Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:27 am BST

PDB ID	:	1B3U
Title	:	CRYSTAL STRUCTURE OF CONSTANT REGULATORY DOMAIN OF HUMAN PP2A, PR65ALPHA
Authors	:	Groves, M.R.; Hanlon, N.; Turowski, P.; Hemmings, B.; Barford, D.
Deposited on	:	1998-12-14
Resolution	:	2.30 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 ⓘ symbol.

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

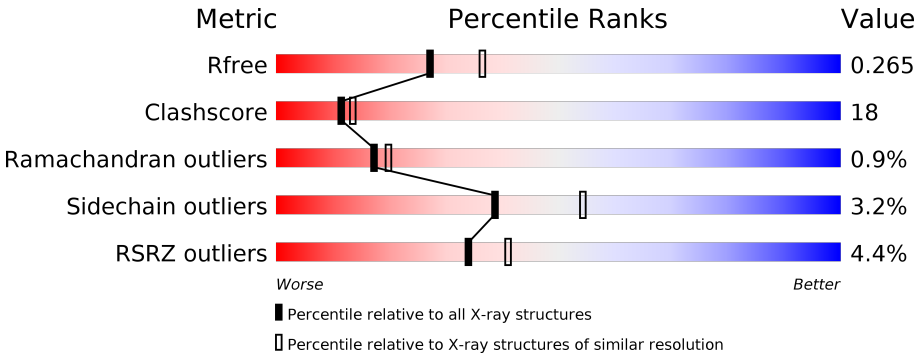
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	588	3% 68% 29%
1	B	588	5% 67% 31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9869 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 PROTEIN (PROTEIN PHOSPHATASE PP2A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4570	2900	770	873	27			
1	B	588	Total	C	N	O	S	0	0	0
			4570	2900	770	873	27			

- Molecule 2 is water.

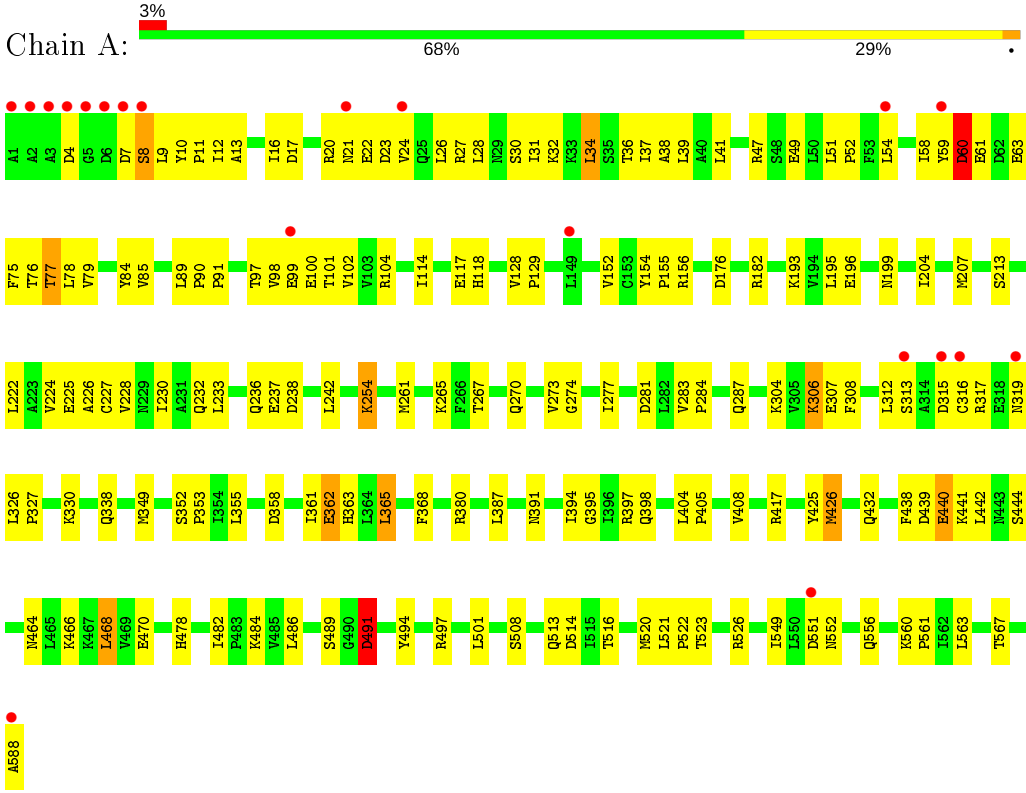
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	421	Total	O	0	0
			421	421		
2	B	308	Total	O	0	0
			308	308		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

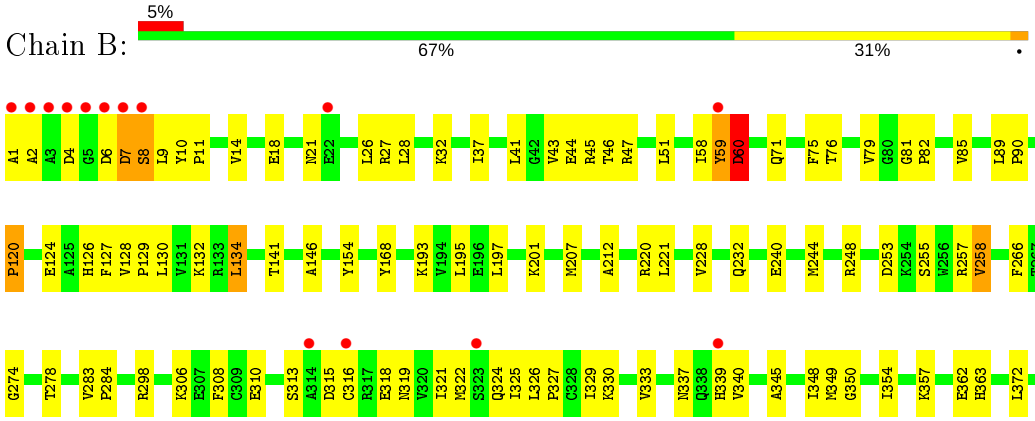
- Molecule 1: PROTEIN (PROTEIN PHOSPHATASE PP2A)

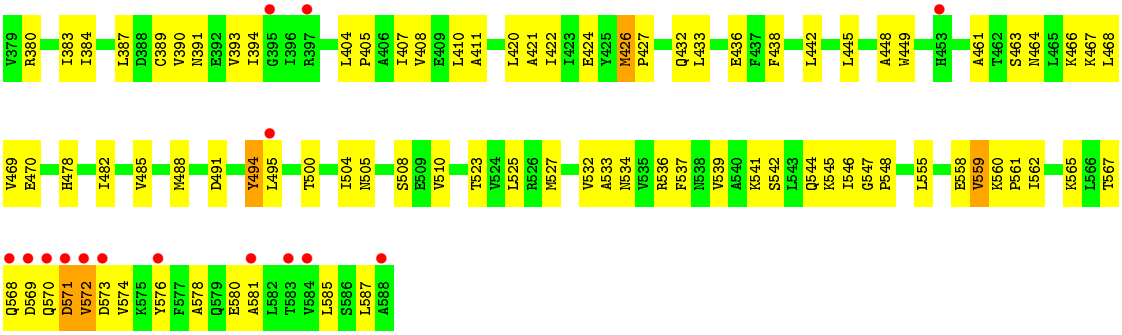
Chain A:



- Molecule 1: PROTEIN (PROTEIN PHOSPHATASE PP2A)

Chain B:




V379 R380 I383 I384 L387 D388 C389 V390 N391 E392 V393 I394 G395 I396 R397 L404 P405 A406 I407 V408 E409 L410 A411 L420 A421 I422 I423 E424 Y425 M426 P427 Q432 L433 E436 F437 F438 L442 L445 A448 W449 H453 A461 T462 S463 N464 L465 K466 K467 L468
V469 E470 H478 I482 V485 M488 D491 Y494 L495 T500 I504 N505 S508 E509 V510 T523 V524 L525 R526 M527 V532 A533 N534 V535 R536 F537 N538 V539 A540 K541 S542 L543 Q544 K545 I546 G547 P548 L555 E558 V559 K560 P561 I562 K565 L566 T567
Q568 D569 Q570 D571 V572 D573 V574 K575 Y576 P577 A578 Q579 E580 A581 L582 T583 V584 L585 S586 L587 A588

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.28Å 112.15Å 122.63Å 90.00° 95.60° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 24.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	82.8 (25.00-2.30) 82.7 (24.93-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	5.32 (at 2.31Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.209 , 0.268 0.206 , 0.265	Depositor DCC
R_{free} test set	1005 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 69.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9869	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 4.33% 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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/4644	0.59	0/6305
1	B	0.30	0/4644	0.57	0/6305
All	All	0.32	0/9288	0.58	0/12610

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

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	4570	0	4666	150	0
1	B	4570	0	4666	175	0
2	A	421	0	0	13	0
2	B	308	0	0	13	0
All	All	9869	0	9332	325	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 (325) 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:101:THR:HG22	1:A:104:ARG:HH22	1.26	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:VAL:HG12	1:B:573:ASP:H	1.29	0.96
1:B:306:LYS:HE2	1:B:350:GLY:HA3	1.49	0.95
1:A:196:GLU:HG2	1:A:199:ASN:HD22	1.39	0.87
1:B:523:THR:O	1:B:527:MET:HG2	1.74	0.87
1:B:8:SER:O	1:B:9:LEU:HD23	1.77	0.82
1:A:101:THR:HG22	1:A:104:ARG:NH2	1.95	0.81
1:B:571:ASP:O	1:B:574:VAL:HG12	1.82	0.80
1:A:361:ILE:HA	1:A:365:LEU:HD22	1.64	0.79
1:A:9:LEU:HD21	1:A:49:GLU:HG3	1.64	0.79
1:B:494:TYR:HD2	1:B:532:VAL:HG11	1.49	0.77
1:B:82:PRO:HA	1:B:85:VAL:HG23	1.64	0.77
1:B:274:GLY:O	1:B:278:THR:HG23	1.84	0.77
1:A:572:VAL:HA	1:A:575:LYS:HE2	1.67	0.76
1:B:316:CYS:HA	1:B:319:ASN:HD22	1.51	0.76
1:B:59:TYR:HD1	1:B:60:ASP:H	1.33	0.75
1:B:59:TYR:HD1	1:B:60:ASP:N	1.86	0.74
1:B:330:LYS:O	1:B:333:VAL:HG12	1.89	0.73
1:B:132:LYS:HE2	1:B:168:TYR:CE1	2.25	0.71
1:B:21:ASN:ND2	1:B:26:LEU:HD23	2.03	0.71
1:A:417:ARG:HG3	2:A:643:HOH:O	1.90	0.71
1:B:572:VAL:HG12	1:B:573:ASP:N	2.06	0.69
1:B:310:GLU:HG2	1:B:354:ILE:HD11	1.74	0.69
1:B:298:ARG:HH12	1:B:340:VAL:HG21	1.58	0.68
1:B:82:PRO:HA	1:B:85:VAL:CG2	2.24	0.68
1:B:76:THR:HG23	1:B:85:VAL:HG22	1.74	0.68
1:A:321:ILE:HG21	1:A:355:LEU:HD21	1.75	0.68
1:B:193:LYS:HB3	1:B:193:LYS:NZ	2.08	0.68
1:B:6:ASP:C	1:B:8:SER:H	1.94	0.67
1:B:505:ASN:HD21	1:B:542:SER:CB	2.06	0.67
1:B:438:PHE:HA	1:B:442:LEU:HD23	1.76	0.67
1:A:24:VAL:HG22	1:A:27:ARG:HH22	1.60	0.67
1:A:196:GLU:HG2	1:A:199:ASN:ND2	2.10	0.67
1:A:76:THR:HG23	1:A:85:VAL:HG12	1.78	0.66
1:B:570:GLN:HB2	1:B:574:VAL:HG11	1.78	0.66
1:B:534:ASN:HA	1:B:537:PHE:CE2	2.31	0.66
1:A:444:SER:HA	1:A:447:MET:HE3	1.78	0.66
1:B:464:ASN:O	1:B:468:LEU:HD13	1.96	0.65
1:B:585:LEU:HB3	1:B:587:LEU:HG	1.78	0.65
1:A:8:SER:HB2	2:A:813:HOH:O	1.97	0.65
1:B:59:TYR:CD1	1:B:60:ASP:N	2.63	0.65
1:B:422:ILE:HG21	2:B:619:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:ASN:HB3	1:B:545:LYS:HD3	1.80	0.64
1:B:6:ASP:C	1:B:8:SER:N	2.51	0.64
1:B:533:ALA:HA	1:B:536:ARG:HE	1.63	0.64
1:A:196:GLU:CG	1:A:199:ASN:HD22	2.09	0.64
1:A:326:LEU:HB3	1:A:327:PRO:HD3	1.80	0.64
1:A:306:LYS:NZ	1:A:306:LYS:HB3	2.13	0.64
1:B:257:ARG:HG3	2:B:784:HOH:O	1.97	0.64
1:B:494:TYR:CD1	1:B:495:LEU:N	2.65	0.63
1:B:565:LYS:HA	1:B:568:GLN:NE2	2.14	0.63
1:A:51:LEU:HB2	1:A:52:PRO:HD3	1.80	0.63
1:A:306:LYS:HD3	2:A:828:HOH:O	1.98	0.62
1:B:253:ASP:CG	1:B:258:VAL:HG11	2.20	0.62
1:B:7:ASP:O	1:B:8:SER:C	2.38	0.62
1:A:395:GLY:HA3	2:A:596:HOH:O	1.99	0.61
1:B:491:ASP:HB3	2:B:680:HOH:O	2.00	0.61
1:A:7:ASP:O	1:A:9:LEU:N	2.33	0.61
1:B:449:TRP:HB3	1:B:461:ALA:HB2	1.82	0.61
1:A:8:SER:HA	2:A:681:HOH:O	2.00	0.61
1:B:37:ILE:N	1:B:37:ILE:HD12	2.16	0.60
1:A:466:LYS:O	1:A:470:GLU:HG3	2.02	0.60
1:B:28:LEU:CD2	1:B:32:LYS:HE3	2.31	0.60
1:A:17:ASP:HA	1:A:20:ARG:NH1	2.17	0.60
1:A:59:TYR:O	1:A:60:ASP:O	2.20	0.60
1:B:494:TYR:HD1	1:B:495:LEU:N	1.98	0.60
1:B:544:GLN:HE21	1:B:581:ALA:HA	1.67	0.59
1:B:345:ALA:HB1	1:B:383:ILE:HG12	1.84	0.59
1:A:438:PHE:HA	1:A:442:LEU:HD23	1.85	0.59
1:A:221:LEU:HD23	1:A:222:LEU:N	2.16	0.59
1:A:238:ASP:HB3	1:A:242:LEU:HD12	1.84	0.59
1:B:37:ILE:H	1:B:37:ILE:HD12	1.67	0.59
1:B:537:PHE:O	1:B:541:LYS:HG3	2.03	0.59
1:B:383:ILE:HG13	2:B:633:HOH:O	2.03	0.58
1:A:39:LEU:HD22	1:A:78:LEU:HD11	1.85	0.58
1:A:444:SER:HA	1:A:447:MET:CE	2.32	0.58
1:B:132:LYS:HG3	1:B:168:TYR:CZ	2.38	0.58
1:A:316:CYS:HA	1:A:319:ASN:HD22	1.69	0.58
1:A:440:GLU:HA	1:A:484:LYS:HE3	1.85	0.58
1:B:494:TYR:CD2	1:B:532:VAL:HG11	2.36	0.58
1:B:565:LYS:HA	1:B:568:GLN:HE21	1.69	0.58
1:B:478:HIS:HA	1:B:482:ILE:HD12	1.86	0.58
1:B:463:SER:O	1:B:467:LYS:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:HD2	1:A:233:LEU:HD21	1.85	0.57
1:B:306:LYS:HG2	1:B:310:GLU:CD	2.25	0.57
1:A:560:LYS:HB3	1:A:561:PRO:HD3	1.86	0.57
1:A:71:GLN:HG3	1:A:75:PHE:CE1	2.39	0.57
1:B:383:ILE:HG21	2:B:633:HOH:O	2.05	0.57
1:B:298:ARG:NH1	1:B:340:VAL:HG21	2.19	0.57
1:B:28:LEU:HD21	1:B:32:LYS:HE3	1.86	0.57
1:A:508:SER:O	1:A:549:ILE:HD13	2.04	0.57
1:A:76:THR:HG23	1:A:85:VAL:CG1	2.35	0.56
1:B:76:THR:HG23	1:B:85:VAL:CG2	2.35	0.56
1:A:491:ASP:O	1:A:497:ARG:HD3	2.05	0.56
1:A:154:TYR:HB3	1:A:155:PRO:HD3	1.87	0.56
1:B:525:LEU:HD22	1:B:562:ILE:HG13	1.87	0.56
1:A:440:GLU:HB3	1:A:484:LYS:NZ	2.20	0.56
1:B:98:VAL:HG12	1:B:99:GLU:N	2.21	0.55
1:B:390:VAL:O	1:B:394:ILE:HG12	2.07	0.55
1:B:306:LYS:CE	1:B:350:GLY:HA3	2.29	0.55
1:B:357:LYS:HG3	1:B:394:ILE:HG22	1.87	0.55
1:B:313:SER:OG	1:B:315:ASP:HB3	2.06	0.55
1:A:439:ASP:HB2	1:A:440:GLU:OE1	2.07	0.55
1:A:387:LEU:H	1:A:432:GLN:HE22	1.55	0.55
1:B:82:PRO:CA	1:B:85:VAL:HG23	2.35	0.55
1:A:228:VAL:O	1:A:232:GLN:HG3	2.05	0.54
1:B:98:VAL:CG1	1:B:99:GLU:N	2.69	0.54
1:A:284:PRO:HA	1:A:287:GLN:HE21	1.72	0.54
1:B:134:LEU:HB3	1:B:146:ALA:HB2	1.90	0.54
1:A:38:ALA:O	1:A:41:LEU:O	2.23	0.54
1:A:76:THR:O	1:A:79:VAL:HG12	2.06	0.54
1:B:372:LEU:O	1:B:380:ARG:HD3	2.08	0.54
1:B:408:VAL:HG22	1:B:445:LEU:HD11	1.90	0.54
1:A:193:LYS:CD	1:A:233:LEU:HD21	2.37	0.54
1:B:404:LEU:HB3	1:B:405:PRO:HD3	1.90	0.53
1:A:10:TYR:N	1:A:11:PRO:HD2	2.24	0.53
1:B:71:GLN:HG3	1:B:75:PHE:CE1	2.43	0.53
1:A:182:ARG:HG2	1:A:219:VAL:HG22	1.91	0.53
1:B:321:ILE:HG23	1:B:322:MET:N	2.22	0.53
1:B:485:VAL:HG12	1:B:500:THR:HG23	1.91	0.53
1:B:508:SER:OG	1:B:546:ILE:HG22	2.09	0.53
1:B:97:THR:O	1:B:97:THR:HG22	2.08	0.53
1:A:358:ASP:O	1:A:362:GLU:HB2	2.09	0.53
1:A:478:HIS:HA	1:A:482:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASP:O	1:A:284:PRO:HD2	2.09	0.52
1:A:267:THR:HG21	1:A:307:GLU:OE1	2.10	0.52
1:B:318:GLU:HA	1:B:321:ILE:HG21	1.91	0.52
1:A:283:VAL:HB	1:A:284:PRO:HD3	1.92	0.52
1:B:221:LEU:C	1:B:221:LEU:HD23	2.30	0.52
1:A:380:ARG:HG3	1:A:425:TYR:OH	2.10	0.52
1:B:324:GLN:O	1:B:327:PRO:HG2	2.10	0.51
1:A:36:THR:OG1	1:A:37:ILE:HD12	2.09	0.51
1:A:98:VAL:HG12	1:A:99:GLU:N	2.24	0.51
1:A:236:GLN:HE22	1:A:274:GLY:HA3	1.76	0.51
1:A:489:SER:O	1:A:497:ARG:HD2	2.11	0.51
1:A:71:GLN:HG3	1:A:75:PHE:HE1	1.76	0.51
1:B:467:LYS:HD3	1:B:470:GLU:OE1	2.11	0.51
1:B:391:ASN:ND2	1:B:433:LEU:HD22	2.25	0.51
1:B:47:ARG:HG2	1:B:79:VAL:HG22	1.92	0.51
1:B:544:GLN:NE2	1:B:581:ALA:HA	2.25	0.51
1:B:380:ARG:HH11	1:B:380:ARG:HG2	1.76	0.50
1:A:128:VAL:HB	1:A:129:PRO:HD3	1.93	0.50
1:A:221:LEU:C	1:A:221:LEU:HD23	2.32	0.50
1:A:37:ILE:HD12	1:A:37:ILE:N	2.26	0.50
1:B:193:LYS:HB3	1:B:193:LYS:HZ2	1.75	0.50
1:B:469:VAL:HG12	1:B:510:VAL:HG11	1.94	0.50
1:B:372:LEU:HD11	1:B:384:ILE:HD11	1.94	0.50
1:A:404:LEU:HB3	1:A:405:PRO:HD3	1.93	0.50
1:B:11:PRO:HG2	1:B:41:LEU:CD2	2.42	0.50
1:B:316:CYS:HA	1:B:319:ASN:ND2	2.24	0.50
1:B:326:LEU:N	1:B:327:PRO:HD2	2.27	0.49
1:B:76:THR:O	1:B:79:VAL:HG12	2.12	0.49
1:A:270:GLN:HE22	1:A:308:PHE:HA	1.77	0.49
1:A:486:LEU:HD22	1:A:523:THR:OG1	2.12	0.49
1:A:28:LEU:CD2	1:A:32:LYS:HE3	2.43	0.49
1:B:10:TYR:N	1:B:11:PRO:HD2	2.28	0.49
1:B:283:VAL:HB	1:B:284:PRO:CD	2.42	0.49
1:A:237:GLU:H	1:A:237:GLU:CD	2.15	0.49
1:B:2:ALA:C	1:B:4:ASP:H	2.15	0.48
1:B:43:VAL:O	1:B:47:ARG:HG3	2.13	0.48
1:B:466:LYS:O	1:B:470:GLU:HG3	2.12	0.48
1:B:81:GLY:HA2	2:B:774:HOH:O	2.12	0.48
1:B:99:GLU:HA	2:B:842:HOH:O	2.13	0.48
1:A:196:GLU:CG	1:A:199:ASN:ND2	2.72	0.48
1:B:420:LEU:O	1:B:424:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:HG22	1:A:97:THR:O	2.13	0.48
1:B:278:THR:O	1:B:283:VAL:HG23	2.14	0.48
1:B:228:VAL:O	1:B:232:GLN:HG3	2.14	0.48
1:B:348:ILE:HG12	1:B:349:MET:HE2	1.94	0.48
1:B:387:LEU:H	1:B:432:GLN:HE22	1.62	0.48
1:A:98:VAL:O	1:A:104:ARG:HD3	2.14	0.48
1:A:349:MET:CE	1:A:368:PHE:HB2	2.44	0.48
1:B:555:LEU:HD11	1:B:587:LEU:HD11	1.96	0.48
1:A:12:ILE:O	1:A:16:ILE:HG13	2.14	0.47
1:A:10:TYR:O	1:A:13:ALA:HB3	2.14	0.47
1:A:325:ILE:HD12	1:A:325:ILE:N	2.28	0.47
1:A:54:LEU:CD2	1:A:58:ILE:HD11	2.44	0.47
1:A:24:VAL:HG22	1:A:27:ARG:NH2	2.28	0.47
1:A:338:GLN:HG3	2:A:635:HOH:O	2.13	0.47
1:B:500:THR:O	1:B:504:ILE:HG13	2.14	0.47
1:A:349:MET:HE1	1:A:368:PHE:HB2	1.97	0.47
1:A:85:VAL:HG11	1:A:117:GLU:HB3	1.97	0.47
1:B:318:GLU:HA	1:B:321:ILE:CG2	2.44	0.47
1:B:445:LEU:O	1:B:448:ALA:HB3	2.14	0.47
1:B:555:LEU:HD21	1:B:587:LEU:HD21	1.96	0.47
1:A:204:ILE:HD13	1:A:207:MET:CE	2.44	0.47
1:A:267:THR:HG23	1:A:304:LYS:HD2	1.96	0.47
1:A:513:GLN:HG3	1:A:549:ILE:O	2.14	0.47
1:A:221:LEU:HG	1:A:261:MET:HG3	1.96	0.47
1:A:265:LYS:HD3	2:A:780:HOH:O	2.13	0.47
1:A:516:THR:HA	1:A:520:MET:HE2	1.97	0.47
1:A:213:SER:HB3	2:A:661:HOH:O	2.15	0.47
1:A:23:ASP:OD2	1:A:26:LEU:HB2	2.14	0.47
1:A:521:LEU:HB3	1:A:522:PRO:HD3	1.96	0.47
1:A:54:LEU:HD22	1:A:58:ILE:HD11	1.97	0.47
1:B:11:PRO:HG2	1:B:41:LEU:HD21	1.96	0.47
1:B:44:GLU:HG3	1:B:45:ARG:N	2.30	0.47
1:A:17:ASP:HA	1:A:20:ARG:HH12	1.78	0.46
1:B:337:ASN:ND2	1:B:339:HIS:HB2	2.30	0.46
1:A:273:VAL:HG21	1:A:277:ILE:HG21	1.96	0.46
1:A:225:GLU:HA	2:A:780:HOH:O	2.16	0.46
1:B:505:ASN:ND2	1:B:542:SER:OG	2.36	0.46
1:A:330:LYS:HE2	2:A:816:HOH:O	2.16	0.46
1:B:533:ALA:HB2	1:B:536:ARG:HH21	1.80	0.46
1:A:552:ASN:O	1:A:556:GLN:HG2	2.16	0.46
1:B:128:VAL:HB	1:B:129:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:GLU:C	1:B:321:ILE:HG22	2.36	0.46
1:B:411:ALA:HB2	2:B:619:HOH:O	2.15	0.46
1:A:37:ILE:H	1:A:37:ILE:HD12	1.80	0.46
1:B:127:PHE:O	1:B:130:LEU:HB3	2.14	0.46
1:B:21:ASN:HD21	1:B:26:LEU:HD23	1.78	0.46
1:A:397:ARG:HG3	2:A:596:HOH:O	2.15	0.46
1:A:27:ARG:O	1:A:30:SER:HB3	2.16	0.45
1:A:526:ARG:HG2	1:A:526:ARG:HH11	1.81	0.45
1:A:563:LEU:O	1:A:567:THR:HG23	2.15	0.45
1:B:132:LYS:HG3	1:B:168:TYR:CE2	2.51	0.45
1:B:207:MET:HA	2:B:787:HOH:O	2.16	0.45
1:A:98:VAL:CG1	1:A:99:GLU:N	2.79	0.45
1:B:555:LEU:O	1:B:559:VAL:HG22	2.15	0.45
1:A:31:ILE:O	1:A:34:LEU:HB2	2.17	0.45
1:A:47:ARG:NH1	1:A:84:TYR:CE2	2.84	0.45
1:A:380:ARG:HD2	1:A:425:TYR:OH	2.15	0.45
1:A:440:GLU:N	1:A:440:GLU:OE1	2.50	0.45
1:B:46:THR:O	1:B:51:LEU:HG	2.16	0.45
1:B:494:TYR:CD1	1:B:494:TYR:C	2.88	0.45
1:A:404:LEU:HD21	1:A:441:LYS:HB3	1.99	0.45
1:B:141:THR:HG21	2:B:842:HOH:O	2.16	0.45
1:B:310:GLU:CG	1:B:354:ILE:HD11	2.45	0.45
1:B:37:ILE:H	1:B:37:ILE:CD1	2.27	0.45
1:A:117:GLU:HA	1:A:117:GLU:OE1	2.17	0.45
1:B:154:TYR:CZ	1:B:195:LEU:HD22	2.51	0.45
1:B:1:ALA:HA	1:B:45:ARG:HH12	1.82	0.45
1:B:567:THR:HG22	1:B:578:ALA:HB3	1.99	0.45
1:A:322:MET:HE2	1:A:363:HIS:CD2	2.51	0.44
1:B:240:GLU:OE2	1:B:244:MET:HG3	2.17	0.44
1:A:154:TYR:CZ	1:A:195:LEU:HD22	2.52	0.44
1:B:426:MET:N	1:B:427:PRO:HD2	2.31	0.44
1:B:547:GLY:N	1:B:548:PRO:HD2	2.32	0.44
1:A:20:ARG:O	1:A:20:ARG:HG2	2.18	0.44
1:A:322:MET:HE3	1:A:326:LEU:HD22	1.98	0.44
1:B:197:LEU:HG	1:B:201:LYS:HE3	1.99	0.44
1:B:89:LEU:HB2	1:B:90:PRO:HD3	1.98	0.44
1:A:397:ARG:HG3	1:A:398:GLN:N	2.33	0.44
1:A:322:MET:CE	1:A:326:LEU:HD22	2.47	0.44
1:A:89:LEU:HB2	1:A:90:PRO:HD3	1.99	0.44
1:A:28:LEU:HD23	1:A:28:LEU:O	2.17	0.44
1:A:440:GLU:HB3	1:A:484:LYS:HZ2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:VAL:HA	1:A:445:LEU:HD21	1.99	0.44
1:B:421:ALA:O	1:B:424:GLU:HB2	2.17	0.44
1:B:488:MET:HA	1:B:491:ASP:OD1	2.18	0.44
1:A:391:ASN:O	1:A:394:ILE:O	2.36	0.43
1:A:426:MET:HB3	1:A:464:ASN:HD21	1.82	0.43
1:B:255:SER:O	1:B:258:VAL:HG13	2.18	0.43
1:A:306:LYS:HZ3	1:A:306:LYS:HB3	1.84	0.43
1:B:120:PRO:O	1:B:124:GLU:HG3	2.18	0.43
1:B:268:GLU:N	1:B:268:GLU:OE1	2.44	0.43
1:B:283:VAL:HB	1:B:284:PRO:HD3	2.01	0.43
1:B:4:ASP:CB	1:B:45:ARG:NH2	2.80	0.43
1:B:555:LEU:CD2	1:B:587:LEU:HD21	2.49	0.43
1:A:90:PRO:HB2	1:A:91:PRO:CD	2.48	0.43
1:B:357:LYS:HA	1:B:393:VAL:HG12	2.01	0.43
1:B:560:LYS:N	1:B:561:PRO:HD2	2.33	0.43
1:B:571:ASP:N	1:B:571:ASP:OD1	2.51	0.43
1:A:224:VAL:O	1:A:227:CYS:HB3	2.19	0.43
1:B:362:GLU:HG2	1:B:363:HIS:CE1	2.53	0.43
1:B:585:LEU:HD23	1:B:587:LEU:CD1	2.48	0.43
1:A:254:LYS:HD2	1:A:254:LYS:HA	1.86	0.43
1:B:306:LYS:O	1:B:310:GLU:HG3	2.19	0.43
1:B:436:GLU:HG2	2:B:812:HOH:O	2.18	0.43
1:B:585:LEU:HD23	1:B:587:LEU:HD12	2.01	0.43
1:A:226:ALA:O	1:A:230:ILE:HG13	2.18	0.42
1:A:273:VAL:HG22	1:A:277:ILE:HD12	2.01	0.42
1:A:352:SER:HB2	1:A:353:PRO:CD	2.48	0.42
1:A:380:ARG:CG	1:A:425:TYR:OH	2.66	0.42
1:A:61:GLU:O	1:A:65:LEU:HG	2.18	0.42
1:B:71:GLN:HG3	1:B:75:PHE:HE1	1.83	0.42
1:A:426:MET:HB3	1:A:464:ASN:ND2	2.34	0.42
1:B:126:HIS:C	1:B:129:PRO:HD2	2.39	0.42
1:B:8:SER:O	1:B:9:LEU:CD2	2.58	0.42
1:B:18:GLU:HB2	2:B:849:HOH:O	2.18	0.42
1:B:270:GLN:HE22	1:B:308:PHE:HA	1.84	0.42
1:B:321:ILE:CG2	1:B:322:MET:N	2.82	0.42
1:A:587:LEU:O	1:A:588:ALA:OXT	2.38	0.42
1:A:77:THR:HG23	1:A:78:LEU:H	1.85	0.42
1:A:21:ASN:OD1	1:A:22:GLU:N	2.53	0.42
1:B:410:LEU:CD1	1:B:422:ILE:HD11	2.50	0.42
1:B:212:ALA:O	1:B:220:ARG:HD2	2.20	0.42
1:B:426:MET:HE3	1:B:426:MET:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:TYR:HD1	1:B:495:LEU:H	1.65	0.42
1:A:39:LEU:CD2	1:A:78:LEU:HD11	2.49	0.42
1:B:410:LEU:CB	1:B:422:ILE:HD11	2.50	0.42
1:B:536:ARG:O	1:B:539:VAL:HB	2.20	0.42
1:A:98:VAL:HG12	1:A:100:GLU:H	1.84	0.41
1:A:114:ILE:O	1:A:118:HIS:HD2	2.03	0.41
1:A:322:MET:HE3	1:A:326:LEU:CD2	2.50	0.41
1:A:387:LEU:H	1:A:432:GLN:NE2	2.17	0.41
1:A:101:THR:HA	1:A:104:ARG:CZ	2.51	0.41
1:A:152:VAL:HG13	2:A:638:HOH:O	2.20	0.41
1:A:176:ASP:HB2	2:A:985:HOH:O	2.19	0.41
1:A:312:LEU:HD13	1:A:320:VAL:HG21	2.03	0.41
1:A:468:LEU:HA	1:A:468:LEU:HD12	1.93	0.41
1:A:154:TYR:N	1:A:155:PRO:CD	2.84	0.41
1:A:365:LEU:HA	1:A:365:LEU:HD12	1.84	0.41
1:B:244:MET:O	1:B:248:ARG:HG3	2.21	0.41
1:B:313:SER:C	1:B:315:ASP:N	2.72	0.41
1:A:365:LEU:O	1:A:368:PHE:HB3	2.21	0.41
1:B:325:ILE:O	1:B:329:ILE:HG12	2.21	0.41
1:B:387:LEU:H	1:B:432:GLN:NE2	2.19	0.41
1:A:28:LEU:HD21	1:A:32:LYS:HE3	2.03	0.41
1:A:77:THR:HG23	1:A:78:LEU:N	2.36	0.41
1:B:14:VAL:O	1:B:18:GLU:HG2	2.21	0.41
1:B:26:LEU:HA	1:B:26:LEU:HD12	1.87	0.41
1:B:21:ASN:O	1:B:27:ARG:HD2	2.21	0.41
1:B:298:ARG:HH11	1:B:298:ARG:CB	2.33	0.41
1:B:348:ILE:HG23	1:B:349:MET:N	2.36	0.41
1:A:100:GLU:OE2	1:A:102:VAL:HG23	2.21	0.41
1:B:576:TYR:O	1:B:580:GLU:HB2	2.21	0.41
1:B:337:ASN:ND2	1:B:339:HIS:H	2.19	0.40
1:B:58:ILE:HD13	1:B:58:ILE:HA	1.94	0.40
1:B:571:ASP:HB2	1:B:572:VAL:H	1.55	0.40
1:A:313:SER:C	1:A:315:ASP:N	2.73	0.40
1:A:4:ASP:HB3	1:A:7:ASP:HB2	2.03	0.40
1:A:8:SER:O	1:A:9:LEU:HD23	2.21	0.40
1:B:407:ILE:O	1:B:408:VAL:C	2.59	0.40
1:B:98:VAL:HG13	2:B:858:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	586/588 (100%)	565 (96%)	16 (3%)	5 (1%)	17	20
1	B	586/588 (100%)	543 (93%)	38 (6%)	5 (1%)	17	20
All	All	1172/1176 (100%)	1108 (94%)	54 (5%)	10 (1%)	17	20

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	317	ARG
1	B	8	SER
1	B	60	ASP
1	B	569	ASP
1	A	8	SER
1	B	572	VAL
1	A	34	LEU
1	A	491	ASP
1	B	389	CYS

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	511/511 (100%)	490 (96%)	21 (4%)	30	43
1	B	511/511 (100%)	499 (98%)	12 (2%)	50	67
All	All	1022/1022 (100%)	989 (97%)	33 (3%)	39	54

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	63	GLU
1	A	77	THR
1	A	156	ARG
1	A	216	GLN
1	A	221	LEU
1	A	254	LYS
1	A	306	LYS
1	A	320	VAL
1	A	322	MET
1	A	362	GLU
1	A	365	LEU
1	A	426	MET
1	A	440	GLU
1	A	451	VAL
1	A	468	LEU
1	A	491	ASP
1	A	494	TYR
1	A	501	LEU
1	A	514	ASP
1	A	551	ASP
1	B	7	ASP
1	B	59	TYR
1	B	60	ASP
1	B	120	PRO
1	B	134	LEU
1	B	258	VAL
1	B	266	PHE
1	B	426	MET
1	B	494	TYR
1	B	558	GLU
1	B	559	VAL
1	B	571	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	118	HIS
1	A	199	ASN
1	A	229	ASN

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Mol	Chain	Res	Type
1	A	249	GLN
1	A	270	GLN
1	A	287	GLN
1	A	319	ASN
1	A	324	GLN
1	A	337	ASN
1	A	363	HIS
1	A	391	ASN
1	A	432	GLN
1	A	505	ASN
1	A	538	ASN
1	B	29	ASN
1	B	229	ASN
1	B	236	GLN
1	B	270	GLN
1	B	319	ASN
1	B	337	ASN
1	B	338	GLN
1	B	363	HIS
1	B	391	ASN
1	B	432	GLN
1	B	443	ASN
1	B	505	ASN
1	B	544	GLN
1	B	568	GLN
1	B	579	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	588/588 (100%)	-0.07	20 (3%)	45	52	12, 31, 71, 101	0
1	B	588/588 (100%)	0.24	32 (5%)	25	32	15, 43, 79, 101	0
All	All	1176/1176 (100%)	0.08	52 (4%)	34	41	12, 35, 75, 101	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	12.0
1	A	1	ALA	11.7
1	A	2	ALA	11.3
1	B	7	ASP	10.5
1	B	2	ALA	10.1
1	B	3	ALA	10.0
1	A	4	ASP	9.0
1	A	7	ASP	8.3
1	B	1	ALA	7.9
1	B	6	ASP	7.7
1	B	588	ALA	6.6
1	A	6	ASP	6.5
1	B	569	ASP	6.3
1	B	8	SER	5.6
1	A	5	GLY	5.6
1	B	5	GLY	5.5
1	B	4	ASP	4.6
1	A	8	SER	4.0
1	B	570	GLN	3.5
1	B	576	TYR	3.3
1	B	584	VAL	3.3
1	A	59	TYR	3.2
1	B	495	LEU	3.2
1	B	339	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	568	GLN	3.0
1	B	22	GLU	3.0
1	B	375	GLU	3.0
1	B	571	ASP	2.9
1	B	453	HIS	2.9
1	B	573	ASP	2.9
1	B	378	GLU	2.8
1	A	588	ALA	2.8
1	A	21	ASN	2.6
1	B	581	ALA	2.6
1	B	397	ARG	2.6
1	B	572	VAL	2.6
1	B	59	TYR	2.4
1	A	24	VAL	2.3
1	B	316	CYS	2.3
1	A	99	GLU	2.3
1	B	395	GLY	2.2
1	A	551	ASP	2.2
1	A	313	SER	2.2
1	B	314	ALA	2.1
1	A	316	CYS	2.1
1	B	377	PRO	2.1
1	A	315	ASP	2.1
1	B	323	SER	2.1
1	B	583	THR	2.1
1	A	54	LEU	2.0
1	A	319	ASN	2.0
1	A	149	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 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.