Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 02:14 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

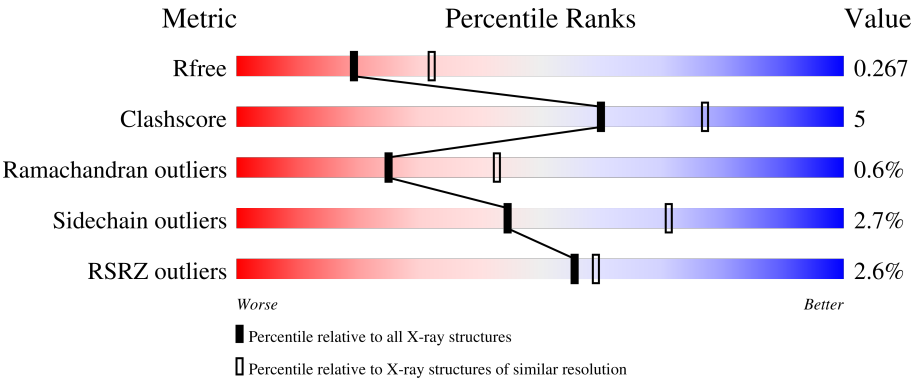
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	574	2% 76% 10% • 12%
1	B	574	4% 76% 11% • 12%
1	C	574	2% 77% 9% • 12%
1	D	574	2% 81% 7% • 11%
1	E	574	2% 83% 7% • 10%

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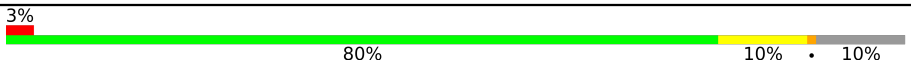
Mol	Chain	Length	Quality of chain
1	F	574	

2 Entry composition (i)

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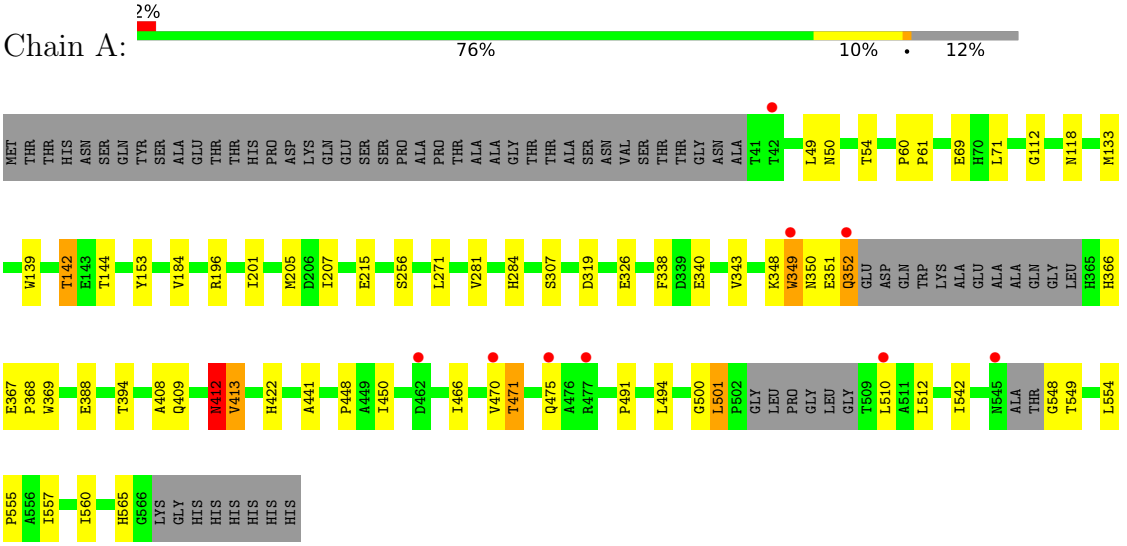
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	119	Total O 119 119	0	0
2	F	87	Total O 87 87	0	0

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.

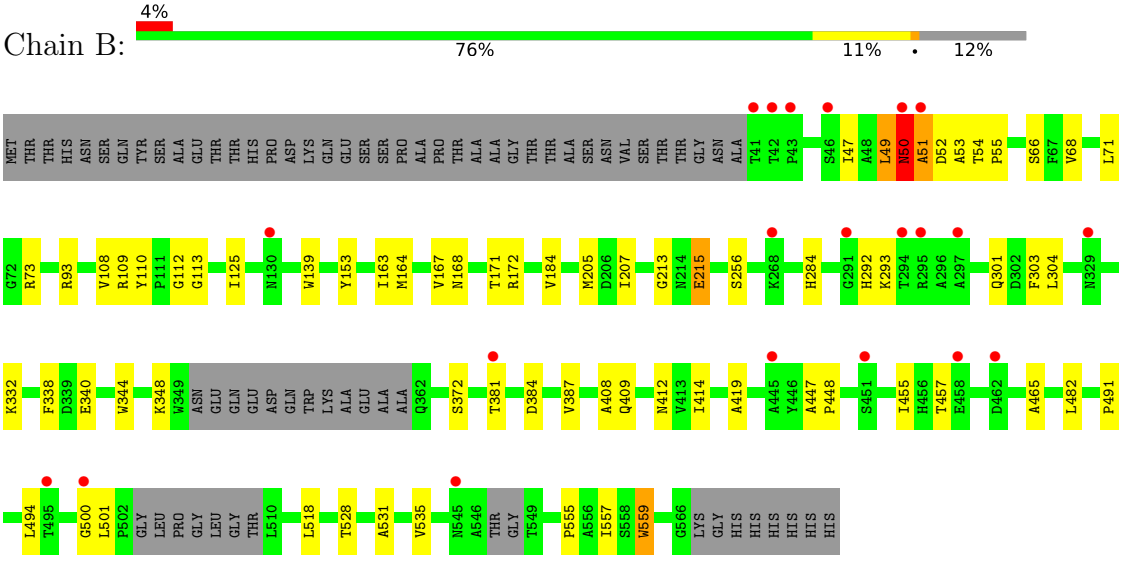
• Molecule 1: ARABINOFURANOSIDASE

Chain A:



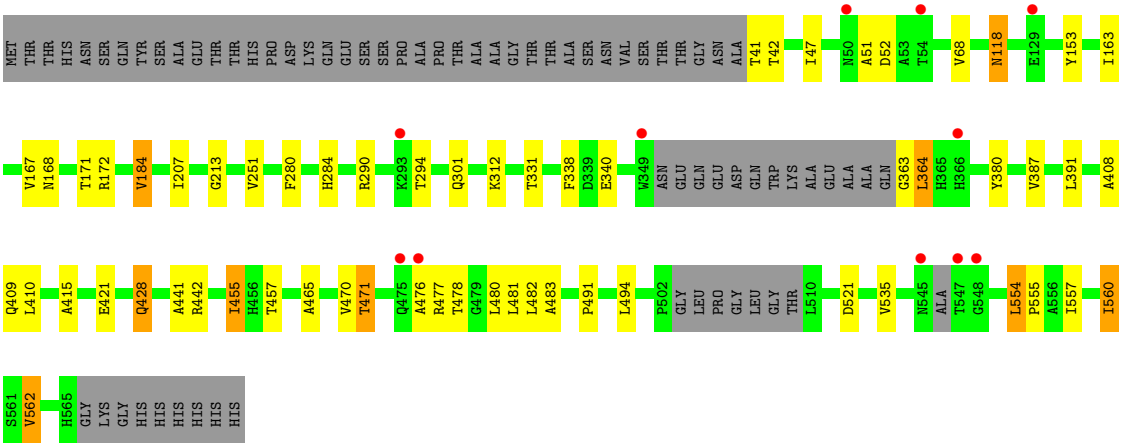
• Molecule 1: ARABINOFURANOSIDASE

Chain B:



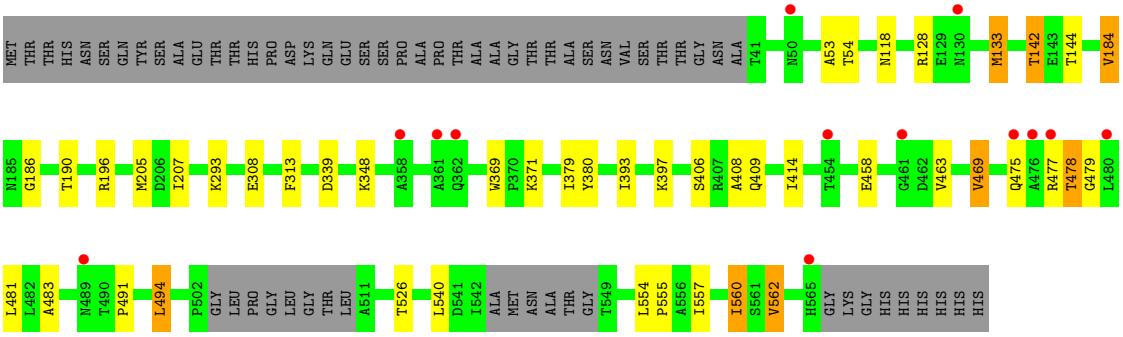
• Molecule 1: ARABINOFURANOSIDASE

Chain C:



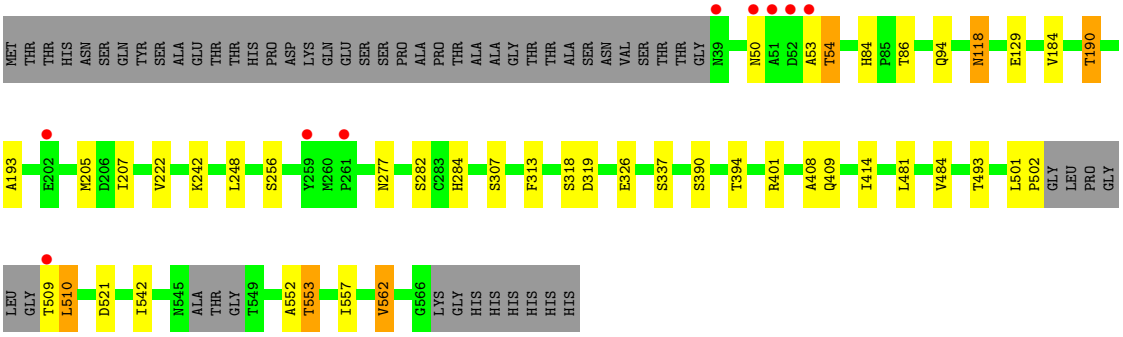
• Molecule 1: ARABINOFURANOSIDASE

Chain D:



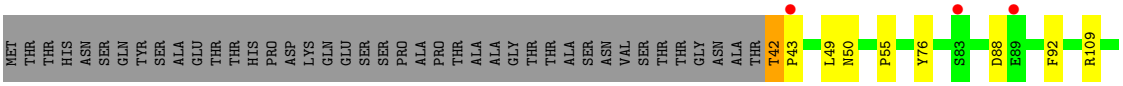
• Molecule 1: ARABINOFURANOSIDASE

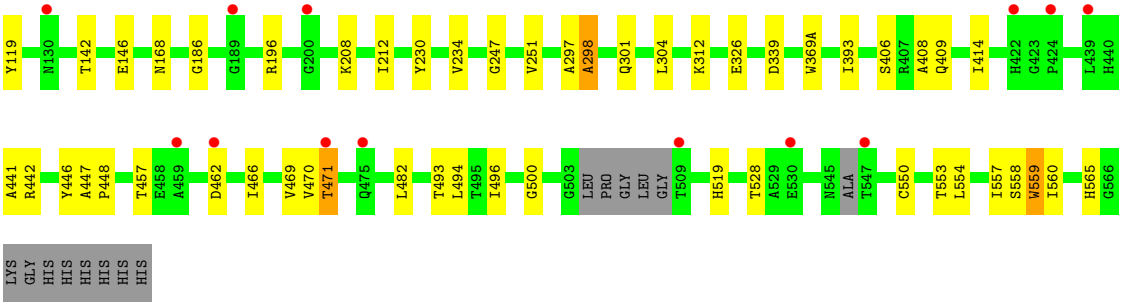
Chain E:



• Molecule 1: ARABINOFURANOSIDASE

Chain F:




Y119 N130 T142 E146 N168 G186 G189 R196 G200 K208 I212 Y230 V234 G247 V251 A297 A298 Q301 L304 K312 E326 D339 W369A I393 S406 R407 A408 Q409 I414 H422 G423 P424 L439 H440
A441 R442 Y446 A447 P448 T457 E458 A459 D462 I466 V469 V470 T471 Q475 L482 T493 L494 T495 I496 G500 G503 LEU PRO GLY LEU GLY T509 H519 T528 A529 E530 N545 ALA T547 C550 T553 L554 I557 S558 W559 I560 H565 G566
LYS GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.02%)	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[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	0.41	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(^{o})	Ideal(^{o})
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 (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	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:O	1:A:475[B]:GLN:NE2	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:C:380:TYR:HD2	1:C:428:GLN:HG2	1.56	0.70
1:D:379:ILE:HG22	1:D:526:THR:HG21	1.74	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:A:326[B]:GLU:OE1	1:A:326[B]:GLU:HA	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:D:380:TYR:O	1:D:526:THR:HG23	2.01	0.61
1:D:540:LEU:HD13	1:D:560:ILE:HD11	1.83	0.61
1:A:557:ILE:HG22	1:A:557:ILE:O	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:54:THR:HG22	1:F:55:PRO:HD2	1.88	0.55
1:A:153:TYR:HB2	1:A:205:MET:HE1	1.89	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:B:301:GLN:HG3	1:B:457:THR:HG22	1.90	0.53
1:D:186:GLY:O	1:D:196:ARG:NH2	2.41	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: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:C:168:ASN:ND2	1:C:171:THR:HG22	2.22	0.51
1:E:256:SER:HA	1:E:284:HIS:HB2	1.93	0.51
1:B:50:ASN:O	1:B:50:ASN:CG	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:NE2	1:A:475[B]:GLN:C	2.65	0.50
1:A:343:VAL:HG23	1:A:388:GLU:HG3	1.94	0.50
1:D:308:GLU:HG3	1:D:463:VAL:HG11	1.93	0.49
1:D:491:PRO:HB3	1:D:555:PRO:HA	1.94	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:B:47:ILE:HG13	1:B:494:LEU:HD11	1.96	0.47
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: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:C:251:VAL:HG22	1:C:280:PHE:HB2	1.97	0.46
1:D:478:THR:HA	1:D:479:GLY:HA3	1.63	0.46
1:C:153:TYR:HA	1:C:163:ILE:HD11	1.98	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: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:B:408:ALA:HA	1:B:409:GLN:HA	1.57	0.45
1:C:47:ILE:CD1	1:C:494:LEU:HD21	2.45	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:307:SER:HB2	1:A:394:THR:OG1	2.17	0.45
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: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:A:133:MET:HG3	1:A:144:THR:HA	1.99	0.45
1:F:297:ALA:N	1:F:298:ALA:HB2	2.32	0.45
1:A:448:PRO:HG2	1:A:450:ILE:HD11	1.97	0.44
1:E:53:ALA:HB1	1:E:54:THR:OG1	2.17	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: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:E:501:LEU:HA	1:E:502:PRO:HD3	1.91	0.44
1:D:184:VAL:HG23	1:D:205:MET:SD	2.58	0.44
1:F:339:ASP:HA	1:F:406:SER:HB2	1.98	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:HD22	1:C:118:ASN:H	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:C:491:PRO:HB3	1:C:555:PRO:HA	2.01	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: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:297:ALA:N	1:F:298:ALA:CB	2.82	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: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:68:VAL:HG23	1:B:110:TYR:HD1	1.84	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:E:282:SER:HA	1:E:337:SER:O	2.18	0.42
1:F:49:LEU:HD21	1:F:470:VAL:HG11	2.01	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:C:480:LEU:CD1	1:C:482:LEU:HG	2.49	0.42
1:F:88:ASP:OD1	1:F:92:PHE:N	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:B:447:ALA:HA	1:B:448:PRO:HD3	1.88	0.42
1:C:42:THR:HG21	1:E:50:ASN:OD1	2.19	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:B:303:PHE:CZ	1:B:387:VAL:HG21	2.55	0.41
1:C:51:ALA:O	1:C:52:ASP:HB2	2.20	0.41
1:C:118:ASN:HD22	1:C:118:ASN:N	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:B:167:VAL:O	1:B:213:GLY:HA2	2.21	0.41
1:F:49:LEU:O	1:F:500:GLY:HA3	2.21	0.41
1:A:60:PRO:HA	1:A:61:PRO:HD3	1.97	0.41
1:A:350:ASN:HA	1:A:351:GLU:HA	1.54	0.41
1:B:292:HIS:CE1	1:B:293:LYS:HG2	2.56	0.41
1:D:142:THR:CG2	1:D:369:TRP:O	2.62	0.41
1:A:367:GLU:HA	1:A:368:PRO:HD3	1.84	0.41
1:A:271:LEU:HD21	1:A:281:VAL:HB	2.03	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:F:447:ALA:HA	1:F:448:PRO:HD3	1.93	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 (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	500/574 (87%)	470 (94%)	26 (5%)	4 (1%)	19	35
1	B	497/574 (87%)	471 (95%)	23 (5%)	3 (1%)	25	43
1	C	496/574 (86%)	473 (95%)	21 (4%)	2 (0%)	34	54
1	D	505/574 (88%)	474 (94%)	28 (6%)	3 (1%)	25	43
1	E	514/574 (90%)	494 (96%)	17 (3%)	3 (1%)	25	43
1	F	514/574 (90%)	490 (95%)	21 (4%)	3 (1%)	25	43
All	All	3026/3444 (88%)	2872 (95%)	136 (4%)	18 (1%)	25	43

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 (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	404/457 (88%)	396 (98%)	8 (2%)	55	79
1	B	402/457 (88%)	393 (98%)	9 (2%)	52	77
1	C	397/457 (87%)	380 (96%)	17 (4%)	29	53
1	D	402/457 (88%)	388 (96%)	14 (4%)	36	62
1	E	414/457 (91%)	403 (97%)	11 (3%)	44	71
1	F	412/457 (90%)	405 (98%)	7 (2%)	60	82
All	All	2431/2742 (89%)	2365 (97%)	66 (3%)	44	71

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

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	412:ASN	C	413:VAL	N	1.10

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	506/574 (88%)	-0.07	9 (1%)	68	71	19, 34, 53, 62	0
1	B	505/574 (87%)	0.47	21 (4%)	36	39	30, 44, 62, 68	0
1	C	504/574 (87%)	-0.14	11 (2%)	62	65	19, 31, 49, 59	0
1	D	511/574 (89%)	0.02	13 (2%)	57	61	18, 34, 61, 73	0
1	E	519/574 (90%)	-0.13	9 (1%)	70	72	21, 32, 46, 54	0
1	F	519/574 (90%)	0.08	16 (3%)	49	52	26, 39, 60, 68	0
All	All	3064/3444 (88%)	0.04	79 (2%)	56	59	18, 36, 57, 73	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	52	ASP	5.9
1	B	50	ASN	5.3
1	B	294	THR	4.8
1	E	39	ASN	4.2
1	C	547	THR	4.1
1	B	51	ALA	3.9
1	F	43	PRO	3.7
1	A	349	TRP	3.7
1	A	510	LEU	3.6
1	D	358	ALA	3.6
1	F	530	GLU	3.6
1	D	50	ASN	3.4
1	D	475	GLN	3.3
1	A	352	GLN	3.3
1	D	489	ASN	3.1
1	F	422	HIS	3.1
1	B	458	GLU	3.1
1	E	509	THR	3.1
1	F	547	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	42	THR	3.0
1	A	475[A]	GLN	3.0
1	D	477	ARG	3.0
1	B	130	ASN	2.9
1	B	46	SER	2.8
1	F	200	GLY	2.8
1	B	43	PRO	2.8
1	D	361	ALA	2.8
1	F	439	LEU	2.8
1	D	480	LEU	2.8
1	B	329	ASN	2.7
1	F	130	ASN	2.7
1	F	189	GLY	2.7
1	C	548	GLY	2.7
1	A	477	ARG	2.7
1	F	471	THR	2.7
1	E	51	ALA	2.6
1	C	54	THR	2.6
1	B	545	ASN	2.6
1	A	545	ASN	2.6
1	C	349	TRP	2.6
1	F	475	GLN	2.6
1	A	462	ASP	2.6
1	E	259	TYR	2.6
1	A	470	VAL	2.5
1	D	362	GLN	2.5
1	F	462	ASP	2.5
1	F	89	GLU	2.5
1	F	424	PRO	2.5
1	E	53	ALA	2.5
1	E	50	ASN	2.4
1	F	509	THR	2.4
1	D	476	ALA	2.4
1	B	451	SER	2.4
1	E	261	PRO	2.4
1	C	293	LYS	2.3
1	C	476	ALA	2.3
1	B	381	THR	2.3
1	D	454	THR	2.3
1	D	461	GLY	2.3
1	B	42	THR	2.2
1	B	500	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	366	HIS	2.2
1	D	565	HIS	2.2
1	C	545	ASN	2.2
1	B	445	ALA	2.1
1	C	50	ASN	2.1
1	C	129	GLU	2.1
1	B	41	THR	2.1
1	B	295	ARG	2.1
1	B	495	THR	2.1
1	E	202	GLU	2.1
1	F	83	SER	2.1
1	B	291	GLY	2.1
1	B	297	ALA	2.1
1	F	459	ALA	2.1
1	D	130	ASN	2.1
1	B	462	ASP	2.0
1	C	475	GLN	2.0
1	B	268	LYS	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.