Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:19 PM GMT

PDB ID	:	3WTU
Title	:	Crystal structure of the complex comprised of ETS1 (V170A), RUNX1, CBF-BETA, and the tcralpha gene enhancer DNA
Authors	:	Shiina, M.; Hamada, K.; Ogata, K.
Deposited on	:	2014-04-21
Resolution	:	2.70 Å(reported)

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

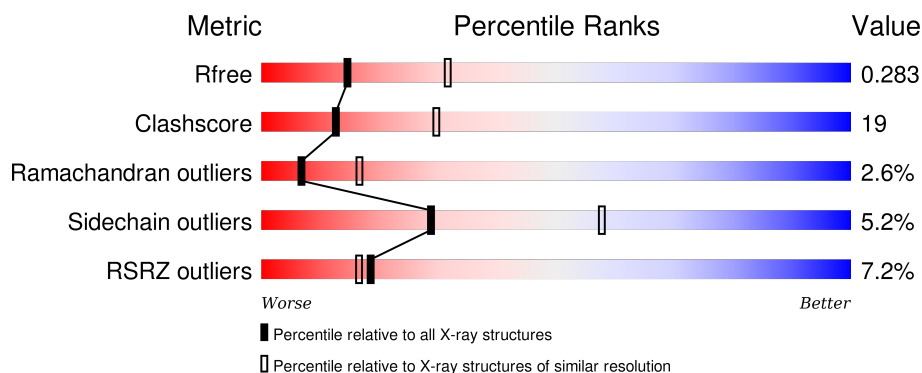|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.
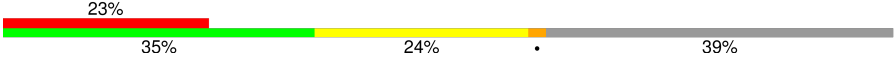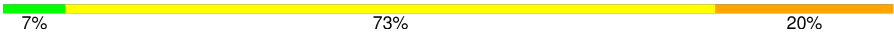
Metric	Percentile Ranks	Value
Rfree		0.283
Clashscore		19
Ramachandran outliers		2.6%
Sidechain outliers		5.2%
RSRZ outliers		7.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 <=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	204	36% 19% • 42%
1	F	204	43% 14% • 42%
2	B	142	6% 52% 36% • 8%
2	G	142	5% 46% 39% 6% 9%
3	C	166	% 49% 21% • 29%

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Mol	Chain	Length	Quality of chain
3	H	166	23% 35% 24% • 39%
4	D	15	7% 73% 20%
4	I	15	7% 73% 20%
5	E	15	73% 27%
5	J	15	73% 27%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7030 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 Runt-related transcription factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			912	572	169	167	4			
1	F	118	Total	C	N	O	S	0	0	0
			912	572	169	167	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	LYS	LEU	ENGINEERED MUTATION	UNP Q03347
A	170	ALA	VAL	ENGINEERED MUTATION	UNP Q03347
F	94	LYS	LEU	ENGINEERED MUTATION	UNP Q03347
F	170	ALA	VAL	ENGINEERED MUTATION	UNP Q03347

- Molecule 2 is a protein called Core-binding factor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	130	Total	C	N	O	S	0	0	0
			1071	671	195	199	6			
2	G	129	Total	C	N	O	S	0	0	0
			1062	666	193	197	6			

- Molecule 3 is a protein called Protein C-ets-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	118	Total	C	N	O	S	0	0	0
			967	627	165	171	4			
3	H	101	Total	C	N	O	S	0	0	0
			853	553	147	149	4			

- Molecule 4 is a DNA chain called DNA (5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total 299	C 144	N 54	O 87	P 14	0	0	0
4	I	15	Total 299	C 144	N 54	O 87	P 14	0	0	0

- Molecule 5 is a DNA chain called DNA (5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP* GP*CP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	15	Total 310	C 148	N 59	O 89	P 14	0	0	0
5	J	15	Total 310	C 148	N 59	O 89	P 14	0	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total 5	O 5	0	0
6	B	4	Total 4	O 4	0	0
6	C	7	Total 7	O 7	0	0
6	F	6	Total 6	O 6	0	0
6	G	2	Total 2	O 2	0	0
6	E	7	Total 7	O 7	0	0
6	I	1	Total 1	O 1	0	0
6	J	3	Total 3	O 3	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 errors 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: Runt-related transcription factor 1

Chain A:

- Molecule 1: Runt-related transcription factor 1

Chain F:

- Molecule 2: Core-binding factor subunit beta

Chain B:

- Molecule 2: Core-binding factor subunit beta

Chain G:

MET P2 R3 V4 Q8 R9 S10 K11 N14 E15 E16 F17 F18 R19 K20 L21 S22 E24 K28 Y29 R33 E38 Q41 F44 Q45 N46 R49 I55 A56 F57 V58 A59 T60 G61 T62 N63 L66 Q67 P70 A71 SER TRP GLN GLY GLU GLN ARG GLN

THR P81 S82 R83 E84 Y85 V86 D87 L88 E89 R90 E91 V95 K98 L103 V106 C107 V108 I109 W110 K111 L116 H117 R118 L119 E126 F127 D128 E129 E130 R131 A132 Q133 Q134 E135 D136 A137 L138 A139 GLN GLN ALA
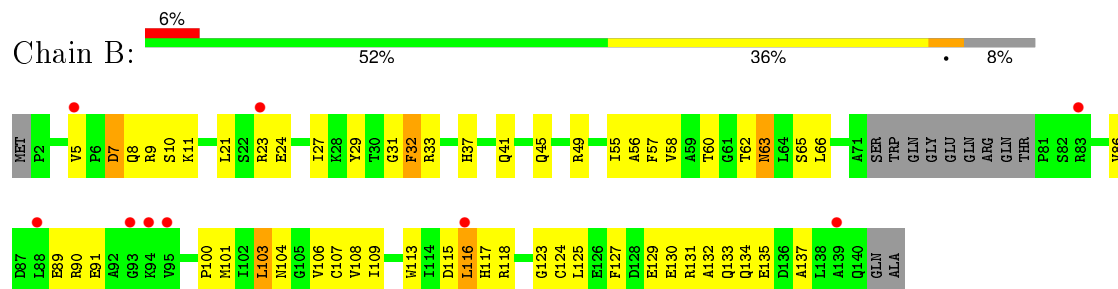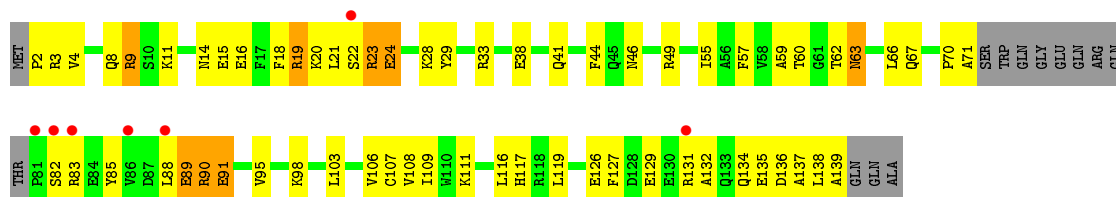
- Molecule 3: Protein C-ets-1

Chain C:
49% 21% 29%

SER LEU GLN ARG VAL PRO SER TYR ASP SER PHE ASP GLU ASP SER PRO TYR PRO ALA ALA LEU PRO ASN HIS LYS PRO LYS GLY THR PHE LYS ASP TYR VAL ARG ASP ARG ALA ASP LEU ASN LYS ASP LYS P319 V320 I321 P322 A323 A324 A325 L326 A327 T330 Q336 L337 W338 L342

E343 L344 L345 S352 F353 I354 T357 G358 D359 E362 F363 K364 L365 V371 R378 K383 M384 N385 Y386 E387 K388 K404 T405 K408 R409 Y410 V411 L418 L421 E427 M432 K436 PRO ASP ALA ASP GLU

- Molecule 3: Protein C-ets-1

Chain H:
23%
35% 24% 39%

SER LEU GLN ARG VAL PRO SER TYR ASP SER PHE ASP GLU ASP SER PRO TYR PRO ALA ALA LEU PRO ASN HIS LYS PRO LYS GLY THR PHE LYS ASP TYR VAL ARG ASP ARG ALA ASP LEU ASN LYS ASP LYS PRO VAL ILE PRO ALA ALA ALA LEU ALA GLY TYR THR GLY SER G333 P334 I335

Q336 L337 W338 Q339 F340 L341 L342 L345 T346 D347 K348 S349 C350 Q351 S352 F353 I354 S355 W356 T357 G358 W361 E362 F363 K364 L365 S366 D367 P368 D369 E370 V371 A372 R373 R374 W375 M384 N385 Y386 E387 K388 L389 S390 L393 Y396 I401 G407 K408 R409 R413 F414 V415

C416 D417 L418 Q419 S420 L421 L422 G423 Y424 T425 P426 E427 E428 L429 H430 A431 M432 L433 ASP VAL LYS PRO ASP ALA ASP GLU

- Molecule 4: DNA (5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3')

Chain D:
7% 73% 20%

G1 A2 A3 G4 C5 C6 A7 C8 A9 T10 C11 C12 T13 C14 T15

- Molecule 4: DNA (5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3')

Chain I:
7% 73% 20%

G1 A2 A3 G4 C5 C6 A7 C8 A9 T10 C11 C12 T13 C14 T15

- Molecule 5: DNA (5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3')

Chain E:
73% 27%

A1 T9 G10 T13 T14 C15

● Molecule 5: DNA (5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3'
)

Chain J: 73%   27%

A1 T9 G10 G11 C15

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.56Å 102.11Å 194.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.70 48.74 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.74-2.70) 98.9 (48.74-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.25 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.232 , 0.282 0.233 , 0.283	Depositor DCC
R_{free} test set	4371 reflections (10.07%)	DCC
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	4 of 43409 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7030	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.53	0/931	0.70	0/1265
1	F	0.59	0/931	0.75	0/1265
2	B	0.42	0/1093	0.56	0/1466
2	G	0.46	0/1084	0.58	0/1454
3	C	0.59	0/994	0.68	0/1342
3	H	0.38	0/877	0.48	0/1181
4	D	0.67	0/334	0.94	1/512 (0.2%)
4	I	0.66	0/334	0.96	1/512 (0.2%)
5	E	0.62	0/348	0.86	0/537
5	J	0.60	0/348	0.80	0/537
All	All	0.53	0/7274	0.69	2/10071 (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
4	D	0	3
4	I	0	3
5	E	0	1
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	4	DG	N9-C1'-C2'	-7.11	99.09	112.60
4	I	4	DG	N9-C1'-C2'	-5.31	102.51	112.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	4	DG	Sidechain
4	D	5	DC	Sidechain
4	D	9	DA	Sidechain
5	E	13	DT	Sidechain
4	I	4	DG	Sidechain
4	I	5	DC	Sidechain
4	I	9	DA	Sidechain

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	912	0	918	39	0
1	F	912	0	918	24	0
2	B	1071	0	1034	48	0
2	G	1062	0	1026	49	0
3	C	967	0	966	25	0
3	H	853	0	847	48	0
4	D	299	0	170	15	0
4	I	299	0	170	20	0
5	E	310	0	171	2	0
5	J	310	0	171	4	0
6	A	5	0	0	0	0
6	B	4	0	0	0	0
6	C	7	0	0	0	0
6	E	7	0	0	0	0
6	F	6	0	0	1	0
6	G	2	0	0	0	0
6	I	1	0	0	0	0
6	J	3	0	0	0	0
All	All	7030	0	6391	259	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 19.

All (259) 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)
4:I:14:DC:H2"	4:I:15:DT:H5'	1.50	0.94
1:A:82:ASN:HD21	1:A:118:ARG:HH11	1.15	0.93
3:H:419:GLN:HE22	3:H:425:THR:HA	1.28	0.93
2:B:60:THR:HG23	2:B:62:THR:H	1.40	0.84
1:F:64:ARG:HA	1:F:71:LEU:HD23	1.60	0.83
2:G:88:LEU:HD23	2:G:95:VAL:HG22	1.62	0.81
2:G:11:LYS:HG3	2:G:15:GLU:HG3	1.64	0.80
1:A:161:THR:H	2:B:104:ASN:HD21	1.29	0.78
1:F:79:TRP:CZ2	1:F:86:PRO:HD3	2.20	0.77
3:H:362:GLU:HB2	3:H:413:ARG:HH11	1.52	0.74
3:C:327:ALA:HA	3:C:421:LEU:HD23	1.70	0.73
1:A:69:ASN:HD21	1:A:95:GLY:H	1.36	0.72
3:H:419:GLN:NE2	3:H:425:THR:HA	2.04	0.72
4:I:14:DC:H2"	4:I:15:DT:C5'	2.19	0.71
1:A:109:ASN:ND2	1:A:112:ASN:H	1.90	0.70
1:F:64:ARG:HA	1:F:71:LEU:CD2	2.23	0.69
4:D:10:DT:H2"	4:D:11:DC:H5'	1.75	0.69
1:A:69:ASN:ND2	1:A:95:GLY:H	1.90	0.68
2:G:60:THR:HG23	2:G:62:THR:H	1.59	0.67
2:G:134:GLN:O	2:G:138:LEU:HG	1.95	0.67
2:B:108:VAL:HG12	2:B:109:ILE:N	2.10	0.67
2:G:55:ILE:HD12	2:G:66:LEU:HD12	1.77	0.67
1:F:175:GLU:OE1	1:F:175:GLU:HA	1.95	0.66
2:G:63:ASN:N	2:G:63:ASN:HD22	1.92	0.66
1:A:111:GLU:HG3	1:A:144:LYS:HZ2	1.61	0.66
1:A:82:ASN:ND2	1:A:118:ARG:HH11	1.91	0.65
1:A:111:GLU:HG3	1:A:144:LYS:NZ	2.11	0.65
4:I:11:DC:H1'	4:I:12:DC:H5"	1.76	0.65
2:B:45:GLN:HE21	2:B:49:ARG:HH12	1.44	0.65
2:B:129:GLU:O	2:B:133:GLN:HG3	1.97	0.65
3:H:372:ALA:HB1	3:H:385:ASN:HA	1.79	0.64
2:B:108:VAL:HG12	2:B:109:ILE:H	1.61	0.64
3:H:365:LEU:HD21	3:H:368:PRO:CA	2.28	0.63
4:I:12:DC:H2'	4:I:13:DT:H72	1.81	0.63
2:G:90:ARG:O	2:G:91:GLU:HB2	1.98	0.63
2:G:8:GLN:HE21	2:G:107:CYS:H	1.46	0.63
3:C:365:LEU:HD23	3:C:371:VAL:HG21	1.79	0.63
1:F:63:VAL:HG22	1:F:64:ARG:N	2.14	0.63
1:A:104:THR:HG22	1:A:151:THR:HB	1.80	0.63
2:G:9:ARG:HG3	2:G:9:ARG:HH11	1.64	0.62
2:B:55:ILE:HD12	2:B:66:LEU:HD12	1.82	0.62
2:B:108:VAL:HG11	2:B:125:LEU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:365:LEU:HD21	3:H:368:PRO:N	2.15	0.61
1:F:164:ARG:HD2	6:F:306:HOH:O	2.01	0.60
3:H:347:ASP:OD2	3:H:349:SER:HB3	2.02	0.60
1:A:70:PHE:CE2	1:A:152:VAL:HG21	2.36	0.60
1:A:106:MET:HE1	2:B:65:SER:HB2	1.84	0.60
1:A:97:VAL:H	1:A:127:GLN:HE22	1.49	0.60
1:A:159:VAL:HG13	2:B:103:LEU:HA	1.84	0.59
2:G:70:PRO:HG3	2:G:85:TYR:CE2	2.37	0.59
3:C:345:LEU:HD21	3:C:354:ILE:HG12	1.84	0.59
4:D:11:DC:H2"	4:D:12:DC:H5'	1.84	0.59
1:A:82:ASN:HD21	1:A:118:ARG:NH1	1.94	0.59
2:B:9:ARG:HA	2:B:127:PHE:CE2	2.38	0.59
3:H:353:PHE:CG	3:H:370:GLU:HG2	2.38	0.59
1:A:145:SER:HB3	1:A:164:ARG:HA	1.84	0.58
3:H:340:PHE:HZ	3:H:374:ARG:HB3	1.69	0.58
2:B:5:VAL:HG11	2:B:11:LYS:HD2	1.85	0.58
1:A:63:VAL:HG12	1:A:72:CYS:O	2.03	0.58
4:I:13:DT:H6	4:I:13:DT:H5'	1.69	0.57
2:G:41:GLN:HG2	2:G:119:LEU:HD21	1.86	0.57
3:C:336:GLN:NE2	3:C:338:TRP:HE1	2.03	0.57
2:G:8:GLN:HE22	2:G:132:ALA:HA	1.70	0.57
1:F:63:VAL:HG12	1:F:72:CYS:O	2.04	0.56
3:H:385:ASN:OD1	3:H:387:GLU:HB2	2.05	0.56
2:G:108:VAL:HG12	2:G:109:ILE:N	2.20	0.56
2:B:134:GLN:O	2:B:137:ALA:HB3	2.05	0.56
3:C:409:ARG:HD2	3:C:410:TYR:CE2	2.40	0.56
1:A:109:ASN:C	1:A:109:ASN:HD22	2.09	0.56
2:G:111:LYS:HD2	2:G:126:GLU:OE1	2.05	0.56
4:D:13:DT:H2"	4:D:14:DC:H5'	1.87	0.56
2:B:89:GLU:O	2:B:91:GLU:N	2.39	0.56
3:H:371:VAL:HA	3:H:374:ARG:HB2	1.87	0.56
1:F:78:HIS:HB3	1:F:173:PRO:HG3	1.88	0.55
4:I:9:DA:H1'	4:I:10:DT:H5"	1.87	0.55
3:H:345:LEU:HD13	3:H:356:TRP:CE2	2.42	0.55
3:H:419:GLN:NE2	3:H:426:PRO:HD3	2.22	0.55
2:G:21:LEU:HD21	2:G:60:THR:HG21	1.88	0.55
4:D:1:DG:O4'	4:I:15:DT:H2'	2.06	0.55
1:A:68:PRO:O	1:A:94:LYS:HD2	2.07	0.55
2:G:132:ALA:O	2:G:136:ASP:HB2	2.07	0.54
2:B:63:ASN:HD22	2:B:63:ASN:N	2.06	0.54
3:C:409:ARG:HG3	3:C:410:TYR:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ASP:HB3	2:B:118:ARG:HB2	1.88	0.54
2:G:8:GLN:HG2	2:G:106:VAL:HA	1.90	0.54
1:A:152:VAL:HG12	1:A:154:THR:HG23	1.90	0.54
2:B:131:ARG:HG2	2:B:131:ARG:HH11	1.73	0.54
4:I:13:DT:H5'	4:I:13:DT:C6	2.42	0.53
4:I:12:DC:C2'	4:I:13:DT:H72	2.37	0.53
3:H:365:LEU:O	3:H:365:LEU:HD23	2.08	0.53
2:B:21:LEU:HD22	2:B:57:PHE:CD1	2.43	0.53
3:H:348:LYS:HD3	3:H:433:LEU:HD23	1.89	0.53
2:B:7:ASP:HB2	2:B:10:SER:HB3	1.89	0.53
4:I:10:DT:H1'	4:I:11:DC:H5'	1.90	0.53
3:H:368:PRO:HG2	3:H:369:ASP:H	1.74	0.53
1:A:112:ASN:HD22	1:A:112:ASN:C	2.12	0.53
4:D:9:DA:H2"	4:D:10:DT:H5'	1.91	0.53
3:H:369:ASP:HB3	3:H:373:ARG:NH2	2.24	0.53
3:H:345:LEU:HD22	3:H:356:TRP:CD1	2.43	0.53
3:H:419:GLN:HE22	3:H:425:THR:CA	2.11	0.52
3:H:353:PHE:HB3	3:H:370:GLU:HG2	1.91	0.52
1:F:167:LYS:C	1:F:168:ILE:HD12	2.29	0.52
2:B:106:VAL:O	2:B:108:VAL:HG23	2.09	0.52
3:H:362:GLU:HB2	3:H:413:ARG:HD2	1.92	0.52
2:G:16:GLU:OE2	2:G:20:LYS:HB2	2.09	0.52
2:B:131:ARG:O	2:B:135:GLU:HB2	2.09	0.52
2:G:11:LYS:HG3	2:G:15:GLU:CG	2.37	0.52
3:C:385:ASN:HD21	3:C:387:GLU:HG3	1.75	0.52
3:C:322:PRO:HG2	3:C:326:LEU:HG	1.91	0.51
2:G:9:ARG:HH11	2:G:9:ARG:CG	2.22	0.51
3:C:405:THR:HG21	3:C:408:LYS:HD2	1.93	0.51
3:H:389:LEU:HD23	3:H:389:LEU:O	2.10	0.51
2:B:37:HIS:O	2:B:41:GLN:HG3	2.11	0.51
4:I:2:DA:H1'	4:I:3:DA:H5'	1.93	0.51
2:B:56:ALA:HB2	2:B:63:ASN:HA	1.93	0.51
1:F:79:TRP:CH2	1:F:86:PRO:HD3	2.46	0.50
1:F:63:VAL:HB	1:F:74:VAL:HG22	1.92	0.50
3:H:369:ASP:HB3	3:H:373:ARG:HH21	1.75	0.50
2:B:8:GLN:HE22	2:B:132:ALA:HA	1.77	0.50
2:B:57:PHE:HB2	2:B:60:THR:HG22	1.94	0.50
3:H:340:PHE:CZ	3:H:374:ARG:HB3	2.46	0.50
1:F:66:ASP:OD2	1:F:161:THR:OG1	2.29	0.50
3:C:327:ALA:HA	3:C:421:LEU:CD2	2.40	0.50
5:E:15:DC:H2'	5:J:1:DA:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:388:LYS:HE2	4:D:10:DT:H2'	1.94	0.49
2:G:19:ARG:HA	2:G:22:SER:OG	2.12	0.49
2:G:23:ARG:O	2:G:24:GLU:C	2.50	0.49
1:A:112:ASN:ND2	1:A:114:SER:H	2.09	0.49
4:D:9:DA:H1'	4:D:10:DT:H5"	1.95	0.49
5:E:9:DT:H2"	5:E:10:DG:C8	2.48	0.48
3:H:401:ILE:HA	3:H:416:CYS:HB3	1.94	0.48
1:F:130:ARG:HH12	1:F:132:ASN:HD22	1.60	0.48
4:I:12:DC:H2"	4:I:13:DT:H5'	1.95	0.48
1:F:102:LEU:N	1:F:102:LEU:HD22	2.28	0.48
3:H:334:PRO:HG2	5:J:11:DG:H4'	1.94	0.48
2:G:106:VAL:HG12	2:G:108:VAL:CG2	2.43	0.48
2:G:131:ARG:HB3	2:G:131:ARG:CZ	2.44	0.48
4:D:5:DC:H1'	4:D:6:DC:H5"	1.96	0.48
3:H:429:LEU:C	3:H:431:ALA:H	2.16	0.48
4:I:11:DC:C2'	4:I:12:DC:H5"	2.44	0.48
4:D:11:DC:H1'	4:D:12:DC:H5"	1.95	0.48
2:G:82:SER:OG	2:G:85:TYR:HB2	2.13	0.48
4:D:1:DG:H2"	4:D:2:DA:OP2	2.13	0.47
2:G:82:SER:OG	2:G:83:ARG:N	2.47	0.47
2:B:41:GLN:HE21	2:B:117:HIS:HA	1.78	0.47
3:H:365:LEU:HD21	3:H:368:PRO:HA	1.96	0.47
4:D:14:DC:H2"	4:D:15:DT:H5'	1.95	0.47
1:A:78:HIS:CD2	1:A:167:LYS:HE3	2.49	0.47
4:I:7:DA:H2"	4:I:8:DC:O5'	2.14	0.47
2:B:55:ILE:HD12	2:B:66:LEU:CD1	2.44	0.47
1:F:136:PHE:CB	1:F:168:ILE:HG12	2.44	0.47
2:B:8:GLN:NE2	2:B:132:ALA:HA	2.30	0.47
3:H:362:GLU:CB	3:H:413:ARG:HD2	2.45	0.47
2:G:108:VAL:HG12	2:G:109:ILE:H	1.79	0.47
1:F:69:ASN:HB2	2:G:2:PRO:O	2.15	0.47
2:G:63:ASN:N	2:G:63:ASN:ND2	2.60	0.47
2:G:106:VAL:HG12	2:G:108:VAL:HG23	1.97	0.47
3:H:393:LEU:HA	3:H:396:TYR:HD2	1.79	0.47
2:B:108:VAL:CG1	2:B:109:ILE:N	2.78	0.46
2:B:29:TYR:CZ	2:B:31:GLY:HA3	2.50	0.46
2:G:16:GLU:OE2	2:G:20:LYS:HD2	2.15	0.46
2:B:45:GLN:HE21	2:B:49:ARG:NH1	2.12	0.46
3:H:345:LEU:HB3	3:H:356:TRP:HE1	1.81	0.46
1:A:112:ASN:HD21	2:B:33:ARG:HH12	1.64	0.46
2:G:3:ARG:NE	2:G:135:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:ILE:HD11	2:B:113:TRP:O	2.15	0.46
3:H:338:TRP:CE2	3:H:339:GLN:HG3	2.51	0.45
1:F:177:ARG:NH1	5:J:11:DG:N7	2.63	0.45
1:A:65:THR:HG23	1:A:70:PHE:O	2.16	0.45
5:J:9:DT:H2"	5:J:10:DG:C8	2.52	0.45
3:H:417:ASP:O	3:H:421:LEU:HD13	2.16	0.45
3:C:385:ASN:HD21	3:C:387:GLU:CG	2.30	0.45
2:B:32:PHE:CD2	2:B:32:PHE:N	2.84	0.45
2:B:57:PHE:HB2	2:B:60:THR:CG2	2.46	0.45
1:A:112:ASN:ND2	2:B:33:ARG:HH12	2.14	0.45
1:F:113:TYR:CZ	2:G:28:LYS:HD2	2.52	0.45
3:C:357:THR:CG2	3:C:362:GLU:HG2	2.47	0.45
3:C:404:LYS:HG3	3:C:405:THR:N	2.31	0.44
2:G:11:LYS:HE3	2:G:15:GLU:OE1	2.18	0.44
2:G:131:ARG:HB3	2:G:131:ARG:NH1	2.33	0.44
2:B:108:VAL:CG1	2:B:109:ILE:H	2.28	0.44
4:D:11:DC:H1'	4:D:12:DC:C5'	2.46	0.44
2:B:45:GLN:OE1	2:B:116:LEU:HD22	2.18	0.44
2:G:71:ALA:HB3	2:G:131:ARG:NE	2.33	0.44
2:B:115:ASP:O	2:B:117:HIS:N	2.50	0.44
3:H:431:ALA:C	3:H:433:LEU:H	2.21	0.44
1:F:63:VAL:CG2	1:F:64:ARG:N	2.79	0.44
3:H:384:MET:HE1	3:H:389:LEU:HB2	1.99	0.44
3:H:390:SER:O	3:H:393:LEU:HB2	2.18	0.44
4:I:8:DC:H2"	4:I:9:DA:C8	2.53	0.44
3:C:404:LYS:HE2	3:C:411:VAL:O	2.17	0.44
1:A:69:ASN:HD21	1:A:95:GLY:N	2.12	0.43
2:G:8:GLN:HB3	2:G:127:PHE:HE2	1.83	0.43
1:A:126:ASN:O	1:A:127:GLN:HB2	2.17	0.43
4:D:10:DT:C2'	4:D:11:DC:H5'	2.47	0.43
3:H:347:ASP:CG	3:H:349:SER:HB3	2.38	0.43
2:B:56:ALA:CB	2:B:63:ASN:HA	2.48	0.43
1:A:149:THR:HG21	2:B:63:ASN:O	2.17	0.43
1:A:109:ASN:HD21	1:A:112:ASN:H	1.64	0.43
3:H:422:LEU:C	3:H:424:TYR:H	2.21	0.43
2:G:46:ASN:O	2:G:49:ARG:HB2	2.18	0.43
1:A:116:GLU:HG2	1:A:137:VAL:HB	2.00	0.43
2:B:21:LEU:HD21	2:B:60:THR:HG21	2.01	0.43
1:A:79:TRP:CZ2	1:A:86:PRO:HD3	2.53	0.43
1:A:115:ALA:HB2	1:A:146:PHE:CZ	2.52	0.43
1:F:63:VAL:HG22	1:F:64:ARG:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:SER:O	1:A:144:LYS:HB3	2.19	0.43
3:C:353:PHE:N	3:C:353:PHE:CD2	2.87	0.43
4:I:11:DC:C1'	4:I:12:DC:H5"	2.47	0.43
3:H:429:LEU:O	3:H:429:LEU:HD23	2.18	0.43
2:G:63:ASN:H	2:G:63:ASN:HD22	1.63	0.43
2:B:131:ARG:HG2	2:B:131:ARG:NH1	2.34	0.43
3:C:364:LYS:HB3	3:C:411:VAL:HG22	2.01	0.42
3:C:324:ALA:HB2	3:C:343:GLU:HG3	2.02	0.42
2:B:86:VAL:HG13	2:B:86:VAL:O	2.19	0.42
1:F:168:ILE:HD12	1:F:168:ILE:N	2.34	0.42
2:G:29:TYR:CD2	2:G:44:PHE:HD2	2.38	0.42
1:A:144:LYS:HE2	3:H:407:GLY:HA2	2.01	0.42
4:D:6:DC:H2"	4:D:7:DA:C8	2.54	0.42
1:A:109:ASN:ND2	1:A:109:ASN:C	2.72	0.42
2:G:9:ARG:NH1	2:G:9:ARG:CG	2.78	0.42
1:A:171:ASP:HB3	1:A:174:ARG:HD2	2.02	0.42
3:C:320:VAL:HG11	3:C:432:MET:HB3	2.01	0.42
4:D:8:DC:H2"	4:D:9:DA:C8	2.55	0.41
2:G:18:PHE:O	2:G:20:LYS:N	2.53	0.41
3:H:421:LEU:C	3:H:422:LEU:HD12	2.40	0.41
3:C:336:GLN:HE21	3:C:338:TRP:HE1	1.67	0.41
2:G:9:ARG:NH1	2:G:129:GLU:OE1	2.53	0.41
3:H:353:PHE:CB	3:H:370:GLU:HG2	2.50	0.41
1:F:112:ASN:HD22	1:F:112:ASN:C	2.23	0.41
4:I:11:DC:H2"	4:I:12:DC:H5"	2.03	0.41
3:C:364:LYS:CB	3:C:411:VAL:HG22	2.50	0.41
3:H:393:LEU:HA	3:H:396:TYR:CD2	2.55	0.41
3:H:361:TRP:HZ2	3:H:419:GLN:HE21	1.67	0.41
2:B:100:PRO:O	2:B:101:MET:HB3	2.21	0.41
3:H:396:TYR:HB3	3:H:401:ILE:HB	2.02	0.41
3:H:336:GLN:H	3:H:339:GLN:HE21	1.68	0.41
1:F:93:ALA:O	1:F:127:GLN:NE2	2.50	0.41
3:C:322:PRO:HB2	3:C:325:ALA:HB3	2.02	0.41
2:G:4:VAL:HG13	2:G:135:GLU:HG2	2.03	0.41
3:C:342:LEU:HA	3:C:342:LEU:HD12	1.94	0.41
1:A:69:ASN:HD22	1:A:94:LYS:HB2	1.85	0.41
3:H:384:MET:HE1	3:H:389:LEU:CA	2.51	0.41
2:G:137:ALA:C	2:G:139:ALA:H	2.24	0.41
1:A:112:ASN:HD22	1:A:113:TYR:N	2.18	0.41
2:G:21:LEU:HD22	2:G:57:PHE:CD1	2.56	0.41
2:G:85:TYR:HA	2:G:98:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:23:ARG:H	2:G:23:ARG:HD3	1.86	0.41
1:A:98:PRO:HG2	1:A:101:THR:OG1	2.21	0.41
4:I:14:DC:C2'	4:I:15:DT:C5'	2.95	0.40
4:I:5:DC:H1'	4:I:6:DC:H5"	2.03	0.40
4:I:6:DC:H2"	4:I:7:DA:C8	2.57	0.40
2:B:8:GLN:HE21	2:B:107:CYS:H	1.68	0.40
3:C:359:ASP:OD2	3:C:359:ASP:C	2.59	0.40
2:B:123:GLY:O	2:B:124:CYS:HB3	2.21	0.40
1:F:114:SER:HB3	2:G:33:ARG:HH11	1.87	0.40
3:H:348:LYS:HA	3:H:351:GLN:CG	2.51	0.40
3:C:418:LEU:HD23	3:C:418:LEU:HA	1.79	0.40
2:B:100:PRO:HA	2:B:109:ILE:HA	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	116/204 (57%)	109 (94%)	7 (6%)	0	100	100
1	F	116/204 (57%)	110 (95%)	5 (4%)	1 (1%)	21	49
2	B	126/142 (89%)	105 (83%)	14 (11%)	7 (6%)	2	3
2	G	125/142 (88%)	109 (87%)	9 (7%)	7 (6%)	2	3
3	C	116/166 (70%)	111 (96%)	5 (4%)	0	100	100
3	H	99/166 (60%)	82 (83%)	14 (14%)	3 (3%)	5	13
All	All	698/1024 (68%)	626 (90%)	54 (8%)	18 (3%)	7	16

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	90	ARG

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Mol	Chain	Res	Type
2	G	91	GLU
2	G	19	ARG
3	H	334	PRO
2	B	32	PHE
2	B	116	LEU
2	B	130	GLU
2	G	116	LEU
3	H	431	ALA
2	B	58	VAL
2	G	14	ASN
2	G	24	GLU
2	G	59	ALA
2	G	89	GLU
2	B	7	ASP
2	B	24	GLU
1	F	110	ASP
3	H	368	PRO

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	99/178 (56%)	91 (92%)	8 (8%)	15	33
1	F	99/178 (56%)	93 (94%)	6 (6%)	23	49
2	B	113/123 (92%)	110 (97%)	3 (3%)	52	82
2	G	112/123 (91%)	103 (92%)	9 (8%)	15	33
3	C	102/145 (70%)	96 (94%)	6 (6%)	24	51
3	H	91/145 (63%)	91 (100%)	0	100	100
All	All	616/892 (69%)	584 (95%)	32 (5%)	29	58

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASN

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Mol	Chain	Res	Type
1	A	104	THR
1	A	109	ASN
1	A	112	ASN
1	A	117	LEU
1	A	144	LYS
1	A	145	SER
1	A	162	TYR
2	B	23	ARG
2	B	63	ASN
2	B	103	LEU
3	C	330	THR
3	C	352	SER
3	C	378	ARG
3	C	383	LYS
3	C	404	LYS
3	C	427	GLU
1	F	62	LEU
1	F	96	ASP
1	F	112	ASN
1	F	139	ARG
1	F	162	TYR
1	F	175	GLU
2	G	9	ARG
2	G	23	ARG
2	G	38	GLU
2	G	63	ASN
2	G	67	GLN
2	G	89	GLU
2	G	90	ARG
2	G	103	LEU
2	G	117	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	82	ASN
1	A	109	ASN
1	A	112	ASN
1	A	119	ASN
1	A	127	GLN
1	A	132	ASN

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Mol	Chain	Res	Type
2	B	8	GLN
2	B	41	GLN
2	B	46	ASN
2	B	104	ASN
2	B	133	GLN
2	B	134	GLN
2	B	140	GLN
3	C	336	GLN
3	C	380	ASN
3	C	385	ASN
1	F	112	ASN
1	F	126	ASN
1	F	132	ASN
2	G	8	GLN
2	G	134	GLN
3	H	336	GLN
3	H	339	GLN
3	H	419	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	118/204 (57%)	0.15	0	100	100	44, 63, 90, 101	0
1	F	118/204 (57%)	0.06	1 (0%)	87	88	43, 54, 74, 101	0
2	B	130/142 (91%)	0.67	9 (6%)	20	18	65, 90, 118, 130	0
2	G	129/142 (90%)	0.49	7 (5%)	29	28	62, 80, 110, 115	0
3	C	118/166 (71%)	0.28	1 (0%)	87	88	40, 62, 91, 101	0
3	H	101/166 (60%)	1.81	38 (37%)	0	0	62, 120, 166, 171	0
4	D	15/15 (100%)	-0.20	0	100	100	51, 55, 68, 69	0
4	I	15/15 (100%)	-0.23	0	100	100	53, 63, 82, 87	0
5	E	15/15 (100%)	-0.28	0	100	100	46, 54, 65, 71	0
5	J	15/15 (100%)	-0.27	0	100	100	51, 61, 76, 81	0
All	All	774/1084 (71%)	0.49	56 (7%)	18	16	40, 71, 125, 171	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	429	LEU	6.5
3	H	421	LEU	6.5
3	H	422	LEU	6.5
3	H	432	MET	6.3
3	H	356	TRP	5.3
3	H	361	TRP	4.8
3	H	341	LEU	4.8
3	H	426	PRO	4.4
3	H	335	ILE	4.2
3	H	433	LEU	4.1
3	H	345	LEU	4.1
3	H	424	TYR	4.1
3	H	337	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
3	H	419	GLN	3.8
3	H	354	ILE	3.7
2	B	116	LEU	3.7
3	H	423	GLY	3.5
3	H	364	LYS	3.3
3	H	427	GLU	3.3
3	H	333	GLY	3.2
2	B	95	VAL	3.2
3	H	342	LEU	3.1
3	H	425	THR	2.9
3	H	374	ARG	2.9
3	H	351	GLN	2.7
3	H	375	TRP	2.7
3	H	430	HIS	2.7
3	H	365	LEU	2.7
3	H	414	PHE	2.7
3	H	346	THR	2.6
3	H	338	TRP	2.6
3	H	409	ARG	2.6
2	G	82	SER	2.5
2	G	22	SER	2.5
3	H	350	CYS	2.5
2	B	88	LEU	2.4
1	F	177	ARG	2.4
3	H	372	ALA	2.4
2	G	83	ARG	2.4
3	H	358	GLY	2.3
3	H	418	LEU	2.3
2	B	83	ARG	2.3
2	G	86	VAL	2.3
2	G	81	PRO	2.2
3	H	420	SER	2.2
2	B	5	VAL	2.2
2	B	23	ARG	2.2
3	C	330	THR	2.2
2	B	93	GLY	2.1
3	H	353	PHE	2.1
2	B	139	ALA	2.1
3	H	363	PHE	2.1
2	G	131	ARG	2.1
2	B	94	LYS	2.1
2	G	88	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	H	366	SER	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.