Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:24 pm BST

PDB ID	:	5Y58
Title	:	Crystal structure of Ku70/80 and TLC1
Authors	:	Chen, H.; Xue, J.; Wu, J.; Lei, M.
Deposited on	:	2017-08-08
Resolution	:	2.80 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 ①) were used in the production of this report:

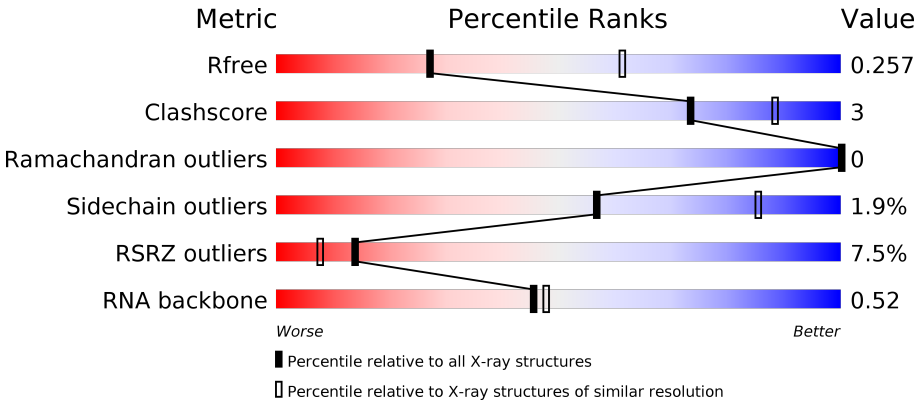
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 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	575	83% 11% • 5%
1	C	575	84% 10% • 5%
1	E	575	7% 84% 11% • 5%
2	B	628	7% 82% 8% • 10%

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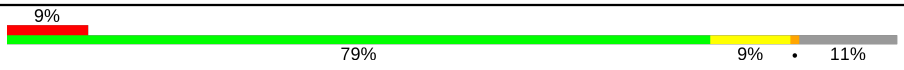
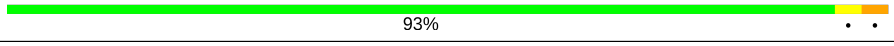
Mol	Chain	Length	Quality of chain
2	D	628	
2	F	628	
3	X	30	
3	Y	30	
3	Z	30	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29320 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 ATP-dependent DNA helicase II subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4549	2926	743	863	17			
1	C	548	Total	C	N	O	S	0	0	0
			4549	2926	743	863	17			
1	E	548	Total	C	N	O	S	0	0	0
			4549	2926	743	863	17			

- Molecule 2 is a protein called ATP-dependent DNA helicase II subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	568	Total	C	N	O	S	0	0	0
			4509	2849	750	887	23			
2	D	560	Total	C	N	O	S	0	0	0
			4442	2812	737	870	23			
2	F	565	Total	C	N	O	S	0	0	0
			4493	2841	747	882	23			

- Molecule 3 is a RNA chain called TLC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	30	Total	C	N	O	P	0	0	0
			641	287	116	208	30			
3	Y	30	Total	C	N	O	P	0	0	0
			641	287	116	208	30			
3	Z	30	Total	C	N	O	P	0	0	0
			641	287	116	208	30			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		

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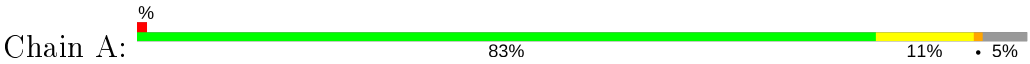
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	66	Total O 66 66	0	0
4	X	14	Total O 14 14	0	0
4	C	19	Total O 19 19	0	0
4	D	48	Total O 48 48	0	0
4	Y	13	Total O 13 13	0	0
4	E	34	Total O 34 34	0	0
4	F	45	Total O 45 45	0	0
4	Z	7	Total O 7 7	0	0

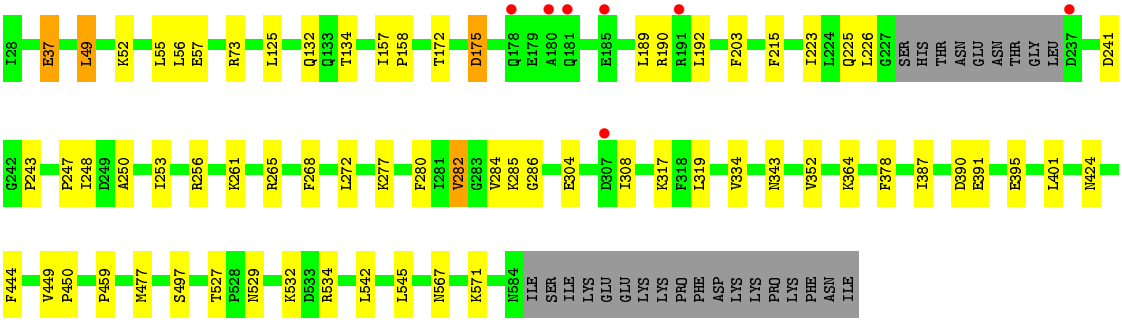
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: ATP-dependent DNA helicase II subunit 1

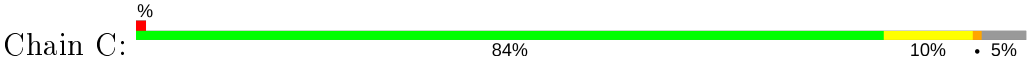
Chain A:

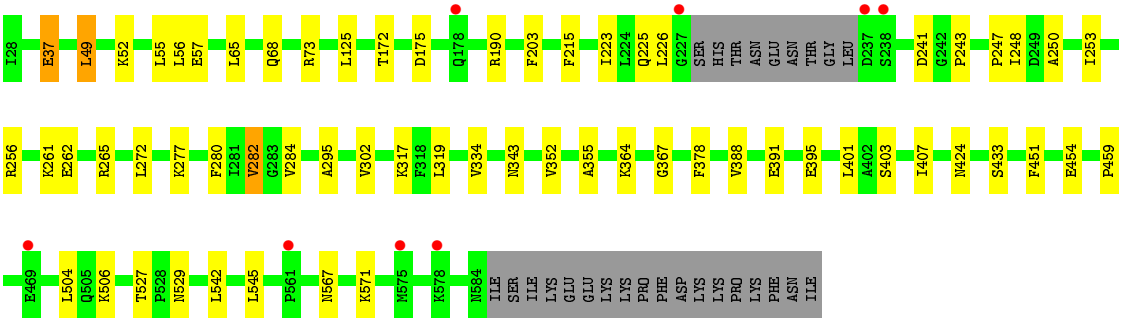




- Molecule 1: ATP-dependent DNA helicase II subunit 1

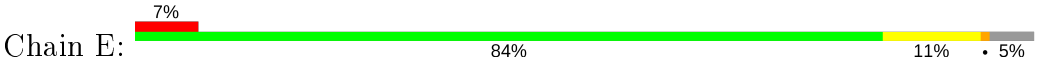
Chain C:

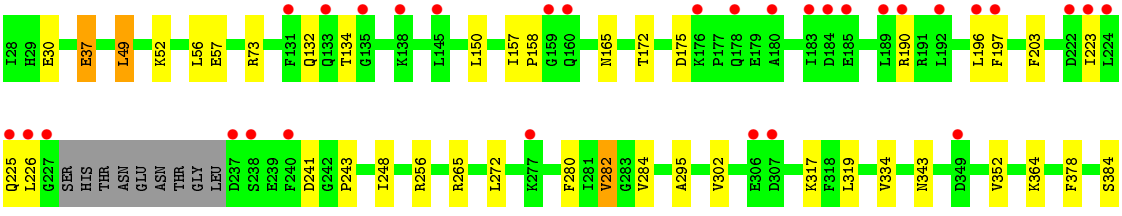


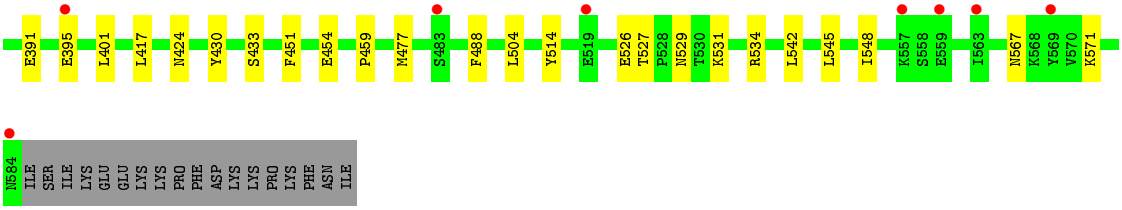


- Molecule 1: ATP-dependent DNA helicase II subunit 1

Chain E:

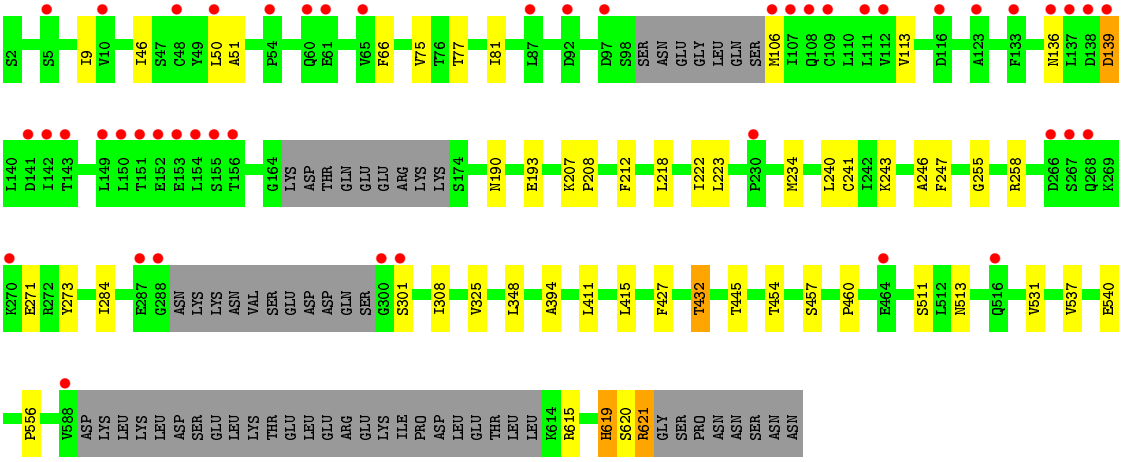






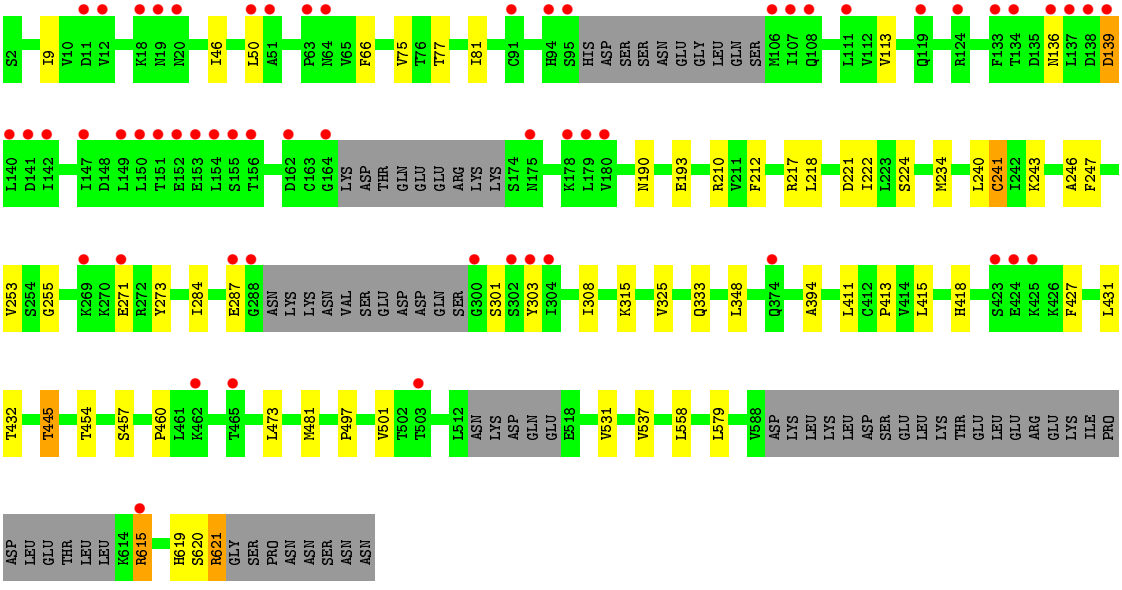
• Molecule 2: ATP-dependent DNA helicase II subunit 2

Chain B:



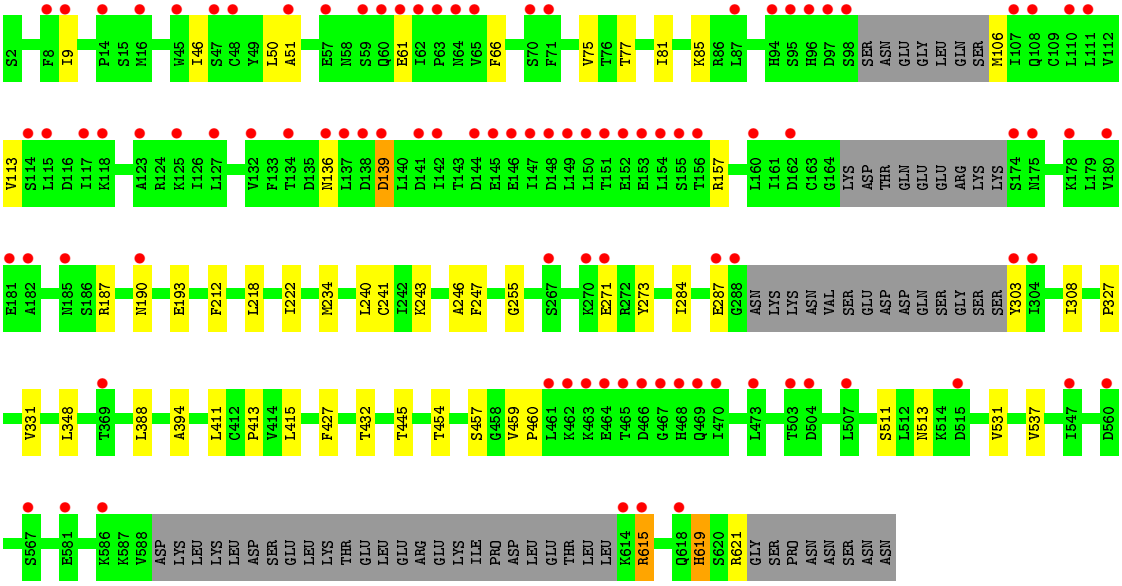
• Molecule 2: ATP-dependent DNA helicase II subunit 2

Chain D:



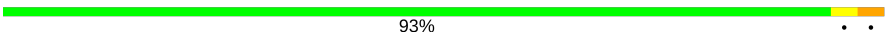
• Molecule 2: ATP-dependent DNA helicase II subunit 2

Chain F:



- Molecule 3: TLC1

Chain X:

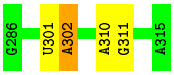


- Molecule 3: TLC1

Chain Y:

- Molecule 3: TLC1

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	116.30Å 115.16Å 115.85Å 77.43° 78.48° 63.73°	Depositor
Resolution (Å)	44.11 – 2.80 48.33 – 2.78	Depositor EDS
% Data completeness (in resolution range)	91.8 (44.11-2.80) 90.6 (48.33-2.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.215 , 0.258 0.218 , 0.257	Depositor DCC
R_{free} test set	5915 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	29320	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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	0.24	0/4647	0.37	0/6253
1	C	0.26	0/4647	0.38	0/6253
1	E	0.25	0/4647	0.37	0/6253
2	B	0.23	0/4583	0.41	0/6203
2	D	0.24	0/4514	0.41	0/6109
2	F	0.25	0/4567	0.42	0/6182
3	X	0.24	0/717	0.72	0/1115
3	Y	0.23	0/717	0.74	0/1115
3	Z	0.29	0/717	0.72	0/1115
All	All	0.25	0/29756	0.43	0/40598

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	258	ARG	Sidechain

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	4549	0	4523	37	0
1	C	4549	0	4523	37	0
1	E	4549	0	4523	36	0
2	B	4509	0	4542	27	0
2	D	4442	0	4488	38	0
2	F	4493	0	4529	33	0
3	X	641	0	323	1	0
3	Y	641	0	323	2	0
3	Z	641	0	323	2	0
4	A	60	0	0	0	0
4	B	66	0	0	0	0
4	C	19	0	0	0	0
4	D	48	0	0	0	0
4	E	34	0	0	0	0
4	F	45	0	0	0	0
4	X	14	0	0	0	0
4	Y	13	0	0	0	0
4	Z	7	0	0	0	0
All	All	29320	0	28097	188	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 3.

All (188) 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:E:30:GLU:HG3	1:E:165:ASN:HB3	1.67	0.74
2:B:212:PHE:HB3	2:B:246:ALA:HB3	1.73	0.70
1:C:506:LYS:HE3	2:D:333:GLN:O	1.91	0.70
1:E:526:GLU:OE2	1:E:534:ARG:HD3	1.91	0.69
2:F:615:ARG:HH21	2:F:619:HIS:HB2	1.57	0.69
2:F:212:PHE:HB3	2:F:246:ALA:HB3	1.75	0.68
2:D:212:PHE:HB3	2:D:246:ALA:HB3	1.76	0.66
2:B:190:ASN:HB2	2:B:193:GLU:HB2	1.78	0.65
1:C:49:LEU:HG	1:C:57:GLU:HG3	1.78	0.65
2:B:255:GLY:HA2	2:B:531:VAL:HG22	1.79	0.65
2:D:394:ALA:HB3	2:D:411:LEU:HB2	1.79	0.64
2:D:190:ASN:HB2	2:D:193:GLU:HB2	1.80	0.64
1:C:52:LYS:HG3	1:C:56:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:GLU:HG2	1:A:395:GLU:HA	1.83	0.61
1:E:49:LEU:HG	1:E:57:GLU:HG3	1.84	0.60
1:A:272:LEU:HB3	1:A:282:VAL:HG12	1.82	0.60
1:A:378:PHE:HA	2:B:432:THR:HG21	1.84	0.59
1:C:378:PHE:HA	2:D:432:THR:HG21	1.85	0.59
2:F:190:ASN:HB2	2:F:193:GLU:HB2	1.83	0.59
1:E:203:PHE:HB2	1:E:243:PRO:HG3	1.83	0.58
1:A:203:PHE:HB2	1:A:243:PRO:HG3	1.85	0.58
1:E:378:PHE:HA	2:F:432:THR:HG21	1.85	0.58
1:C:190:ARG:HG3	1:C:223:ILE:HA	1.86	0.57
1:C:203:PHE:HB2	1:C:243:PRO:HG3	1.86	0.57
2:F:255:GLY:HA2	2:F:531:VAL:HG22	1.85	0.57
2:B:394:ALA:HB3	2:B:411:LEU:HB2	1.86	0.57
1:C:272:LEU:HB3	1:C:282:VAL:HG12	1.86	0.57
2:D:255:GLY:HA2	2:D:531:VAL:HG22	1.86	0.56
1:A:190:ARG:HG3	1:A:223:ILE:HA	1.87	0.56
1:E:284:VAL:HG12	1:E:401:LEU:HD11	1.87	0.56
1:E:52:LYS:HG3	1:E:56:LEU:HD23	1.86	0.56
1:A:49:LEU:HG	1:A:57:GLU:HG3	1.88	0.56
1:A:52:LYS:HG3	1:A:56:LEU:HD23	1.88	0.56
1:E:352:VAL:HG22	2:F:537:VAL:HG21	1.88	0.55
2:F:394:ALA:HB3	2:F:411:LEU:HB2	1.88	0.55
1:E:317:LYS:HE2	1:E:319:LEU:HD21	1.89	0.54
2:D:9:ILE:HD11	2:D:113:VAL:HG21	1.88	0.54
1:C:284:VAL:HG12	1:C:401:LEU:HD11	1.90	0.54
2:F:218:LEU:HB3	2:F:240:LEU:HB2	1.90	0.54
1:C:352:VAL:HG22	2:D:537:VAL:HG21	1.90	0.54
1:E:190:ARG:HG3	1:E:223:ILE:HA	1.90	0.53
2:D:218:LEU:HB3	2:D:240:LEU:HB2	1.89	0.53
1:E:248:ILE:HD13	1:E:256:ARG:HD3	1.90	0.53
1:E:527:THR:HG22	1:E:529:ASN:H	1.74	0.52
1:E:30:GLU:CG	1:E:165:ASN:HB3	2.36	0.52
2:F:234:MET:HE3	2:F:243:LYS:HG2	1.92	0.52
1:C:317:LYS:HE2	1:C:319:LEU:HD21	1.93	0.51
2:D:325:VAL:HG23	2:D:619:HIS:HE1	1.74	0.51
2:F:51:ALA:HB1	2:F:106:MET:HG2	1.92	0.51
1:E:73:ARG:HD2	1:E:265:ARG:HH21	1.75	0.51
2:B:218:LEU:HB3	2:B:240:LEU:HB2	1.92	0.51
2:D:46:ILE:HG12	2:D:75:VAL:HG22	1.93	0.51
2:F:9:ILE:HD11	2:F:113:VAL:HG21	1.93	0.51
2:B:540:GLU:HG3	2:B:556:PRO:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:271:GLU:HB3	2:D:273:TYR:HE1	1.76	0.51
2:B:620:SER:O	2:B:621:ARG:HB2	2.10	0.51
1:A:317:LYS:HE2	1:A:319:LEU:HD21	1.93	0.50
1:E:272:LEU:HB3	1:E:282:VAL:HG12	1.91	0.50
1:A:226:LEU:HB2	1:A:241:ASP:HA	1.93	0.50
1:A:542:LEU:HD22	2:B:222:ILE:HD12	1.94	0.50
1:E:542:LEU:HD22	2:F:222:ILE:HD12	1.92	0.50
1:A:175:ASP:OD1	1:A:215:PHE:HA	2.12	0.50
1:C:302:VAL:HB	2:D:615:ARG:NH2	2.26	0.50
1:E:132:GLN:HB3	1:E:134:THR:HG23	1.94	0.50
1:E:391:GLU:HG2	1:E:395:GLU:HA	1.94	0.50
1:E:459:PRO:HG3	2:F:247:PHE:CD1	2.47	0.50
1:C:451:PHE:HB2	1:C:454:GLU:HG3	1.94	0.49
1:C:567:ASN:O	1:C:571:LYS:HG2	2.12	0.49
2:D:50:LEU:HD12	2:D:66:PHE:HD2	1.77	0.49
2:F:50:LEU:HD12	2:F:66:PHE:HD2	1.77	0.49
1:C:542:LEU:HD22	2:D:222:ILE:HD12	1.93	0.49
1:A:37:GLU:HB3	1:A:172:THR:HA	1.94	0.49
2:B:9:ILE:HD11	2:B:113:VAL:HG21	1.93	0.49
2:D:454:THR:HG22	2:D:460:PRO:HA	1.94	0.49
2:B:51:ALA:HB1	2:B:106:MET:HG2	1.94	0.48
1:C:55:LEU:HD23	1:C:125:LEU:HD13	1.95	0.48
1:C:545:LEU:HB2	2:D:222:ILE:HD11	1.95	0.48
1:A:334:VAL:HG12	1:A:343:ASN:HB2	1.95	0.48
1:A:352:VAL:HG22	2:B:537:VAL:HG21	1.95	0.48
1:C:73:ARG:HD2	1:C:265:ARG:HH21	1.79	0.48
1:E:514:TYR:CE2	2:F:621:ARG:HG3	2.49	0.48
1:E:150:LEU:HD13	1:E:196:LEU:HD23	1.96	0.48
1:A:248:ILE:HD13	1:A:256:ARG:HD3	1.95	0.48
1:C:226:LEU:HB2	1:C:241:ASP:HA	1.96	0.48
1:A:73:ARG:HD2	1:A:265:ARG:HH21	1.79	0.47
2:B:50:LEU:HD12	2:B:66:PHE:HD2	1.78	0.47
1:E:30:GLU:HG3	1:E:165:ASN:CB	2.42	0.47
2:F:415:LEU:HD22	2:F:427:PHE:HB3	1.97	0.47
2:B:46:ILE:HG12	2:B:75:VAL:HG22	1.95	0.47
2:D:620:SER:O	2:D:621:ARG:HB2	2.15	0.47
1:C:334:VAL:HG12	1:C:343:ASN:HB2	1.97	0.47
2:F:284:ILE:HG23	2:F:308:ILE:HG12	1.97	0.47
2:F:46:ILE:HG12	2:F:75:VAL:HG22	1.96	0.47
2:B:77:THR:O	2:B:81:ILE:HG12	2.16	0.46
2:D:415:LEU:HD22	2:D:427:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:LYS:HE2	2:B:223:LEU:HD11	1.97	0.46
2:F:287:GLU:HA	2:F:303:TYR:HA	1.98	0.46
2:F:136:ASN:HB3	2:F:139:ASP:HB2	1.98	0.46
1:A:284:VAL:HG12	1:A:401:LEU:HD11	1.96	0.46
1:E:295:ALA:HB2	1:E:504:LEU:HD23	1.98	0.46
1:E:545:LEU:HB2	2:F:222:ILE:HD11	1.98	0.46
1:A:459:PRO:HG3	2:B:247:PHE:CD1	2.51	0.45
2:D:284:ILE:HG23	2:D:308:ILE:HG12	1.98	0.45
1:E:157:ILE:HA	1:E:158:PRO:HD2	1.73	0.45
2:F:388:LEU:HG	2:F:413:PRO:HB2	1.97	0.45
2:F:77:THR:O	2:F:81:ILE:HG12	2.17	0.45
2:B:234:MET:HE3	2:B:243:LYS:HG2	1.97	0.45
2:F:81:ILE:HG22	2:F:85:LYS:HE2	1.98	0.45
3:Z:310:A:H2'	3:Z:311:G:C8	2.52	0.45
1:C:459:PRO:HG3	2:D:247:PHE:CD1	2.52	0.45
1:E:226:LEU:HB2	1:E:241:ASP:HA	1.99	0.45
1:A:189:LEU:HD23	1:A:192:LEU:HD12	1.99	0.45
2:D:77:THR:O	2:D:81:ILE:HG12	2.17	0.45
3:Y:302:A:H2'	3:Y:302:A:N3	2.32	0.45
1:C:65:LEU:HG	1:C:261:LYS:HD3	1.99	0.45
2:D:221:ASP:HB3	2:D:224:SER:HB2	1.99	0.45
3:Z:302:A:N3	3:Z:302:A:H2'	2.32	0.45
1:E:37:GLU:HB3	1:E:172:THR:HA	1.98	0.44
1:C:37:GLU:HB3	1:C:172:THR:HA	1.99	0.44
1:E:526:GLU:OE2	1:E:531:LYS:HA	2.18	0.44
3:X:302:A:H2'	3:X:302:A:N3	2.32	0.44
2:B:511:SER:C	2:B:513:ASN:H	2.21	0.44
1:C:367:GLY:HA2	2:D:481:MET:HB3	2.00	0.44
2:F:454:THR:HG22	2:F:460:PRO:HA	2.00	0.44
2:F:271:GLU:HB3	2:F:273:TYR:HE1	1.83	0.43
1:E:334:VAL:HG12	1:E:343:ASN:HB2	1.99	0.43
1:C:248:ILE:HD13	1:C:256:ARG:HD3	2.00	0.43
3:Y:310:A:H2'	3:Y:311:G:C8	2.53	0.43
1:C:364:LYS:HB3	1:C:364:LYS:HE2	1.85	0.43
1:C:527:THR:HG22	1:C:529:ASN:H	1.82	0.43
2:D:473:LEU:HB2	2:D:579:LEU:HD13	2.00	0.43
1:A:55:LEU:HD23	1:A:125:LEU:HD13	1.99	0.43
2:B:284:ILE:HG23	2:B:308:ILE:HG12	2.00	0.43
1:E:567:ASN:O	1:E:571:LYS:HG2	2.18	0.43
1:A:364:LYS:HB3	1:A:364:LYS:HE2	1.83	0.43
2:D:136:ASN:HB3	2:D:139:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:SER:O	1:C:407:ILE:HG12	2.19	0.42
1:A:567:ASN:O	1:A:571:LYS:HG2	2.19	0.42
1:C:277:LYS:HB3	1:C:277:LYS:HE2	1.87	0.42
2:B:207:LYS:HA	2:B:208:PRO:HD3	1.91	0.42
2:D:234:MET:HE3	2:D:243:LYS:HG2	2.02	0.42
1:C:355:ALA:HB1	2:D:558:LEU:HB2	2.01	0.42
1:A:157:ILE:HA	1:A:158:PRO:HD2	1.73	0.42
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.90	0.42
1:C:295:ALA:HB2	1:C:504:LEU:HD23	2.02	0.42
1:A:387:ILE:HB	1:A:444:PHE:HB2	2.02	0.42
1:A:527:THR:HG22	1:A:529:ASN:H	1.84	0.42
2:B:415:LEU:HD22	2:B:427:PHE:HB3	2.02	0.42
1:E:197:PHE:HD2	1:E:226:LEU:HD21	1.84	0.42
1:A:277:LYS:HB3	1:A:277:LYS:HE2	1.87	0.42
1:A:304:GLU:HA	1:A:308:ILE:O	2.20	0.42
2:B:271:GLU:HB3	2:B:273:TYR:HE1	1.84	0.42
1:C:391:GLU:HG2	1:C:395:GLU:HA	2.00	0.42
1:A:250:ALA:HA	1:A:253:ILE:HG13	2.02	0.41
2:B:454:THR:HG22	2:B:460:PRO:HA	2.00	0.41
2:D:413:PRO:HA	2:D:431:LEU:HD23	2.02	0.41
2:D:620:SER:O	2:D:621:ARG:CB	2.68	0.41
2:F:287:GLU:HG3	2:F:303:TYR:HB3	2.01	0.41
2:F:157:ARG:HH22	2:F:187:ARG:HH12	1.68	0.41
1:A:215:PHE:HB3	1:A:247:PRO:HB3	2.02	0.41
1:A:545:LEU:HB2	2:B:222:ILE:HD11	2.02	0.41
1:E:302:VAL:HB	2:F:615:ARG:NH2	2.35	0.41
2:D:271:GLU:HB3	2:D:273:TYR:CE1	2.56	0.41
1:C:302:VAL:HB	2:D:615:ARG:HH22	1.85	0.41
1:C:262:GLU:HB2	2:D:445:THR:HG23	2.02	0.41
1:A:285:LYS:HG3	1:A:390:ASP:HB2	2.02	0.41
1:C:454:GLU:HG2	2:D:253:VAL:HG22	2.02	0.41
2:D:418:HIS:CE1	2:D:497:PRO:HG3	2.55	0.41
1:E:488:PHE:CE1	1:E:548:ILE:HG23	2.56	0.41
2:F:459:VAL:HA	2:F:460:PRO:HD3	1.91	0.41
1:A:261:LYS:HE3	1:A:261:LYS:HB3	1.94	0.41
2:B:325:VAL:HG23	2:B:619:HIS:CE1	2.55	0.41
1:E:364:LYS:HB3	1:E:364:LYS:HE2	1.90	0.41
1:A:268:PHE:CE1	1:A:286:GLY:HA3	2.55	0.41
2:D:325:VAL:HB	2:D:619:HIS:HE2	1.86	0.41
2:F:327:PRO:O	2:F:331:VAL:HG23	2.21	0.41
2:B:136:ASN:HB3	2:B:139:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ALA:HA	1:C:253:ILE:HG13	2.02	0.41
2:D:287:GLU:HA	2:D:303:TYR:HA	2.03	0.41
2:F:271:GLU:HB3	2:F:273:TYR:CE1	2.56	0.41
1:A:449:VAL:HA	1:A:450:PRO:HD3	1.97	0.40
1:C:215:PHE:HB3	1:C:247:PRO:HB3	2.02	0.40
1:E:417:LEU:HB2	1:E:430:TYR:HB2	2.01	0.40
1:E:451:PHE:HB2	1:E:454:GLU:HG3	2.03	0.40
2:F:511:SER:C	2:F:513:ASN:H	2.25	0.40
1:A:132:GLN:HB3	1:A:134:THR:HG23	2.04	0.40
2:D:217:ARG:HG2	2:D:241:CYS:SG	2.61	0.40
1:C:68:GLN:OE1	1:C:261:LYS:HE2	2.22	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	544/575 (95%)	529 (97%)	15 (3%)	0	100	100
1	C	544/575 (95%)	526 (97%)	18 (3%)	0	100	100
1	E	544/575 (95%)	527 (97%)	17 (3%)	0	100	100
2	B	558/628 (89%)	539 (97%)	19 (3%)	0	100	100
2	D	548/628 (87%)	531 (97%)	17 (3%)	0	100	100
2	F	555/628 (88%)	536 (97%)	19 (3%)	0	100	100
All	All	3293/3609 (91%)	3188 (97%)	105 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	510/536 (95%)	500 (98%)	10 (2%)	55 84
1	C	510/536 (95%)	501 (98%)	9 (2%)	59 86
1	E	510/536 (95%)	500 (98%)	10 (2%)	55 84
2	B	527/585 (90%)	517 (98%)	10 (2%)	57 85
2	D	519/585 (89%)	508 (98%)	11 (2%)	53 84
2	F	525/585 (90%)	517 (98%)	8 (2%)	65 89
All	All	3101/3363 (92%)	3043 (98%)	58 (2%)	57 85

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	49	LEU
1	A	175	ASP
1	A	225	GLN
1	A	280	PHE
1	A	282	VAL
1	A	424	ASN
1	A	477	MET
1	A	497	SER
1	A	534	ARG
2	B	139	ASP
2	B	241	CYS
2	B	301	SER
2	B	348	LEU
2	B	432	THR
2	B	445	THR
2	B	457	SER
2	B	615	ARG
2	B	619	HIS
2	B	621	ARG
1	C	37	GLU
1	C	49	LEU

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Mol	Chain	Res	Type
1	C	175	ASP
1	C	225	GLN
1	C	280	PHE
1	C	282	VAL
1	C	388	VAL
1	C	424	ASN
1	C	433	SER
2	D	139	ASP
2	D	210	ARG
2	D	241	CYS
2	D	301	SER
2	D	315	LYS
2	D	348	LEU
2	D	445	THR
2	D	457	SER
2	D	501	VAL
2	D	615	ARG
2	D	621	ARG
1	E	37	GLU
1	E	49	LEU
1	E	175	ASP
1	E	225	GLN
1	E	280	PHE
1	E	282	VAL
1	E	384	SER
1	E	424	ASN
1	E	433	SER
1	E	477	MET
2	F	61	GLU
2	F	139	ASP
2	F	241	CYS
2	F	348	LEU
2	F	445	THR
2	F	457	SER
2	F	615	ARG
2	F	619	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	229	ASN
2	F	619	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	X	29/30 (96%)	2 (6%)	0
3	Y	29/30 (96%)	2 (6%)	0
3	Z	29/30 (96%)	2 (6%)	0
All	All	87/90 (96%)	6 (6%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	X	301	U
3	X	302	A
3	Y	301	U
3	Y	302	A
3	Z	301	U
3	Z	302	A

There are no RNA pucker outliers to report.

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	548/575 (95%)	-0.16	7 (1%) 77 72	16, 51, 99, 142	0
1	C	548/575 (95%)	-0.27	8 (1%) 73 68	17, 46, 94, 150	0
1	E	548/575 (95%)	0.45	39 (7%) 16 9	29, 71, 130, 181	0
2	B	568/628 (90%)	0.22	47 (8%) 11 6	16, 64, 143, 204	0
2	D	560/628 (89%)	0.29	58 (10%) 6 3	19, 64, 149, 189	0
2	F	565/628 (89%)	0.85	97 (17%) 1 1	22, 82, 163, 200	0
3	X	30/30 (100%)	-0.21	0 100 100	32, 55, 109, 130	0
3	Y	30/30 (100%)	-0.13	0 100 100	34, 57, 100, 122	0
3	Z	30/30 (100%)	-0.14	0 100 100	35, 55, 116, 126	0
All	All	3427/3699 (92%)	0.22	256 (7%) 14 8	16, 60, 140, 204	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	145	GLU	8.7
2	F	60	GLN	8.5
2	B	150	LEU	8.3
2	B	97	ASP	7.6
2	F	59	SER	7.4
2	B	108	GLN	7.2
2	D	106	MET	6.9
1	A	178	GLN	6.8
2	D	423	SER	6.5
2	F	137	LEU	6.5
2	B	154	LEU	6.4
2	F	94	HIS	6.3
2	D	137	LEU	6.2
2	F	149	LEU	6.0
2	D	155	SER	5.7

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Mol	Chain	Res	Type	RSRZ
2	D	425	LYS	5.7
2	F	462	LYS	5.7
2	F	178	LYS	5.5
2	F	174	SER	5.4
1	E	307	ASP	5.4
2	B	149	LEU	5.3
2	F	125	LYS	5.3
2	F	107	ILE	5.3
2	F	97	ASP	5.1
2	F	123	ALA	5.1
2	F	155	SER	5.1
2	D	153	GLU	5.0
1	E	135	GLY	5.0
2	D	95	SER	5.0
1	E	240	PHE	5.0
2	F	466	ASP	4.9
2	F	148	ASP	4.9
2	F	96	HIS	4.9
2	B	152	GLU	4.8
2	F	288	GLY	4.7
2	F	65	VAL	4.7
2	F	614	LYS	4.7
2	F	141	ASP	4.7
2	F	111	LEU	4.6
2	F	51	ALA	4.6
2	B	151	THR	4.6
2	B	155	SER	4.5
1	E	237	ASP	4.5
2	F	504	ASP	4.4
2	F	98	SER	4.4
2	D	154	LEU	4.4
2	D	150	LEU	4.4
2	B	138	ASP	4.4
2	D	134	THR	4.3
2	D	149	LEU	4.3
2	F	152	GLU	4.3
2	F	62	ILE	4.3
2	F	465	THR	4.3
2	B	300	GLY	4.3
2	F	134	THR	4.3
2	F	160	LEU	4.3
2	F	464	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	180	ALA	4.2
2	F	470	ILE	4.2
2	D	51	ALA	4.2
2	F	115	LEU	4.1
2	D	50	LEU	4.1
2	B	153	GLU	4.1
2	F	142	ILE	4.1
2	F	150	LEU	4.0
2	F	267	SER	4.0
2	D	142	ILE	4.0
2	F	469	GLN	4.0
2	F	114	SER	3.9
2	F	182	ALA	3.9
2	D	108	GLN	3.9
1	E	227	GLY	3.9
2	D	462	LYS	3.8
2	F	9	ILE	3.8
2	F	461	LEU	3.7
1	C	238	SER	3.7
2	F	108	GLN	3.7
2	F	162	ASP	3.6
1	E	196	LEU	3.6
1	E	225	GLN	3.6
2	F	138	ASP	3.6
1	E	160	GLN	3.6
2	D	140	LEU	3.5
2	F	151	THR	3.5
2	B	464	GLU	3.5
1	E	131	PHE	3.4
2	F	61	GLU	3.4
2	F	87	LEU	3.4
2	F	473	LEU	3.4
1	E	183	ILE	3.4
2	D	178	LYS	3.3
2	F	154	LEU	3.3
1	E	185	GLU	3.3
2	B	60	GLN	3.3
2	F	48	CYS	3.2
2	B	288	GLY	3.2
1	E	197	PHE	3.2
1	C	237	ASP	3.2
2	B	301	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	95	SER	3.2
1	E	557	LYS	3.1
2	D	152	GLU	3.1
2	B	50	LEU	3.1
2	F	63	PRO	3.1
2	D	303	TYR	3.1
2	B	107	ILE	3.1
1	A	237	ASP	3.1
1	C	578	LYS	3.1
2	F	147	ILE	3.1
1	E	176	LYS	3.0
2	B	133	PHE	3.0
2	F	64	ASN	3.0
1	A	181	GLN	3.0
2	D	162	ASP	3.0
2	F	468	HIS	3.0
2	D	503	THR	3.0
2	F	287	GLU	3.0
2	F	190	ASN	2.9
1	E	584	ASN	2.9
1	E	178	GLN	2.9
2	F	270	LYS	2.9
2	F	144	ASP	2.9
2	D	136	ASN	2.9
2	D	111	LEU	2.9
2	F	110	LEU	2.9
2	F	615	ARG	2.9
2	B	136	ASN	2.9
2	D	180	VAL	2.8
2	F	47	SER	2.8
2	D	107	ILE	2.8
2	B	92	ASP	2.8
2	D	175	ASN	2.8
2	D	269	LYS	2.8
1	E	559	GLU	2.8
1	E	190	ARG	2.8
2	F	304	ILE	2.8
2	F	118	LYS	2.8
2	B	143	THR	2.8
1	A	185	GLU	2.8
2	F	14	PRO	2.8
2	B	270	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	20	ASN	2.7
2	F	515	ASP	2.7
2	D	156	THR	2.7
2	D	288	GLY	2.7
1	E	563	ILE	2.7
2	B	516	GLN	2.7
1	E	238	SER	2.7
2	B	137	LEU	2.7
2	B	268	GLN	2.7
2	F	560	ASP	2.7
2	B	10	VAL	2.6
2	D	302	SER	2.6
2	D	147	ILE	2.6
2	D	18	LYS	2.6
2	F	127	LEU	2.6
1	E	222	ASP	2.6
2	D	271	GLU	2.6
1	E	277	LYS	2.6
2	D	64	ASN	2.6
2	F	136	ASN	2.6
2	F	271	GLU	2.6
2	F	180	VAL	2.5
2	D	287	GLU	2.5
2	B	112	VAL	2.5
1	E	184	ASP	2.5
2	F	547	ILE	2.5
1	E	306	GLU	2.5
2	B	111	LEU	2.5
2	F	70	SER	2.5
2	B	65	VAL	2.4
1	E	133	GLN	2.4
1	E	192	LEU	2.4
2	B	109	CYS	2.4
2	F	567	SER	2.4
1	C	575	MET	2.4
2	F	8	PHE	2.4
2	F	467	GLY	2.4
2	D	465	THR	2.4
2	F	153	GLU	2.4
2	D	133	PHE	2.4
1	E	226	LEU	2.4
2	D	138	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	581	GLU	2.4
2	D	300	GLY	2.4
1	C	561	PRO	2.4
2	B	116	ASP	2.4
2	D	11	ASP	2.4
2	B	287	GLU	2.3
2	B	230	PRO	2.3
1	A	180	ALA	2.3
1	C	227	GLY	2.3
2	D	63	PRO	2.3
2	D	374	GLN	2.3
2	F	618	GLN	2.3
2	D	139	ASP	2.3
2	B	142	ILE	2.3
2	D	19	ASN	2.3
1	C	178	GLN	2.3
1	E	569	TYR	2.3
2	B	266	ASP	2.3
2	B	156	THR	2.3
2	B	139	ASP	2.2
1	E	159	GLY	2.2
2	F	463	LYS	2.2
2	D	424	GLU	2.2
1	E	145	LEU	2.2
1	E	395	GLU	2.2
2	D	119	GLN	2.2
2	D	151	THR	2.2
2	F	303	TYR	2.2
2	F	139	ASP	2.2
1	E	223	ILE	2.2
2	F	57	GLU	2.2
1	E	349	ASP	2.2
2	B	123	ALA	2.2
2	F	146	GLU	2.2
1	E	519	GLU	2.2
2	F	16	MET	2.2
2	D	164	GLY	2.1
1	E	483	SER	2.1
2	D	94	HIS	2.1
2	B	588	VAL	2.1
2	F	132	VAL	2.1
2	F	175	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	138	LYS	2.1
2	F	586	LYS	2.1
2	B	5	SER	2.1
2	F	45	TRP	2.1
2	D	179	LEU	2.1
2	D	615	ARG	2.1
2	B	267	SER	2.1
1	C	469	GLU	2.1
2	F	507	LEU	2.1
2	D	304	ILE	2.1
2	D	91	CYS	2.1
2	F	181	GLU	2.1
2	B	87	LEU	2.1
2	B	141	ASP	2.1
1	E	189	LEU	2.1
2	F	156	THR	2.1
2	B	61	GLU	2.1
2	B	106	MET	2.1
1	A	307	ASP	2.0
2	F	369	THR	2.0
2	B	54	PRO	2.0
2	F	185	ASN	2.0
2	F	503	THR	2.0
2	B	48	CYS	2.0
1	A	191	ARG	2.0
2	F	117	ILE	2.0
2	F	71	PHE	2.0
2	D	141	ASP	2.0
2	D	12	VAL	2.0
2	D	124	ARG	2.0
1	E	224	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.