Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:19 PM GMT

PDB ID	:	3WTS
Title	:	Crystal structure of the complex comprised of ETS1, RUNX1, CBFBETA, and the tcralpha gene enhancer DNA
Authors	:	Shiina, M.; Hamada, K.; Ogata, K.
Deposited on	:	2014-04-21
Resolution	:	2.35 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

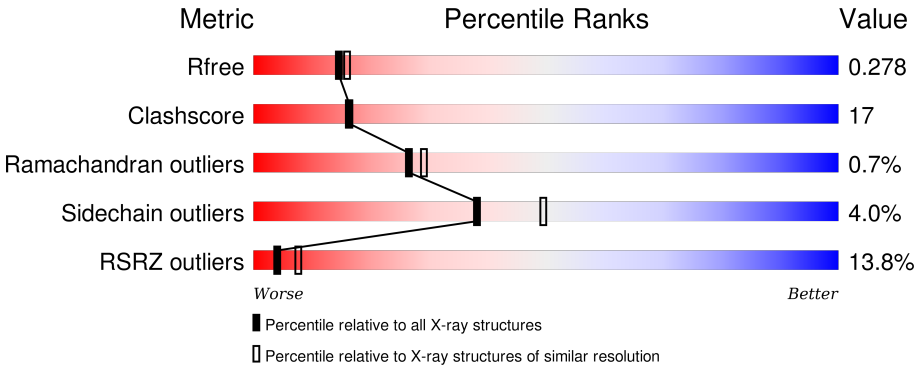
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	205	43% 13% 42%
1	F	205	44% 12% 42%
2	B	142	20% 53% 37% 8%
2	G	142	11% 65% 25% 9%
3	C	166	2% 56% 14% 29%

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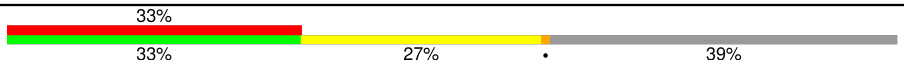
Mol	Chain	Length	Quality of chain
3	H	166	
4	D	15	
4	I	15	
5	E	15	
5	J	15	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7094 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	119	Total	C	N	O	S	0	0	0
			922	579	170	168	5			
1	F	118	Total	C	N	O	S	0	0	0
			914	574	169	167	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MET	-	EXPRESSION TAG	UNP Q03347
A	94	LYS	LEU	ENGINEERED MUTATION	UNP Q03347
F	59	MET	-	EXPRESSION TAG	UNP Q03347
F	94	LYS	LEU	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 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	C	N	O	P	0	0	0
			299	144	54	87	14			
4	I	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			

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

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

- Molecule 6 is water.

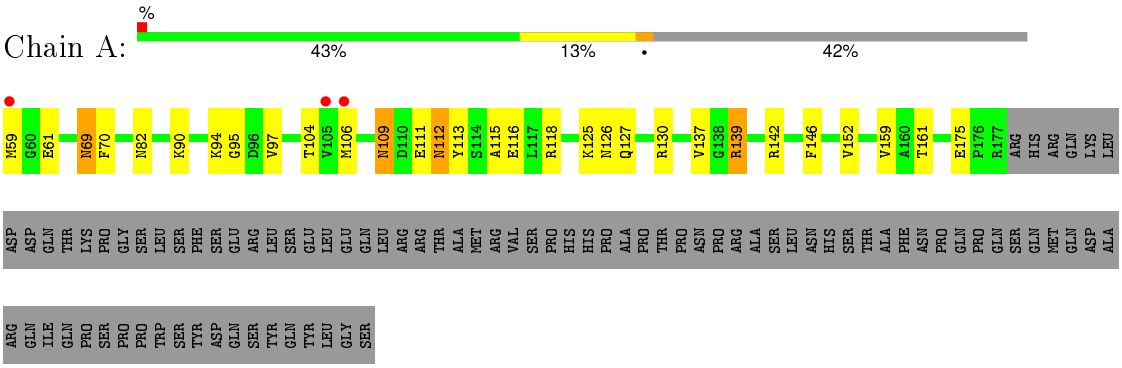
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	B	3	Total	O	0	0
			3	3		
6	C	16	Total	O	0	0
			16	16		
6	F	13	Total	O	0	0
			13	13		
6	G	3	Total	O	0	0
			3	3		
6	D	7	Total	O	0	0
			7	7		
6	E	14	Total	O	0	0
			14	14		
6	I	2	Total	O	0	0
			2	2		
6	J	11	Total	O	0	0
			11	11		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

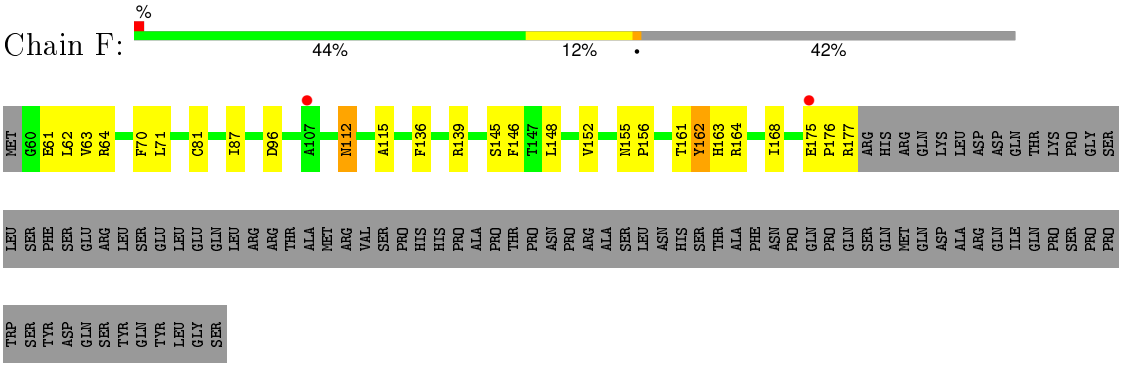
• Molecule 1: Runt-related transcription factor 1

Chain A:



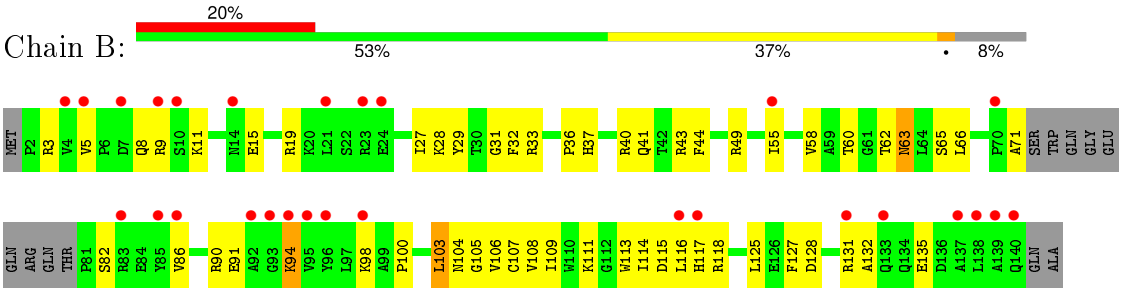
• Molecule 1: Runt-related transcription factor 1

Chain F:



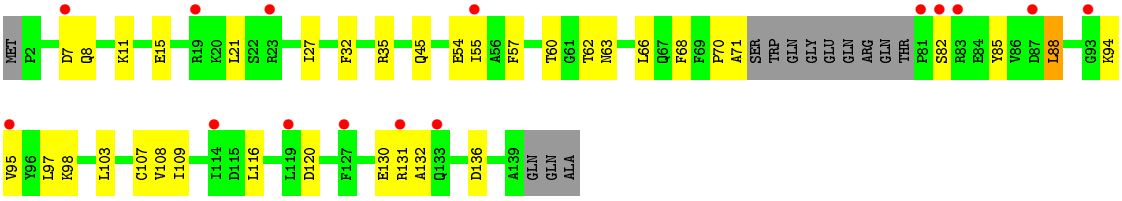
• Molecule 2: Core-binding factor subunit beta

Chain B:



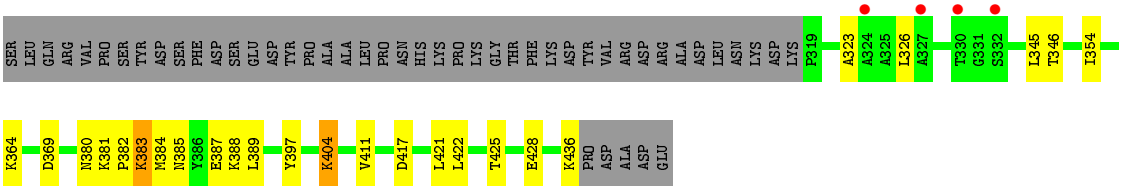
• Molecule 2: Core-binding factor subunit beta

Chain G:



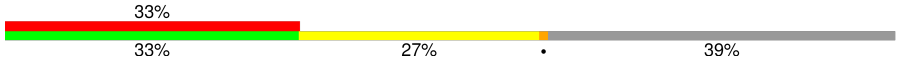
• Molecule 3: Protein C-ets-1

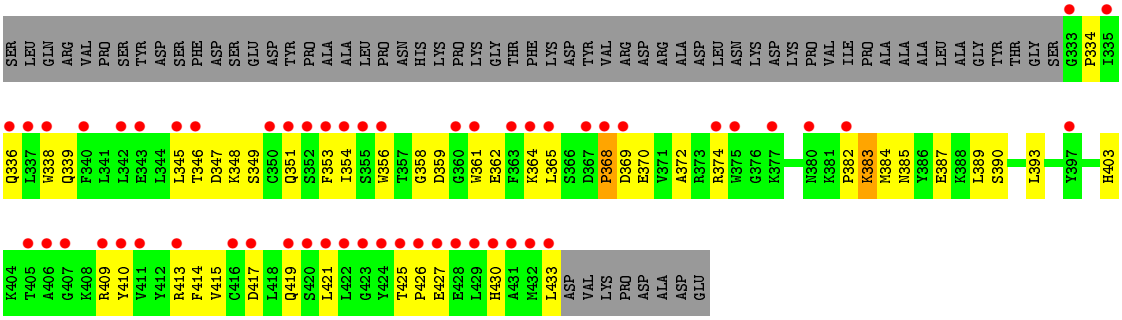
Chain C:



• Molecule 3: Protein C-ets-1

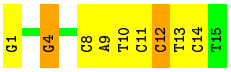
Chain H:





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

Chain D:



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

Chain I:

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

Chain E:

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

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.72Å 102.06Å 194.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.99 – 2.35 44.99 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.99-2.35) 98.9 (44.99-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.34Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.249 , 0.279 0.249 , 0.278	Depositor DCC
R_{free} test set	6608 reflections (10.13%)	DCC
Wilson B-factor (Å^2)	64.1	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 65218 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7094	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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, 0.375 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	0.40	0/941	0.62	0/1278
1	F	0.48	0/933	0.68	0/1268
2	B	0.34	0/1093	0.49	0/1466
2	G	0.36	0/1084	0.50	0/1454
3	C	0.44	0/994	0.58	0/1342
3	H	0.32	0/877	0.43	0/1181
4	D	0.61	0/334	0.94	1/512 (0.2%)
4	I	0.58	0/334	0.88	1/512 (0.2%)
5	E	0.52	0/348	0.82	0/537
5	J	0.47	0/348	0.74	0/537
All	All	0.43	0/7286	0.63	2/10087 (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	2
4	I	0	2
5	E	0	1
All	All	0	5

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'	-5.84	101.50	112.60
4	I	4	DG	N9-C1'-C2'	-5.10	102.91	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	12	DC	Sidechain
4	D	4	DG	Sidechain
5	E	113	DT	Sidechain
4	I	4	DG	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	922	0	931	33	0
1	F	914	0	922	23	0
2	B	1071	0	1034	50	0
2	G	1062	0	1026	31	0
3	C	967	0	966	20	0
3	H	853	0	847	47	0
4	D	299	0	170	13	0
4	I	299	0	170	16	0
5	E	310	0	171	2	0
5	J	310	0	171	5	0
6	A	18	0	0	2	0
6	B	3	0	0	0	0
6	C	16	0	0	1	0
6	D	7	0	0	2	0
6	E	14	0	0	0	0
6	F	13	0	0	0	0
6	G	3	0	0	2	0
6	I	2	0	0	0	0
6	J	11	0	0	0	0
All	All	7094	0	6408	224	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 17.

All (224) 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:82:ASN:HD21	1:A:118:ARG:HH11	1.14	0.94
1:A:69:ASN:HD21	1:A:95:GLY:H	1.17	0.90
3:H:345:LEU:HB3	3:H:356:TRP:HE1	1.38	0.86
4:I:10:DT:H2"	4:I:11:DC:H5'	1.63	0.79
1:A:69:ASN:ND2	1:A:95:GLY:H	1.80	0.79
1:A:109:ASN:ND2	1:A:112:ASN:H	1.79	0.79
4:D:10:DT:H2"	4:D:11:DC:H5'	1.63	0.79
3:H:362:GLU:HB2	3:H:413:ARG:HH11	1.47	0.76
1:A:97:VAL:H	1:A:127:GLN:HE22	1.34	0.75
4:I:11:DC:H1'	4:I:12:DC:H5"	1.71	0.73
1:A:161:THR:H	2:B:104:ASN:HD21	1.41	0.69
2:G:60:THR:HG23	2:G:62:THR:H	1.57	0.68
1:A:104:THR:HG23	6:A:307:HOH:O	1.93	0.68
2:B:71:ALA:HB2	2:B:131:ARG:HD3	1.77	0.67
1:A:109:ASN:C	1:A:109:ASN:HD22	1.99	0.65
1:A:69:ASN:HD22	1:A:94:LYS:HB2	1.62	0.65
3:H:356:TRP:O	3:H:364:LYS:HE2	1.97	0.65
2:B:108:VAL:HG12	2:B:109:ILE:N	2.13	0.64
2:B:106:VAL:O	2:B:108:VAL:HG23	1.99	0.62
4:D:11:DC:H1'	4:D:12:DC:H5"	1.82	0.62
2:B:108:VAL:HG11	2:B:125:LEU:HB3	1.81	0.62
3:H:348:LYS:HA	3:H:351:GLN:HE21	1.65	0.61
1:F:115:ALA:HB2	1:F:146:PHE:CZ	2.36	0.60
2:B:55:ILE:HG12	2:B:114:ILE:HD11	1.84	0.60
3:H:336:GLN:H	3:H:339:GLN:HE21	1.50	0.60
1:F:64:ARG:HA	1:F:71:LEU:HD23	1.83	0.60
2:G:85:TYR:HA	2:G:98:LYS:HB3	1.82	0.59
4:I:11:DC:H2"	4:I:12:DC:H5"	1.84	0.59
3:H:336:GLN:H	3:H:339:GLN:NE2	2.01	0.59
3:H:409:ARG:HH11	5:J:101:DA:H3'	1.68	0.58
5:E:115:DC:H2'	5:J:101:DA:O4'	2.04	0.58
4:D:13:DT:H2"	4:D:14:DC:H5'	1.85	0.58
2:B:108:VAL:HG12	2:B:109:ILE:H	1.67	0.58
1:F:70:PHE:CE2	1:F:152:VAL:HG21	2.39	0.58
4:I:11:DC:C2'	4:I:12:DC:H5"	2.33	0.58
2:B:41:GLN:HE21	2:B:117:HIS:HA	1.69	0.57
3:C:425:THR:OG1	3:C:428:GLU:HG3	2.04	0.57
3:C:345:LEU:HD21	3:C:354:ILE:HG12	1.85	0.57
1:A:69:ASN:HD21	1:A:95:GLY:N	1.95	0.57
2:G:71:ALA:HB1	2:G:131:ARG:HE	1.70	0.56
3:H:359:ASP:HB3	3:H:413:ARG:NH1	2.20	0.56
2:B:63:ASN:HD22	2:B:63:ASN:N	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:VAL:HG22	1:F:64:ARG:N	2.20	0.56
3:C:382:PRO:HG2	3:C:383:LYS:HD3	1.88	0.56
3:H:347:ASP:OD2	3:H:349:SER:HB3	2.06	0.56
3:H:346:THR:HG22	3:H:433:LEU:HD11	1.88	0.56
3:H:348:LYS:O	3:H:351:GLN:HG2	2.05	0.56
2:B:109:ILE:HD11	2:B:128:ASP:OD1	2.06	0.55
1:A:70:PHE:CE2	1:A:152:VAL:HG21	2.42	0.55
2:G:55:ILE:HD13	2:G:66:LEU:HD12	1.89	0.54
3:H:389:LEU:HD23	3:H:389:LEU:O	2.07	0.54
4:I:9:DA:H1'	4:I:10:DT:H5"	1.90	0.54
2:G:132:ALA:O	2:G:136:ASP:HB2	2.07	0.54
2:B:5:VAL:HG11	2:B:11:LYS:HG3	1.90	0.54
1:A:69:ASN:ND2	1:A:94:LYS:HB2	2.23	0.54
3:H:361:TRP:HB3	3:H:414:PHE:HB2	1.90	0.53
2:G:108:VAL:HG22	2:G:109:ILE:H	1.73	0.53
3:H:365:LEU:HD21	3:H:368:PRO:CA	2.38	0.53
2:G:8:GLN:HE21	2:G:107:CYS:H	1.57	0.53
2:B:5:VAL:HG12	2:B:105:GLY:O	2.09	0.53
4:D:10:DT:C2'	4:D:11:DC:H5'	2.35	0.53
4:D:9:DA:H1'	4:D:10:DT:H5"	1.89	0.53
4:I:11:DC:C1'	4:I:12:DC:H5"	2.37	0.52
2:B:28:LYS:HE3	2:B:58:VAL:HG21	1.91	0.52
1:A:142:ARG:HD3	5:E:115:DC:H4'	1.91	0.52
1:F:161:THR:HG21	1:F:163:HIS:CE1	2.44	0.52
2:B:15:GLU:O	2:B:19:ARG:HG3	2.09	0.52
3:H:372:ALA:HB1	3:H:385:ASN:HA	1.91	0.52
2:G:95:VAL:HG13	2:G:116:LEU:HD21	1.91	0.52
2:G:82:SER:OG	2:G:85:TYR:HB2	2.09	0.52
1:F:87:ILE:HD12	1:F:87:ILE:O	2.09	0.52
1:F:136:PHE:CB	1:F:168:ILE:HG12	2.40	0.51
3:C:385:ASN:OD1	3:C:388:LYS:HG3	2.10	0.51
1:A:109:ASN:HD21	1:A:112:ASN:H	1.52	0.51
4:I:11:DC:H2"	4:I:12:DC:C5'	2.40	0.51
2:G:108:VAL:HG22	2:G:109:ILE:N	2.25	0.51
2:B:37:HIS:O	2:B:41:GLN:HG3	2.10	0.51
2:G:71:ALA:CB	2:G:131:ARG:HE	2.23	0.51
1:A:139:ARG:HB2	1:A:139:ARG:HH11	1.75	0.51
1:A:109:ASN:ND2	1:A:111:GLU:H	2.08	0.51
3:H:365:LEU:HD21	3:H:368:PRO:HA	1.93	0.51
3:H:425:THR:HB	3:H:426:PRO:HD2	1.93	0.51
3:C:364:LYS:CB	3:C:411:VAL:HG22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:389:LEU:HD23	3:C:389:LEU:C	2.30	0.51
3:H:409:ARG:HH11	5:J:101:DA:C3'	2.24	0.51
1:F:145:SER:OG	1:F:164:ARG:HA	2.11	0.51
1:A:159:VAL:HG13	2:B:103:LEU:HA	1.93	0.51
2:B:60:THR:HG23	2:B:62:THR:H	1.76	0.51
2:B:55:ILE:HD13	2:B:66:LEU:HD12	1.92	0.50
2:B:71:ALA:CB	2:B:131:ARG:HD3	2.41	0.50
1:A:112:ASN:HD21	2:B:33:ARG:HH12	1.59	0.50
2:G:68:PHE:CZ	2:G:97:LEU:HD13	2.46	0.50
1:A:139:ARG:HD3	1:A:139:ARG:N	2.27	0.50
3:H:348:LYS:HE3	3:H:433:LEU:HA	1.93	0.49
4:D:1:DG:O4'	4:I:15:DT:H2'	2.12	0.49
3:H:368:PRO:HG2	3:H:369:ASP:H	1.76	0.49
3:H:345:LEU:HB3	3:H:356:TRP:NE1	2.17	0.49
4:D:8:DC:H2"	4:D:9:DA:C8	2.48	0.49
4:D:8:DC:H2'	6:D:102:HOH:O	2.11	0.49
2:B:115:ASP:HB3	2:B:118:ARG:HB2	1.95	0.49
2:B:98:LYS:HE2	2:B:111:LYS:HD3	1.94	0.48
4:D:11:DC:H2"	4:D:12:DC:C5'	2.43	0.48
1:A:115:ALA:HB2	1:A:146:PHE:CZ	2.48	0.48
3:H:348:LYS:NZ	3:H:433:LEU:HD23	2.29	0.48
3:H:409:ARG:HD3	3:H:410:TYR:CE2	2.49	0.48
1:A:109:ASN:ND2	1:A:109:ASN:C	2.67	0.48
2:G:32:PHE:HB3	2:G:35:ARG:CG	2.43	0.48
2:B:29:TYR:CZ	2:B:31:GLY:HA3	2.48	0.48
2:B:49:ARG:HH11	2:B:49:ARG:HG3	1.78	0.48
3:H:374:ARG:HH11	3:H:374:ARG:HG2	1.79	0.48
2:G:21:LEU:HD21	2:G:60:THR:HG21	1.96	0.48
2:G:27:ILE:HB	2:G:55:ILE:CG2	2.43	0.48
1:A:90:LYS:HD3	1:A:130:ARG:HG2	1.95	0.48
2:G:70:PRO:HG3	2:G:85:TYR:CE2	2.49	0.47
3:C:364:LYS:HB3	3:C:411:VAL:HG22	1.95	0.47
1:A:116:GLU:HB3	1:A:137:VAL:HB	1.96	0.47
1:A:82:ASN:ND2	1:A:118:ARG:HH11	1.95	0.47
2:B:98:LYS:HE2	2:B:111:LYS:CD	2.45	0.47
2:B:29:TYR:CE1	2:B:44:PHE:HB2	2.48	0.47
1:F:148:LEU:HB2	1:F:162:TYR:HB3	1.97	0.47
3:H:359:ASP:HB3	3:H:413:ARG:HH12	1.80	0.47
2:B:100:PRO:HB3	2:B:109:ILE:CD1	2.44	0.47
3:H:409:ARG:HB3	5:J:102:DG:OP1	2.15	0.47
4:I:2:DA:H1'	4:I:3:DA:H5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:ARG:NH1	5:J:111:DG:N7	2.63	0.47
3:C:397:TYR:OH	3:C:404:LYS:HB2	2.14	0.47
3:C:385:ASN:HD21	3:C:387:GLU:HB2	1.80	0.46
4:I:13:DT:H5'	4:I:13:DT:C6	2.50	0.46
3:C:385:ASN:ND2	3:C:387:GLU:HB2	2.30	0.46
1:A:112:ASN:ND2	2:B:33:ARG:HH12	2.14	0.46
1:F:146:PHE:HD1	1:F:168:ILE:HD13	1.81	0.46
4:D:11:DC:H2"	4:D:12:DC:H5'	1.97	0.46
2:B:27:ILE:HD11	2:B:113:TRP:O	2.16	0.46
3:H:348:LYS:HA	3:H:351:GLN:NE2	2.29	0.46
3:C:326:LEU:HB3	3:C:421:LEU:O	2.16	0.45
4:D:9:DA:H2"	4:D:10:DT:H5'	1.98	0.45
3:H:348:LYS:HZ2	3:H:433:LEU:HD23	1.80	0.45
3:H:365:LEU:HD21	3:H:368:PRO:N	2.31	0.45
2:G:68:PHE:CE1	2:G:97:LEU:HB3	2.51	0.45
2:G:131:ARG:NH1	2:G:131:ARG:HB3	2.32	0.45
3:C:323:ALA:HB2	3:C:346:THR:HG21	1.99	0.45
3:C:436:LYS:HB2	3:C:436:LYS:NZ	2.32	0.45
1:A:109:ASN:HD22	1:A:112:ASN:H	1.59	0.45
1:F:63:VAL:O	1:F:71:LEU:HD23	2.16	0.45
2:G:88:LEU:HD12	2:G:88:LEU:N	2.32	0.45
3:H:336:GLN:HE21	4:I:7:DA:H3'	1.82	0.44
2:G:55:ILE:HG22	6:G:202:HOH:O	2.18	0.44
2:B:86:VAL:HG13	2:B:86:VAL:O	2.18	0.44
1:F:146:PHE:CD1	1:F:168:ILE:HD13	2.53	0.44
3:H:368:PRO:HG2	3:H:369:ASP:OD1	2.18	0.44
3:H:409:ARG:HD3	3:H:410:TYR:CD2	2.52	0.44
3:C:417:ASP:O	3:C:421:LEU:HD13	2.17	0.44
3:H:358:GLY:HA2	3:H:430:HIS:CE1	2.53	0.44
1:A:106:MET:HE1	2:B:65:SER:N	2.32	0.44
3:C:326:LEU:HD13	3:C:422:LEU:HA	2.00	0.44
2:G:63:ASN:N	2:G:63:ASN:HD22	2.16	0.44
3:C:383:LYS:HD3	3:C:383:LYS:H	1.83	0.43
3:H:338:TRP:CE2	3:H:339:GLN:HG3	2.52	0.43
3:H:385:ASN:OD1	3:H:387:GLU:HB2	2.17	0.43
4:I:13:DT:H5'	4:I:13:DT:H6	1.82	0.43
4:I:8:DC:H2"	4:I:9:DA:C8	2.53	0.43
2:G:11:LYS:O	2:G:15:GLU:HB2	2.18	0.43
2:B:8:GLN:O	2:B:127:PHE:HE2	2.02	0.43
2:B:32:PHE:CE2	2:B:43:ARG:HD3	2.52	0.43
3:H:425:THR:C	3:H:427:GLU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:419:GLN:HE22	3:H:425:THR:HA	1.84	0.43
2:B:8:GLN:NE2	2:B:107:CYS:H	2.17	0.43
1:A:139:ARG:HD2	6:A:317:HOH:O	2.18	0.43
2:B:108:VAL:CG1	2:B:109:ILE:N	2.82	0.43
2:G:32:PHE:HB3	2:G:35:ARG:HG3	2.01	0.43
3:H:389:LEU:HD23	3:H:389:LEU:C	2.39	0.43
1:F:81:CYS:HB3	1:F:168:ILE:CG2	2.49	0.42
2:G:45:GLN:HG2	6:G:201:HOH:O	2.19	0.42
1:A:112:ASN:HD22	1:A:112:ASN:C	2.21	0.42
2:G:71:ALA:HB2	2:G:131:ARG:HD2	2.01	0.42
2:G:8:GLN:NE2	2:G:107:CYS:H	2.17	0.42
3:H:345:LEU:HD21	3:H:354:ILE:HG12	2.01	0.42
1:A:126:ASN:O	1:A:127:GLN:HB2	2.19	0.42
1:F:161:THR:HG22	1:F:162:TYR:N	2.35	0.42
4:I:8:DC:OP1	4:I:8:DC:H4'	2.19	0.42
3:C:384:MET:HE3	6:D:104:HOH:O	2.19	0.42
3:H:390:SER:HA	3:H:393:LEU:HD12	2.01	0.42
1:F:175:GLU:OE1	1:F:175:GLU:HA	2.20	0.42
2:B:3:ARG:HH21	2:B:135:GLU:CD	2.22	0.42
4:I:10:DT:C2'	4:I:11:DC:H5'	2.40	0.42
2:G:27:ILE:HD12	2:G:55:ILE:HG21	2.02	0.42
2:B:82:SER:HB2	2:B:86:VAL:HG12	2.02	0.42
1:F:63:VAL:HG22	1:F:64:ARG:H	1.84	0.42
3:H:361:TRP:HZ2	3:H:419:GLN:HE21	1.68	0.42
1:A:106:MET:HE1	2:B:65:SER:HB2	2.01	0.42
2:G:57:PHE:HB2	2:G:60:THR:HG22	2.01	0.42
2:B:118:ARG:HG2	2:B:118:ARG:HH11	1.84	0.42
1:F:175:GLU:HA	1:F:176:PRO:HD3	1.97	0.41
3:C:381:LYS:HE2	4:D:9:DA:H4'	2.02	0.41
1:A:113:TYR:CE2	2:B:28:LYS:HD2	2.55	0.41
3:H:345:LEU:HD22	3:H:356:TRP:CD1	2.55	0.41
2:G:94:LYS:HA	2:G:116:LEU:HG	2.02	0.41
2:B:32:PHE:CD2	2:B:32:PHE:N	2.88	0.41
3:H:354:ILE:HG13	3:H:364:LYS:O	2.20	0.41
3:H:365:LEU:HD22	3:H:410:TYR:CD1	2.56	0.41
4:I:9:DA:H2"	4:I:10:DT:H5'	2.02	0.41
2:G:54:GLU:C	2:G:55:ILE:HD12	2.40	0.41
2:B:90:ARG:O	2:B:91:GLU:HB2	2.20	0.41
2:B:8:GLN:HE22	2:B:132:ALA:HA	1.86	0.41
1:F:61:GLU:HG3	1:F:62:LEU:HD13	2.03	0.41
1:F:136:PHE:HB3	1:F:168:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:PHE:CD2	2:B:43:ARG:HD3	2.55	0.41
3:H:417:ASP:O	3:H:421:LEU:HD13	2.21	0.41
3:H:353:PHE:CG	3:H:370:GLU:HG2	2.55	0.41
1:F:136:PHE:HB2	1:F:168:ILE:HG12	2.01	0.41
2:B:27:ILE:HB	2:B:55:ILE:CG2	2.51	0.41
1:F:155:ASN:HA	1:F:156:PRO:HA	1.95	0.41
1:F:112:ASN:HD22	1:F:112:ASN:C	2.22	0.41
2:B:41:GLN:NE2	2:B:117:HIS:HA	2.35	0.41
2:B:36:PRO:O	2:B:40:ARG:HG3	2.21	0.41
2:B:94:LYS:HZ2	2:B:94:LYS:HB3	1.85	0.41
2:B:9:ARG:HA	2:B:127:PHE:CE2	2.56	0.40
2:B:98:LYS:HE2	2:B:111:LYS:CE	2.51	0.40
2:G:68:PHE:HB3	2:G:85:TYR:HB3	2.03	0.40
4:D:12:DC:H2'	4:D:13:DT:H72	2.02	0.40
1:A:125:LYS:O	1:A:126:ASN:HB2	2.22	0.40
3:C:387:GLU:HG2	6:C:511:HOH:O	2.20	0.40
3:C:364:LYS:HB2	3:C:411:VAL:HG22	2.03	0.40
3:H:403:HIS:ND1	3:H:415:VAL:HG21	2.37	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	117/205 (57%)	111 (95%)	6 (5%)	0	100 100
1	F	116/205 (57%)	111 (96%)	5 (4%)	0	100 100
2	B	126/142 (89%)	109 (86%)	16 (13%)	1 (1%)	24 26
2	G	125/142 (88%)	112 (90%)	13 (10%)	0	100 100
3	C	116/166 (70%)	114 (98%)	2 (2%)	0	100 100
3	H	99/166 (60%)	82 (83%)	13 (13%)	4 (4%)	4 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	699/1026 (68%)	639 (91%)	55 (8%)	5 (1%)	26 29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	382	PRO
3	H	383	LYS
2	B	116	LEU
3	H	368	PRO
3	H	334	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	101/180 (56%)	94 (93%)	7 (7%)	19 21
1	F	100/180 (56%)	96 (96%)	4 (4%)	38 49
2	B	113/123 (92%)	110 (97%)	3 (3%)	52 67
2	G	112/123 (91%)	107 (96%)	5 (4%)	34 43
3	C	102/145 (70%)	98 (96%)	4 (4%)	39 51
3	H	91/145 (63%)	89 (98%)	2 (2%)	60 75
All	All	619/896 (69%)	594 (96%)	25 (4%)	38 49

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	MET
1	A	61	GLU
1	A	69	ASN
1	A	109	ASN
1	A	112	ASN
1	A	139	ARG
1	A	175	GLU

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Mol	Chain	Res	Type
2	B	63	ASN
2	B	94	LYS
2	B	103	LEU
3	C	369	ASP
3	C	380	ASN
3	C	383	LYS
3	C	404	LYS
1	F	96	ASP
1	F	112	ASN
1	F	139	ARG
1	F	162	TYR
2	G	7	ASP
2	G	88	LEU
2	G	103	LEU
2	G	120	ASP
2	G	130	GLU
3	H	383	LYS
3	H	384	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) 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
2	B	8	GLN
2	B	41	GLN
2	B	104	ASN
2	B	134	GLN
3	C	380	ASN
1	F	112	ASN
1	F	127	GLN
1	F	163	HIS
2	G	8	GLN
2	G	67	GLN
2	G	134	GLN
3	H	336	GLN
3	H	339	GLN

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Mol	Chain	Res	Type
3	H	351	GLN
3	H	419	GLN
3	H	430	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	119/205 (58%)	0.71	3 (2%) 61 73	42, 57, 81, 113	0
1	F	118/205 (57%)	0.58	2 (1%) 73 83	38, 51, 71, 94	0
2	B	130/142 (91%)	1.31	28 (21%) 1 2	62, 87, 113, 127	0
2	G	129/142 (90%)	1.09	15 (11%) 6 11	56, 78, 106, 111	0
3	C	118/166 (71%)	0.65	4 (3%) 49 62	38, 58, 87, 95	0
3	H	101/166 (60%)	2.71	55 (54%) 0 0	61, 116, 154, 158	0
4	D	15/15 (100%)	0.01	0 100 100	46, 51, 60, 61	0
4	I	15/15 (100%)	0.10	0 100 100	50, 61, 75, 78	0
5	E	15/15 (100%)	-0.09	0 100 100	41, 48, 61, 61	0
5	J	15/15 (100%)	-0.00	0 100 100	45, 56, 68, 71	0
All	All	775/1086 (71%)	1.05	107 (13%) 4 8	38, 67, 125, 158	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	433	LEU	9.3
3	H	353	PHE	9.1
3	H	429	LEU	8.5
3	H	421	LEU	8.3
1	A	59	MET	7.1
3	H	360	GLY	7.0
3	C	332	SER	6.8
3	H	431	ALA	6.7
3	C	330	THR	6.4
2	B	92	ALA	6.1
2	B	93	GLY	6.0
3	H	335	ILE	6.0
3	H	375	TRP	5.9

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Mol	Chain	Res	Type	RSRZ
3	H	422	LEU	5.6
3	H	424	TYR	5.6
3	H	354	ILE	5.6
3	H	426	PRO	5.5
2	G	93	GLY	5.4
3	H	419	GLN	5.2
3	H	425	THR	5.2
3	H	338	TRP	5.0
3	C	327	ALA	4.8
3	H	356	TRP	4.7
3	H	351	GLN	4.4
3	H	432	MET	4.4
2	G	133	GLN	4.2
2	B	138	LEU	4.0
3	H	407	GLY	4.0
2	B	139	ALA	4.0
3	H	365	LEU	4.0
3	H	361	TRP	4.0
2	B	116	LEU	4.0
3	H	420	SER	4.0
3	H	337	LEU	4.0
2	B	94	LYS	3.9
3	H	350	CYS	3.9
2	G	95	VAL	3.9
3	H	430	HIS	3.8
3	H	364	LYS	3.8
2	G	82	SER	3.8
3	H	345	LEU	3.7
3	H	423	GLY	3.7
2	B	5	VAL	3.6
3	H	417	ASP	3.6
2	G	7	ASP	3.5
3	H	342	LEU	3.5
3	H	427	GLU	3.5
3	H	409	ARG	3.3
3	H	346	THR	3.3
3	H	406	ALA	3.3
2	G	83	ARG	3.3
2	B	4	VAL	3.2
2	B	140	GLN	3.1
2	B	86	VAL	3.1
2	B	96	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	83	ARG	3.1
2	B	10	SER	3.0
3	H	374	ARG	3.0
2	B	137	ALA	3.0
2	B	23	ARG	3.0
3	H	413	ARG	2.9
2	B	14	ASN	2.8
2	B	117	HIS	2.8
3	H	405	THR	2.8
3	H	340	PHE	2.7
2	B	133	GLN	2.7
3	H	428	GLU	2.7
1	F	175	GLU	2.7
3	H	411	VAL	2.6
2	G	55	ILE	2.6
2	G	127	PHE	2.6
3	H	352	SER	2.5
2	G	119	LEU	2.5
3	H	343	GLU	2.5
2	B	131	ARG	2.5
2	B	9	ARG	2.5
2	G	131	ARG	2.5
2	G	23	ARG	2.5
2	B	21	LEU	2.4
3	H	368	PRO	2.4
2	B	55	ILE	2.4
2	G	81	PRO	2.4
2	B	7	ASP	2.4
1	A	105	VAL	2.4
2	G	87	ASP	2.4
3	H	377	LYS	2.4
3	H	380	ASN	2.4
3	H	410	TYR	2.4
2	B	70	PRO	2.4
3	H	363	PHE	2.3
3	H	333	GLY	2.3
2	G	19	ARG	2.3
3	H	355	SER	2.3
2	B	85	TYR	2.3
3	H	397	TYR	2.2
2	B	98	LYS	2.2
3	H	367	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	H	336	GLN	2.1
3	C	324	ALA	2.1
3	H	369	ASP	2.1
3	H	416	CYS	2.1
3	H	382	PRO	2.1
2	B	95	VAL	2.1
1	F	107	ALA	2.1
2	G	114	ILE	2.1
2	B	24	GLU	2.0
1	A	106	MET	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.