



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:43 AM GMT

PDB ID : 2Y2W
Title : Elucidation of the substrate specificity and protein structure of AbfB, a family 51 alpha-L-arabinofuranosidase from Bifidobacterium longum.
Authors : Lagaert, S.; Schoepe, J.; Delcour, J.A.; Lavigne, R.; Strelkov, S.V.; Courtin, C.M.; Mikkelsen, N.E.; Sandgren, M.; Volckaert, G.
Deposited on : 2010-12-16
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

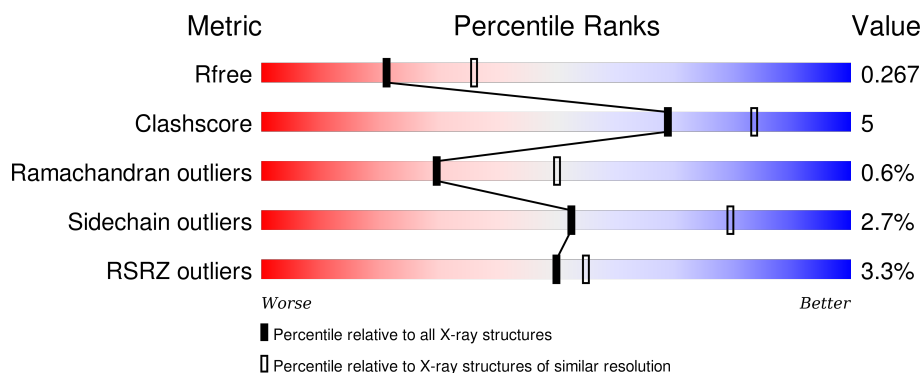
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	574	<div> <div>2%</div> <div>76% 10% • 12%</div> </div>
1	B	574	<div> <div>5%</div> <div>76% 11% • 12%</div> </div>
1	C	574	<div> <div>2%</div> <div>77% 9% • 12%</div> </div>
1	D	574	<div> <div>3%</div> <div>81% 7% • 11%</div> </div>
1	E	574	<div> <div>2%</div> <div>83% 7% • 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	574	<div><div></div><div>3%</div><div>80%</div><div>10%</div><div>•</div><div>10%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24278 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 ARABINOFURANOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	2	1
			3907	2457	668	759	23			
1	B	505	Total	C	N	O	S	0	0	0
			3881	2441	665	752	23			
1	C	504	Total	C	N	O	S	0	0	0
			3855	2426	660	746	23			
1	D	511	Total	C	N	O	S	0	0	0
			3930	2473	674	761	22			
1	E	519	Total	C	N	O	S	0	1	0
			4014	2521	689	781	23			
1	F	519	Total	C	N	O	S	0	1	1
			3992	2510	681	778	23			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	567	LYS	-	EXPRESSION TAG	UNP Q841V6
A	568	GLY	-	EXPRESSION TAG	UNP Q841V6
A	569	HIS	-	EXPRESSION TAG	UNP Q841V6
A	570	HIS	-	EXPRESSION TAG	UNP Q841V6
A	571	HIS	-	EXPRESSION TAG	UNP Q841V6
A	572	HIS	-	EXPRESSION TAG	UNP Q841V6
A	573	HIS	-	EXPRESSION TAG	UNP Q841V6
A	574	HIS	-	EXPRESSION TAG	UNP Q841V6
B	567	LYS	-	EXPRESSION TAG	UNP Q841V6
B	568	GLY	-	EXPRESSION TAG	UNP Q841V6
B	569	HIS	-	EXPRESSION TAG	UNP Q841V6
B	570	HIS	-	EXPRESSION TAG	UNP Q841V6
B	571	HIS	-	EXPRESSION TAG	UNP Q841V6
B	572	HIS	-	EXPRESSION TAG	UNP Q841V6
B	573	HIS	-	EXPRESSION TAG	UNP Q841V6
B	574	HIS	-	EXPRESSION TAG	UNP Q841V6
C	567	LYS	-	EXPRESSION TAG	UNP Q841V6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	568	GLY	-	EXPRESSION TAG	UNP Q841V6
C	569	HIS	-	EXPRESSION TAG	UNP Q841V6
C	570	HIS	-	EXPRESSION TAG	UNP Q841V6
C	571	HIS	-	EXPRESSION TAG	UNP Q841V6
C	572	HIS	-	EXPRESSION TAG	UNP Q841V6
C	573	HIS	-	EXPRESSION TAG	UNP Q841V6
C	574	HIS	-	EXPRESSION TAG	UNP Q841V6
D	567	LYS	-	EXPRESSION TAG	UNP Q841V6
D	568	GLY	-	EXPRESSION TAG	UNP Q841V6
D	569	HIS	-	EXPRESSION TAG	UNP Q841V6
D	570	HIS	-	EXPRESSION TAG	UNP Q841V6
D	571	HIS	-	EXPRESSION TAG	UNP Q841V6
D	572	HIS	-	EXPRESSION TAG	UNP Q841V6
D	573	HIS	-	EXPRESSION TAG	UNP Q841V6
D	574	HIS	-	EXPRESSION TAG	UNP Q841V6
E	567	LYS	-	EXPRESSION TAG	UNP Q841V6
E	568	GLY	-	EXPRESSION TAG	UNP Q841V6
E	569	HIS	-	EXPRESSION TAG	UNP Q841V6
E	570	HIS	-	EXPRESSION TAG	UNP Q841V6
E	571	HIS	-	EXPRESSION TAG	UNP Q841V6
E	572	HIS	-	EXPRESSION TAG	UNP Q841V6
E	573	HIS	-	EXPRESSION TAG	UNP Q841V6
E	574	HIS	-	EXPRESSION TAG	UNP Q841V6
F	567	LYS	-	EXPRESSION TAG	UNP Q841V6
F	568	GLY	-	EXPRESSION TAG	UNP Q841V6
F	569	HIS	-	EXPRESSION TAG	UNP Q841V6
F	570	HIS	-	EXPRESSION TAG	UNP Q841V6
F	571	HIS	-	EXPRESSION TAG	UNP Q841V6
F	572	HIS	-	EXPRESSION TAG	UNP Q841V6
F	573	HIS	-	EXPRESSION TAG	UNP Q841V6
F	574	HIS	-	EXPRESSION TAG	UNP Q841V6

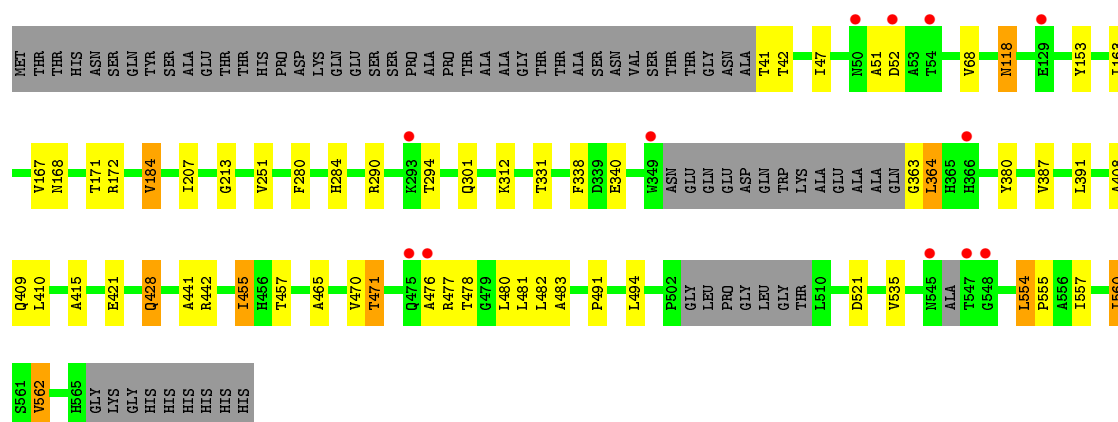
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	130	Total O 130 130	0	0
2	B	105	Total O 105 105	0	0
2	C	135	Total O 135 135	0	0
2	D	123	Total O 123 123	0	0

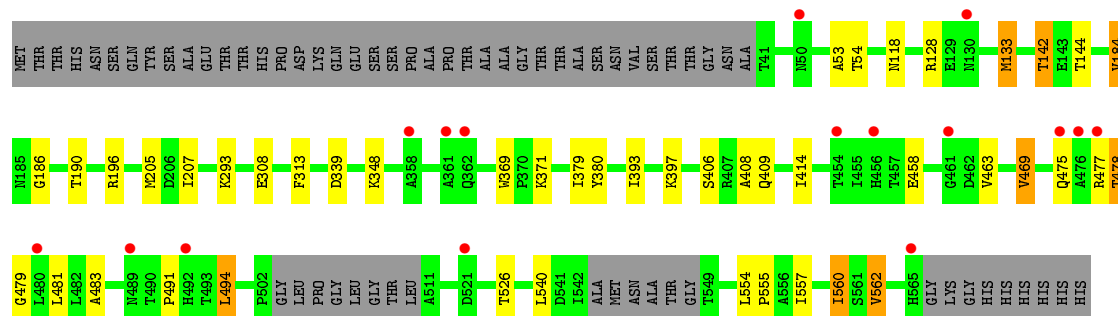
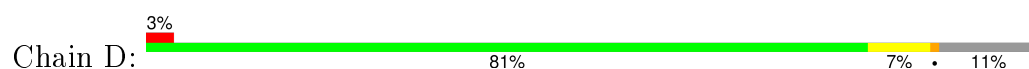
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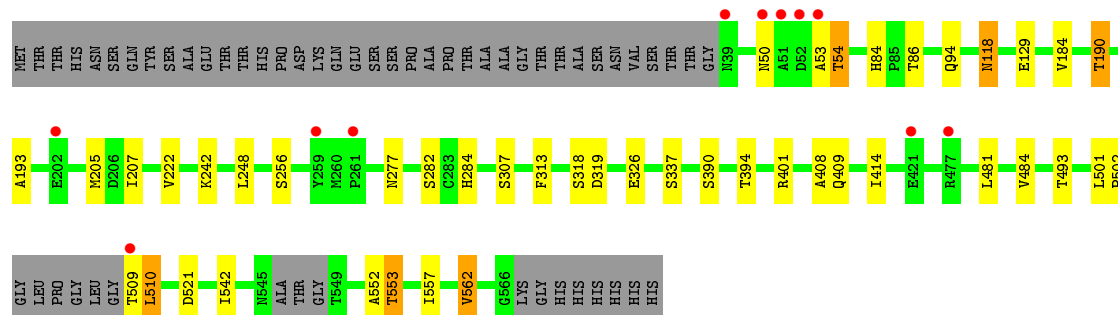
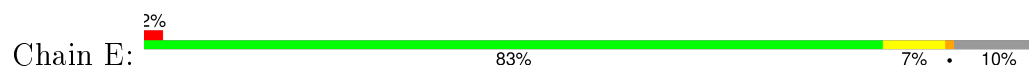
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	119	Total	O	0	0
			119	119		
2	F	87	Total	O	0	0
			87	87		



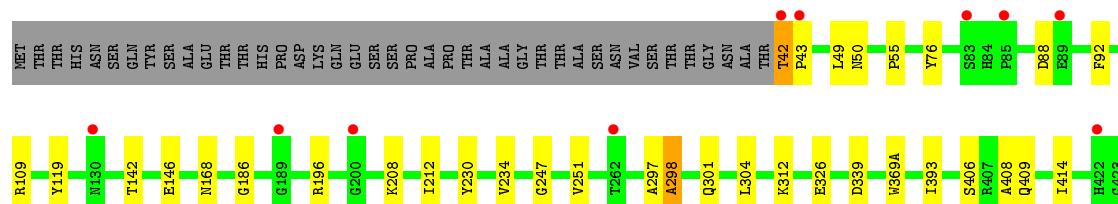
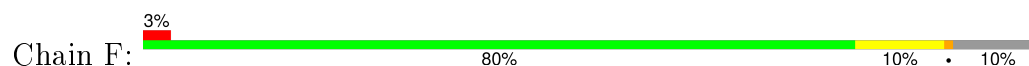
• Molecule 1: ARABINOFURANOSIDASE

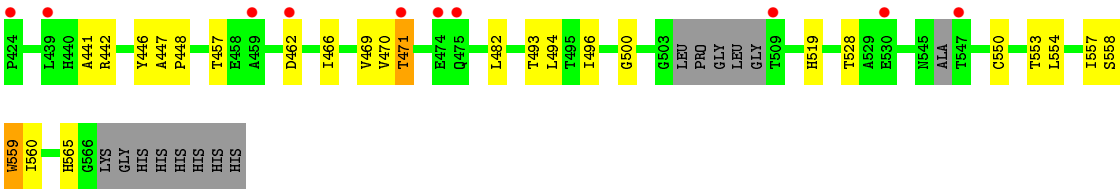


• Molecule 1: ARABINOFURANOSIDASE



• Molecule 1: ARABINOFURANOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.47Å 165.81Å 184.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.50) 99.8 (19.98-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.270 0.218 , 0.267	Depositor DCC
R_{free} test set	5782 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 115158 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24278	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.41	2/4008 (0.0%)	0.59	5/5469 (0.1%)
1	B	0.36	0/3981	0.52	0/5431
1	C	0.32	0/3955	0.50	0/5398
1	D	0.32	0/4035	0.48	0/5509
1	E	0.33	0/4119	0.49	0/5621
1	F	0.32	1/4100 (0.0%)	0.49	0/5596
All	All	0.34	3/24198 (0.0%)	0.51	5/33024 (0.0%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	ASN	C-N	-10.38	1.10	1.34
1	A	565	HIS	C-N	-5.29	1.23	1.33
1	F	565	HIS	C-N	-5.00	1.24	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ASN	O-C-N	-13.44	101.20	122.70
1	A	413	VAL	N-CA-CB	11.07	135.85	111.50
1	A	412	ASN	CA-C-N	8.30	135.46	117.20
1	A	412	ASN	C-N-CA	7.24	139.79	121.70
1	A	413	VAL	N-CA-C	-6.16	94.36	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	412	ASN	Mainchain,Peptide

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	3907	0	3688	49	0
1	B	3881	0	3681	41	0
1	C	3855	0	3645	37	0
1	D	3930	0	3696	27	0
1	E	4014	0	3792	23	0
1	F	3992	0	3770	40	0
2	A	130	0	0	0	0
2	B	105	0	0	0	0
2	C	135	0	0	0	0
2	D	123	0	0	1	0
2	E	119	0	0	0	0
2	F	87	0	0	0	0
All	All	24278	0	22272	212	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 5.

All (212) 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:548:GLY:HA2	1:A:549:THR:HB	1.39	1.04
1:F:297:ALA:HB3	1:F:298:ALA:HB2	1.44	0.96
1:A:475[B]:GLN:NE2	1:A:475[B]:GLN:O	2.02	0.92
1:B:518:LEU:HB3	1:B:559:TRP:HD1	1.35	0.89
1:C:168:ASN:HD21	1:C:171:THR:HG22	1.44	0.81
1:A:351:GLU:HG2	1:A:352:GLN:N	1.99	0.78
1:F:297:ALA:CB	1:F:298:ALA:HB2	2.15	0.77
1:D:142:THR:HG22	1:D:369:TRP:O	1.84	0.76
1:B:518:LEU:HB3	1:B:559:TRP:CD1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:GLY:HA2	1:A:549:THR:CB	2.13	0.76
1:D:53:ALA:HA	1:D:54:THR:OG1	1.86	0.75
1:A:500:GLY:O	1:F:50:ASN:HB2	1.87	0.75
1:A:512:LEU:HD13	1:A:542:ILE:HD12	1.67	0.74
1:D:142:THR:HG23	1:D:371:LYS:HG3	1.70	0.73
1:C:476:ALA:H	1:C:477:ARG:HA	1.53	0.73
1:B:168:ASN:HD21	1:B:171:THR:HG22	1.56	0.71
1:D:379:ILE:HG22	1:D:526:THR:HG21	1.74	0.70
1:C:380:TYR:HD2	1:C:428:GLN:HG2	1.56	0.70
1:D:379:ILE:HG22	1:D:526:THR:CG2	2.23	0.69
1:A:351:GLU:HG2	1:A:352:GLN:H	1.57	0.69
1:C:483:ALA:HB3	1:C:560:ILE:HD11	1.74	0.68
1:C:476:ALA:HB3	1:C:478:THR:H	1.58	0.68
1:D:393:ILE:HG12	1:D:469:VAL:HG22	1.76	0.68
1:A:284:HIS:HD2	1:A:340:GLU:HB2	1.58	0.68
1:D:397:LYS:HG3	1:D:469:VAL:HG12	1.78	0.66
1:F:186:GLY:O	1:F:196:ARG:NH2	2.28	0.66
1:B:49:LEU:O	1:B:51:ALA:N	2.30	0.65
1:B:50:ASN:O	1:B:50:ASN:ND2	2.30	0.65
1:B:66:SER:O	1:B:108:VAL:HA	1.96	0.64
1:A:184:VAL:HG21	1:A:207:ILE:HD12	1.79	0.64
1:E:509:THR:HB	1:E:510:LEU:CB	2.28	0.63
1:D:133:MET:HG3	1:D:144:THR:HA	1.81	0.63
1:C:476:ALA:N	1:C:477:ARG:HA	2.12	0.63
1:A:142:THR:HG22	1:A:369:TRP:O	1.99	0.62
1:B:184:VAL:HG11	1:B:207:ILE:HD12	1.83	0.61
1:D:380:TYR:O	1:D:526:THR:HG23	2.01	0.61
1:C:47:ILE:HD12	1:C:494:LEU:HD21	1.82	0.61
1:C:483:ALA:HB3	1:C:560:ILE:CD1	2.31	0.61
1:A:326[B]:GLU:HA	1:A:326[B]:GLU:OE1	2.01	0.61
1:D:540:LEU:HD13	1:D:560:ILE:HD11	1.83	0.61
1:A:557:ILE:O	1:A:557:ILE:HG22	2.01	0.61
1:A:49:LEU:HD22	1:A:501:LEU:HD11	1.83	0.60
1:A:49:LEU:HD11	1:A:470:VAL:HG21	1.83	0.60
1:E:184:VAL:HG11	1:E:207:ILE:HD12	1.84	0.60
1:B:51:ALA:HA	1:B:52:ASP:C	2.21	0.60
1:A:284:HIS:CD2	1:A:340:GLU:HB2	2.38	0.58
1:B:500:GLY:HA3	1:B:501:LEU:HG	1.86	0.58
1:E:84:HIS:ND1	1:E:86:THR:HG22	2.19	0.58
1:A:475[B]:GLN:HE21	1:A:475[B]:GLN:C	2.06	0.58
1:F:448:PRO:HG3	1:F:470:VAL:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:466:ILE:HG21	1:F:494:LEU:HD21	1.85	0.57
1:B:304:LEU:HD21	1:B:557:ILE:HG12	1.86	0.57
1:B:215:GLU:HG3	1:B:256:SER:HB3	1.87	0.57
1:E:190:THR:HG22	1:E:193:ALA:H	1.70	0.57
1:F:142:THR:HG23	1:F:369(A):TRP:HB2	1.87	0.57
1:D:397:LYS:HG3	1:D:469:VAL:CG1	2.34	0.57
1:E:184:VAL:HG13	1:E:205:MET:HB2	1.87	0.56
1:F:482:LEU:HD22	1:F:559:TRP:CH2	2.41	0.56
1:A:475[B]:GLN:HE21	1:A:475[B]:GLN:CA	2.18	0.56
1:C:284:HIS:HD2	1:C:340:GLU:HB2	1.70	0.56
1:F:297:ALA:HB3	1:F:298:ALA:CB	2.29	0.55
1:F:297:ALA:CA	1:F:298:ALA:HB2	2.37	0.55
1:A:153:TYR:HB2	1:A:205:MET:HE1	1.89	0.55
1:A:54:THR:HG22	1:F:55:PRO:HD2	1.88	0.55
1:A:494:LEU:HD23	1:A:554:LEU:HD13	1.88	0.55
1:B:168:ASN:ND2	1:B:171:THR:HG22	2.21	0.55
1:A:153:TYR:HB2	1:A:205:MET:CE	2.37	0.54
1:D:186:GLY:O	1:D:196:ARG:NH2	2.41	0.53
1:B:301:GLN:HG3	1:B:457:THR:HG22	1.90	0.53
1:F:109:ARG:HD2	1:F:339:ASP:HB2	1.90	0.53
1:C:284:HIS:CD2	1:C:340:GLU:HB2	2.44	0.52
1:E:118:ASN:HB3	1:E:222:VAL:HG21	1.90	0.52
1:D:494:LEU:HD21	1:D:554:LEU:HD13	1.92	0.52
1:B:51:ALA:HA	1:B:53:ALA:N	2.25	0.51
1:D:477:ARG:O	1:D:478:THR:HB	2.10	0.51
1:D:393:ILE:HG23	1:D:469:VAL:HG13	1.91	0.51
1:C:168:ASN:ND2	1:C:171:THR:HG22	2.22	0.51
1:A:466:ILE:HG21	1:A:494:LEU:HD11	1.92	0.51
1:B:455:ILE:HD11	1:B:465:ALA:HA	1.92	0.51
1:E:256:SER:HA	1:E:284:HIS:HB2	1.93	0.51
1:B:50:ASN:CG	1:B:50:ASN:O	2.50	0.50
1:A:184:VAL:HG23	1:A:205:MET:SD	2.51	0.50
1:B:344:TRP:HA	1:B:414:ILE:HD11	1.92	0.50
1:A:50:ASN:HB2	1:F:500:GLY:O	2.12	0.50
1:F:496:ILE:HB	1:F:550:CYS:HB2	1.93	0.50
1:A:475[B]:GLN:C	1:A:475[B]:GLN:NE2	2.65	0.50
1:A:343:VAL:HG23	1:A:388:GLU:HG3	1.94	0.50
1:D:491:PRO:HB3	1:D:555:PRO:HA	1.94	0.49
1:D:308:GLU:HG3	1:D:463:VAL:HG11	1.93	0.49
1:A:349:TRP:CG	1:A:349:TRP:O	2.64	0.49
1:C:441:ALA:HA	1:C:471:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:481:LEU:HB3	1:E:562:VAL:HG13	1.93	0.49
1:B:528:THR:HG23	1:B:531:ALA:H	1.78	0.49
1:E:509:THR:CA	1:E:510:LEU:CB	2.91	0.49
1:C:494:LEU:HD22	1:C:554:LEU:HD11	1.95	0.49
1:F:212:ILE:HG12	1:F:251:VAL:O	2.13	0.49
1:F:446:TYR:HB2	1:F:470:VAL:HG13	1.95	0.48
1:C:301:GLN:HG3	1:C:457:THR:HG22	1.94	0.48
1:B:109:ARG:HA	1:B:164:MET:HB3	1.96	0.48
1:B:51:ALA:HA	1:B:52:ASP:CB	2.43	0.48
1:B:73:ARG:HG2	1:B:372:SER:HB2	1.96	0.48
1:A:71:LEU:HD13	1:A:139:TRP:CD2	2.49	0.48
1:C:380:TYR:CD2	1:C:428:GLN:HG2	2.43	0.47
1:D:483:ALA:HB3	1:D:560:ILE:HG22	1.95	0.47
1:E:86:THR:HG23	1:E:94:GLN:H	1.78	0.47
1:B:47:ILE:HG13	1:B:494:LEU:HD11	1.96	0.47
1:D:128:ARG:NH2	2:D:2016:HOH:O	2.48	0.47
1:B:184:VAL:HG13	1:B:205:MET:HB2	1.97	0.47
1:F:230:TYR:O	1:F:234:VAL:HG22	2.15	0.47
1:B:47:ILE:HD12	1:B:494:LEU:HD21	1.97	0.47
1:A:348:LYS:O	1:A:348:LYS:HG2	2.14	0.47
1:B:171:THR:HG23	1:B:172:ARG:HG3	1.95	0.47
1:F:230:TYR:CZ	1:F:234:VAL:HG11	2.50	0.47
1:B:71:LEU:HG	1:B:139:TRP:CE2	2.50	0.46
1:B:482:LEU:HD22	1:B:559:TRP:CZ3	2.50	0.46
1:C:415:ALA:O	1:C:428:GLN:NE2	2.43	0.46
1:D:408:ALA:HA	1:D:409:GLN:HA	1.65	0.46
1:C:363:GLY:O	1:C:364:LEU:CB	2.64	0.46
1:C:554:LEU:HD22	1:C:560:ILE:HG21	1.97	0.46
1:E:390:SER:HB3	1:E:484:VAL:HG21	1.98	0.46
1:D:478:THR:HA	1:D:479:GLY:HA3	1.63	0.46
1:C:251:VAL:HG22	1:C:280:PHE:HB2	1.97	0.46
1:C:408:ALA:HA	1:C:409:GLN:HA	1.57	0.46
1:E:53:ALA:HA	1:E:54:THR:HG23	1.98	0.46
1:C:153:TYR:HA	1:C:163:ILE:HD11	1.98	0.46
1:A:441:ALA:HA	1:A:471:THR:HG21	1.98	0.45
1:E:408:ALA:HA	1:E:409:GLN:HA	1.65	0.45
1:C:47:ILE:CD1	1:C:494:LEU:HD21	2.45	0.45
1:B:408:ALA:HA	1:B:409:GLN:HA	1.57	0.45
1:C:387:VAL:O	1:C:391:LEU:HG	2.16	0.45
1:C:455:ILE:HD11	1:C:465:ALA:HA	1.99	0.45
1:B:491:PRO:HB3	1:B:555:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ALA:HA	1:A:409:GLN:HA	1.64	0.45
1:F:119:TYR:H	1:F:168:ASN:ND2	2.15	0.45
1:A:307:SER:HB2	1:A:394:THR:OG1	2.17	0.45
1:A:184:VAL:HG22	1:A:205:MET:HB2	1.99	0.45
1:A:215:GLU:HG2	1:A:256:SER:HA	1.98	0.45
1:F:297:ALA:N	1:F:298:ALA:HB2	2.32	0.45
1:A:133:MET:HG3	1:A:144:THR:HA	1.99	0.45
1:E:53:ALA:HB1	1:E:54:THR:OG1	2.17	0.44
1:A:448:PRO:HG2	1:A:450:ILE:HD11	1.97	0.44
1:A:69:GLU:HG3	1:A:112:GLY:HA2	1.98	0.44
1:F:519:HIS:HB2	1:F:558:SER:HB3	1.98	0.44
1:A:49:LEU:HD21	1:A:470:VAL:HB	1.99	0.44
1:E:501:LEU:HA	1:E:502:PRO:HD3	1.91	0.44
1:D:184:VAL:HG21	1:D:207:ILE:HD12	2.00	0.44
1:E:307:SER:HB2	1:E:394:THR:OG1	2.17	0.44
1:F:339:ASP:HA	1:F:406:SER:HB2	1.98	0.44
1:D:184:VAL:HG23	1:D:205:MET:SD	2.58	0.44
1:C:167:VAL:O	1:C:213:GLY:HA2	2.18	0.44
1:A:554:LEU:HD21	1:A:560:ILE:HG12	1.99	0.44
1:E:318:SER:HB3	1:E:401:ARG:HD3	1.99	0.44
1:C:442:ARG:H	1:C:471:THR:HG21	1.83	0.43
1:C:118:ASN:H	1:C:118:ASN:HD22	1.66	0.43
1:D:339:ASP:O	1:D:406:SER:HB2	2.19	0.43
1:F:208:LYS:HE3	1:F:247:GLY:O	2.19	0.43
1:F:119:TYR:H	1:F:168:ASN:HD22	1.64	0.43
1:F:408:ALA:HA	1:F:409:GLN:HA	1.60	0.43
1:C:491:PRO:HB3	1:C:555:PRO:HA	2.01	0.43
1:F:297:ALA:N	1:F:298:ALA:CB	2.82	0.43
1:A:319:ASP:HB3	1:F:326:GLU:HG2	2.00	0.43
1:D:481:LEU:HB3	1:D:562:VAL:HG13	2.01	0.43
1:F:42:THR:HA	1:F:43:PRO:HD2	1.74	0.43
1:F:554:LEU:HD22	1:F:560:ILE:HG21	2.00	0.43
1:F:297:ALA:CA	1:F:298:ALA:CB	2.97	0.43
1:B:68:VAL:HG23	1:B:110:TYR:HD1	1.84	0.42
1:A:196:ARG:HD2	1:A:201:ILE:O	2.18	0.42
1:B:54:THR:HA	1:B:55:PRO:HD3	1.65	0.42
1:B:49:LEU:O	1:B:50:ASN:C	2.57	0.42
1:B:284:HIS:CD2	1:B:340:GLU:HB2	2.55	0.42
1:E:493:THR:HA	1:E:553:THR:HA	2.00	0.42
1:F:49:LEU:HD21	1:F:470:VAL:HG11	2.01	0.42
1:E:282:SER:HA	1:E:337:SER:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:393:ILE:HG23	1:F:469:VAL:HB	2.00	0.42
1:F:88:ASP:OD1	1:F:92:PHE:N	2.49	0.42
1:C:480:LEU:CD1	1:C:482:LEU:HG	2.49	0.42
1:F:442:ARG:O	1:F:471:THR:HG23	2.20	0.42
1:A:49:LEU:HD22	1:A:501:LEU:CD1	2.49	0.42
1:B:381:THR:HG23	1:B:384:ASP:H	1.85	0.42
1:C:42:THR:HG21	1:E:50:ASN:OD1	2.19	0.42
1:B:447:ALA:HA	1:B:448:PRO:HD3	1.88	0.42
1:A:348:LYS:O	1:A:350:ASN:N	2.50	0.42
1:C:171:THR:HG23	1:C:172:ARG:HG3	2.02	0.42
1:F:441:ALA:HA	1:F:471:THR:HG21	2.02	0.42
1:F:493:THR:HG22	1:F:553:THR:HG23	2.02	0.42
1:B:93:ARG:NH1	1:B:419:ALA:HB1	2.35	0.41
1:B:153:TYR:HA	1:B:163:ILE:HD11	2.02	0.41
1:A:475[B]:GLN:HE21	1:A:475[B]:GLN:HA	1.84	0.41
1:D:184:VAL:CG2	1:D:205:MET:SD	3.08	0.41
1:E:542:ILE:HG23	1:E:552:ALA:HB2	2.02	0.41
1:F:301:GLN:HG3	1:F:457:THR:HG22	2.02	0.41
1:C:51:ALA:O	1:C:52:ASP:HB2	2.20	0.41
1:B:303:PHE:CZ	1:B:387:VAL:HG21	2.55	0.41
1:C:118:ASN:N	1:C:118:ASN:HD22	2.18	0.41
1:C:184:VAL:HG11	1:C:207:ILE:HD12	2.03	0.41
1:A:491:PRO:HB3	1:A:555:PRO:HA	2.02	0.41
1:F:49:LEU:O	1:F:500:GLY:HA3	2.21	0.41
1:B:167:VAL:O	1:B:213:GLY:HA2	2.21	0.41
1:A:350:ASN:HA	1:A:351:GLU:HA	1.54	0.41
1:D:142:THR:CG2	1:D:369:TRP:O	2.62	0.41
1:A:60:PRO:HA	1:A:61:PRO:HD3	1.97	0.41
1:B:292:HIS:CE1	1:B:293:LYS:HG2	2.56	0.41
1:A:367:GLU:HA	1:A:368:PRO:HD3	1.84	0.41
1:F:447:ALA:HA	1:F:448:PRO:HD3	1.93	0.40
1:B:112:GLY:HA2	1:B:113:GLY:HA3	1.86	0.40
1:E:242:LYS:HG3	1:E:277:ASN:HB3	2.02	0.40
1:A:271:LEU:HD21	1:A:281:VAL:HB	2.03	0.40
1:C:470:VAL:HG22	1:C:481:LEU:HD13	2.02	0.40
1:C:481:LEU:HB3	1:C:562:VAL:HG13	2.03	0.40
1:F:76:TYR:HE1	1:F:146:GLU:HB2	1.86	0.40
1:E:509:THR:CB	1:E:510:LEU:CB	2.99	0.40
1:C:68:VAL:HG12	1:C:410:LEU:HB3	2.04	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	500/574 (87%)	470 (94%)	26 (5%)	4 (1%)	24	41
1	B	497/574 (87%)	471 (95%)	23 (5%)	3 (1%)	30	50
1	C	496/574 (86%)	473 (95%)	21 (4%)	2 (0%)	39	61
1	D	505/574 (88%)	474 (94%)	28 (6%)	3 (1%)	30	50
1	E	514/574 (90%)	494 (96%)	17 (3%)	3 (1%)	30	50
1	F	514/574 (90%)	490 (95%)	21 (4%)	3 (1%)	30	50
All	All	3026/3444 (88%)	2872 (95%)	136 (4%)	18 (1%)	30	50

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	50	ASN
1	E	510	LEU
1	F	298	ALA
1	A	349	TRP
1	D	478	THR
1	C	364	LEU
1	A	366	HIS
1	B	51	ALA
1	A	412	ASN
1	B	412	ASN
1	D	557	ILE
1	E	414	ILE
1	F	414	ILE
1	A	413	VAL
1	D	414	ILE
1	C	557	ILE
1	F	557	ILE
1	E	557	ILE

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	404/457 (88%)	396 (98%)	8 (2%)	63	86
1	B	402/457 (88%)	393 (98%)	9 (2%)	60	84
1	C	397/457 (87%)	380 (96%)	17 (4%)	35	61
1	D	402/457 (88%)	388 (96%)	14 (4%)	43	70
1	E	414/457 (91%)	403 (97%)	11 (3%)	52	79
1	F	412/457 (90%)	405 (98%)	7 (2%)	68	89
All	All	2431/2742 (89%)	2365 (97%)	66 (3%)	52	79

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	142	THR
1	A	338	PHE
1	A	352	GLN
1	A	422	HIS
1	A	471	THR
1	A	501	LEU
1	A	510	LEU
1	B	49	LEU
1	B	50	ASN
1	B	125	ILE
1	B	215	GLU
1	B	332	LYS
1	B	338	PHE
1	B	348	LYS
1	B	535	VAL
1	B	559	TRP
1	C	41	THR
1	C	118	ASN
1	C	184	VAL
1	C	290	ARG
1	C	294	THR

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Mol	Chain	Res	Type
1	C	312	LYS
1	C	331	THR
1	C	338	PHE
1	C	421	GLU
1	C	428	GLN
1	C	455	ILE
1	C	471	THR
1	C	521	ASP
1	C	535	VAL
1	C	554	LEU
1	C	560	ILE
1	C	562	VAL
1	D	118	ASN
1	D	133	MET
1	D	142	THR
1	D	184	VAL
1	D	190	THR
1	D	293	LYS
1	D	313	PHE
1	D	348	LYS
1	D	458	GLU
1	D	469	VAL
1	D	475	GLN
1	D	494	LEU
1	D	560	ILE
1	D	562	VAL
1	E	54	THR
1	E	118	ASN
1	E	129	GLU
1	E	190	THR
1	E	248	LEU
1	E	313	PHE
1	E	319	ASP
1	E	326	GLU
1	E	521	ASP
1	E	553	THR
1	E	562	VAL
1	F	42	THR
1	F	304	LEU
1	F	312	LYS
1	F	462	ASP
1	F	471	THR

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Mol	Chain	Res	Type
1	F	528	THR
1	F	559	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS
1	B	50	ASN
1	B	90	ASN
1	B	94	GLN
1	B	195	GLN
1	B	516	GLN
1	C	140	HIS
1	C	366	HIS
1	D	157	GLN
1	D	362	GLN
1	D	475	GLN
1	D	492	HIS
1	F	84	HIS
1	F	195	GLN
1	F	239	HIS
1	F	485	ASN

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, 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	506/574 (88%)	-0.01	13 (2%) 59 63	19, 34, 53, 62	0
1	B	505/574 (87%)	0.54	28 (5%) 29 32	30, 44, 62, 68	0
1	C	504/574 (87%)	-0.09	12 (2%) 62 66	19, 31, 49, 59	0
1	D	511/574 (89%)	0.07	16 (3%) 52 57	18, 34, 61, 73	0
1	E	519/574 (90%)	-0.08	11 (2%) 67 71	21, 32, 46, 54	0
1	F	519/574 (90%)	0.14	20 (3%) 43 48	26, 39, 60, 68	0
All	All	3064/3444 (88%)	0.09	100 (3%) 50 55	18, 36, 57, 73	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	52	ASP	6.3
1	B	50	ASN	5.6
1	B	294	THR	5.1
1	E	39	ASN	4.4
1	C	547	THR	4.4
1	B	51	ALA	4.2
1	F	43	PRO	3.9
1	A	510	LEU	3.8
1	A	349	TRP	3.8
1	D	358	ALA	3.7
1	F	530	GLU	3.7
1	D	50	ASN	3.6
1	A	352	GLN	3.5
1	D	475	GLN	3.4
1	B	458	GLU	3.3
1	E	509	THR	3.3
1	F	547	THR	3.3
1	F	422	HIS	3.2
1	D	489	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	42	THR	3.2
1	D	477	ARG	3.1
1	A	475[A]	GLN	3.1
1	B	130	ASN	3.0
1	F	200	GLY	3.0
1	D	361	ALA	3.0
1	B	43	PRO	3.0
1	B	46	SER	2.9
1	F	189	GLY	2.9
1	F	439	LEU	2.9
1	F	130	ASN	2.9
1	C	548	GLY	2.9
1	D	480	LEU	2.8
1	F	471	THR	2.8
1	B	329	ASN	2.8
1	A	477	ARG	2.8
1	C	349	TRP	2.8
1	A	545	ASN	2.8
1	C	54	THR	2.8
1	B	545	ASN	2.8
1	E	51	ALA	2.8
1	A	462	ASP	2.8
1	F	462	ASP	2.7
1	A	470	VAL	2.7
1	F	475	GLN	2.7
1	E	53	ALA	2.7
1	F	509	THR	2.6
1	D	362	GLN	2.6
1	E	50	ASN	2.6
1	E	259	TYR	2.6
1	F	424	PRO	2.5
1	D	476	ALA	2.5
1	F	89	GLU	2.5
1	E	261	PRO	2.5
1	C	476	ALA	2.5
1	B	451	SER	2.5
1	D	454	THR	2.5
1	C	293	LYS	2.5
1	B	381	THR	2.5
1	B	500	GLY	2.4
1	C	366	HIS	2.4
1	D	461	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	42	THR	2.3
1	B	445	ALA	2.3
1	B	495	THR	2.3
1	C	50	ASN	2.3
1	B	297	ALA	2.2
1	C	545	ASN	2.2
1	D	565	HIS	2.2
1	B	295	ARG	2.2
1	F	83	SER	2.2
1	B	291	GLY	2.2
1	B	41	THR	2.2
1	C	129	GLU	2.2
1	E	202	GLU	2.2
1	F	459	ALA	2.1
1	C	475	GLN	2.1
1	D	130	ASN	2.1
1	D	492	HIS	2.1
1	B	544	MET	2.1
1	A	365	HIS	2.1
1	B	282	SER	2.1
1	B	462	ASP	2.1
1	B	471	THR	2.1
1	F	42	THR	2.1
1	F	474	GLU	2.1
1	B	362	GLN	2.1
1	A	331	THR	2.1
1	E	477	ARG	2.1
1	C	52	ASP	2.1
1	B	268	LYS	2.1
1	B	496	ILE	2.1
1	A	261	PRO	2.1
1	D	521	ASP	2.1
1	B	477	ARG	2.0
1	A	366	HIS	2.0
1	F	85	PRO	2.0
1	F	262	THR	2.0
1	E	421	GLU	2.0
1	D	456	HIS	2.0
1	B	347	ASP	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.