:427:ARG:CZ	2:A:2060:HOH:O	2.68	0.41
1:A:182:ILE:HG23	1:A:183:PHE:CE1	2.55	0.40
1:A:349:GLU:O	1:A:351:VAL:N	2.55	0.40
1:A:505:ILE:HA	1:A:506:PRO:HD3	1.85	0.40
1:A:537:MET:HE3	1:A:544:VAL:HG22	1.98	0.40
1:A:259:LEU:HD23	1:A:259:LEU:C	2.42	0.40
1:A:460:ARG:NE	1:A:460:ARG:HA	2.37	0.40
1:B:199:LYS:HD2	1:B:199:LYS:C	2.42	0.40
1:A:267:MET:HA	1:A:267:MET:CE	2.52	0.40
1:A:421:ARG:HA	1:A:471:GLN:O	2.21	0.40
1:A:581:ILE:HD11	1:A:611:LYS:HG2	2.04	0.40
1:B:386:SER:H	1:B:389:THR:HG22	1.86	0.40
1:A:303:ARG:HA	1:A:303:ARG:HD2	1.78	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	438/451 (97%)	373 (85%)	49 (11%)	16 (4%)	3	2
1	B	439/451 (97%)	400 (91%)	37 (8%)	2 (0%)	29	40
All	All	877/902 (97%)	773 (88%)	86 (10%)	18 (2%)	7	7

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	HIS
1	A	436	ASP
1	A	465	PRO
1	A	576	ASN
1	A	176	PRO
1	A	197	ALA
1	A	199	LYS
1	A	399	THR
1	A	401	ASP
1	B	445	GLY
1	B	253	GLY
1	A	173	GLU
1	A	400	ASN
1	A	412	GLU
1	A	445	GLY
1	A	350	TRP
1	A	467	ASN
1	A	395	ILE

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	373/384 (97%)	356 (95%)	17 (5%)	27	42
1	B	377/384 (98%)	351 (93%)	26 (7%)	15	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	750/768 (98%)	707 (94%)	43 (6%)	20 32

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	ASP
1	A	181	ASP
1	A	184	ARG
1	A	187	ARG
1	A	202	ARG
1	A	257	VAL
1	A	273	ILE
1	A	290	ASP
1	A	399	THR
1	A	417	PHE
1	A	426	ARG
1	A	434	LEU
1	A	460	ARG
1	A	499	ASN
1	A	520	ASP
1	A	600	ILE
1	A	603	ASP
1	B	173	GLU
1	B	179	GLU
1	B	184	ARG
1	B	193	LEU
1	B	199	LYS
1	B	213	LYS
1	B	233	GLU
1	B	236	ARG
1	B	262	HIS
1	B	266	THR
1	B	288	PHE
1	B	319	PRO
1	B	333	MET
1	B	342	ARG
1	B	378	ASN
1	B	407	THR
1	B	410	ILE
1	B	416	ASN
1	B	421	ARG
1	B	526	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	538	ARG
1	B	549	ARG
1	B	579	VAL
1	B	600	ILE
1	B	603	ASP
1	B	605	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	HIS
1	A	329	ASN
1	A	369	ASN
1	A	378	ASN
1	A	384	GLN
1	A	456	GLN
1	A	464	ASN
1	A	467	ASN
1	A	499	ASN
1	B	262	HIS
1	B	279	ASN
1	B	329	ASN
1	B	348	HIS
1	B	384	GLN
1	B	400	ASN
1	B	451	HIS
1	B	456	GLN
1	B	481	ASN
1	B	569	ASN
1	B	576	ASN

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 monosaccharides 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	442/451 (98%)	0.83	68 (15%)	2	1	24, 57, 96, 99	1 (0%)
1	B	443/451 (98%)	0.33	19 (4%)	35	32	19, 41, 64, 82	1 (0%)
All	All	885/902 (98%)	0.58	87 (9%)	7	6	19, 47, 91, 99	2 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	PRO	10.3
1	A	395	ILE	7.7
1	B	518	ALA	7.7
1	A	330	ALA	7.4
1	A	377	LYS	6.3
1	A	344	TRP	5.6
1	B	519	ILE	5.1
1	A	392	SER	5.0
1	A	391	ASP	5.0
1	A	466	LYS	4.9
1	A	399	THR	4.8
1	A	397	THR	4.5
1	A	469	ASN	4.2
1	A	236	ARG	4.2
1	A	417	PHE	4.1
1	A	467	ASN	4.1
1	A	415	ALA	4.0
1	A	414	GLY	4.0
1	A	180	ASP	3.9
1	B	242	TYR	3.9
1	B	254	ARG	3.8
1	B	467	ASN	3.7
1	A	398	ARG	3.7
1	B	575	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	503	GLY	3.6
1	A	464	ASN	3.6
1	A	468	GLU	3.6
1	A	418	LYS	3.5
1	A	181	ASP	3.5
1	B	465	PRO	3.5
1	B	252	THR	3.5
1	A	394	TYR	3.5
1	A	343	SER	3.3
1	A	465	PRO	3.3
1	B	500	THR	3.2
1	A	383	ILE	3.2
1	A	473	ILE	3.1
1	A	358	THR	3.1
1	A	322	ARG	3.1
1	A	502	GLU	3.1
1	B	501	PRO	3.0
1	A	402	TRP	3.0
1	A	470	ASP	3.0
1	B	436	ASP	2.9
1	A	366	LYS	2.9
1	A	346	SER	2.9
1	A	472	TYR	2.8
1	B	502	GLU	2.8
1	A	327	GLN	2.8
1	A	345	ASN	2.7
1	B	345	ASN	2.7
1	A	332	ILE	2.7
1	A	230	GLU	2.7
1	A	184	ARG	2.6
1	B	481	ASN	2.6
1	A	481	ASN	2.6
1	A	374	CYS	2.6
1	A	194	HIS	2.6
1	A	378	ASN	2.6
1	A	411	SER	2.6
1	A	234	ALA	2.5
1	A	501	PRO	2.5
1	A	354	PHE	2.5
1	B	468	GLU	2.5
1	A	445	GLY	2.5
1	A	172	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	361	PHE	2.4
1	A	393	GLU	2.4
1	B	520	ASP	2.3
1	A	463	ARG	2.3
1	A	387	ARG	2.3
1	A	412	GLU	2.3
1	B	312	ILE	2.3
1	A	419	ALA	2.3
1	A	351	VAL	2.3
1	B	517	ASP	2.3
1	A	352	THR	2.3
1	A	422	VAL	2.2
1	A	435	THR	2.2
1	A	480	GLU	2.2
1	A	357	LYS	2.2
1	A	380	LYS	2.2
1	B	282	ILE	2.1
1	A	420	GLU	2.1
1	A	379	GLY	2.0
1	A	462	GLY	2.0
1	A	235	LEU	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 monosaccharides 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.