Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:48 AM GMT

PDB ID	:	3Q2T
Title	:	Crystal Structure of CFIm68 RRM/CFIm25/RNA complex
Authors	:	Yang, Q.; Coseno, M.; Gilmartin, G.M.; Doublie, S.
Deposited on	:	2010-12-20
Resolution	:	3.06 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:

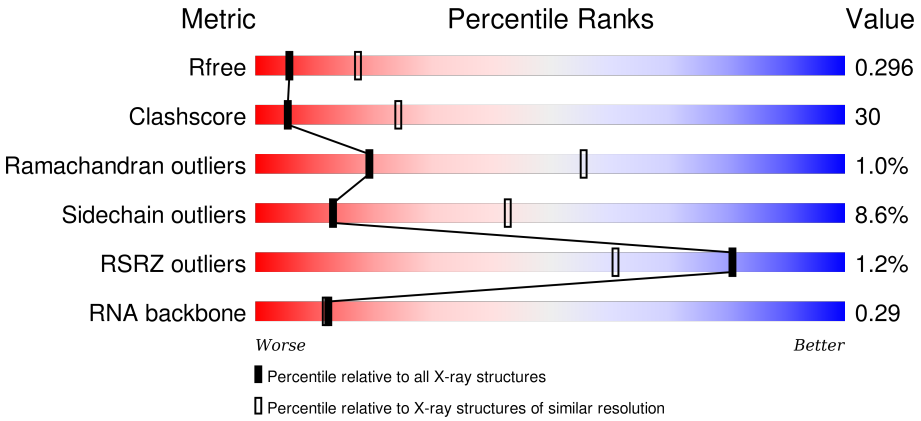
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.06 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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)
RNA backbone	2183	1035 (3.50-2.62)

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	207	53% 43%
1	B	207	50% 44%
2	C	229	21% 17% 59%
2	D	229	17% 20% 60%

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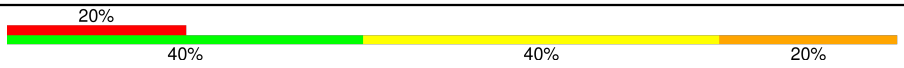
Mol	Chain	Length	Quality of chain
3	E	5	
3	F	5	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5035 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 Cleavage and polyadenylation specificity factor subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	4	2	0
			1699	1106	286	303	4			
1	B	203	Total	C	N	O	S	8	0	0
			1672	1089	282	297	4			

- Molecule 2 is a protein called Cleavage and polyadenylation specificity factor subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	93	Total	C	N	O	S	0	0	0
			731	465	125	139	2			
2	D	92	Total	C	N	O	S	0	0	0
			726	462	124	138	2			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	159	VAL	CYS	ENGINEERED MUTATION	UNP Q16630
C	236	HIS	-	EXPRESSION TAG	UNP Q16630
C	237	HIS	-	EXPRESSION TAG	UNP Q16630
C	238	HIS	-	EXPRESSION TAG	UNP Q16630
C	239	HIS	-	EXPRESSION TAG	UNP Q16630
C	240	HIS	-	EXPRESSION TAG	UNP Q16630
C	241	HIS	-	EXPRESSION TAG	UNP Q16630
D	159	VAL	CYS	ENGINEERED MUTATION	UNP Q16630
D	236	HIS	-	EXPRESSION TAG	UNP Q16630
D	237	HIS	-	EXPRESSION TAG	UNP Q16630
D	238	HIS	-	EXPRESSION TAG	UNP Q16630
D	239	HIS	-	EXPRESSION TAG	UNP Q16630
D	240	HIS	-	EXPRESSION TAG	UNP Q16630
D	241	HIS	-	EXPRESSION TAG	UNP Q16630

- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	P	10	0	0
			102	47	16	35	4			
3	F	5	Total	C	N	O	P	8	0	0
			102	47	16	35	4			

- Molecule 4 is water.

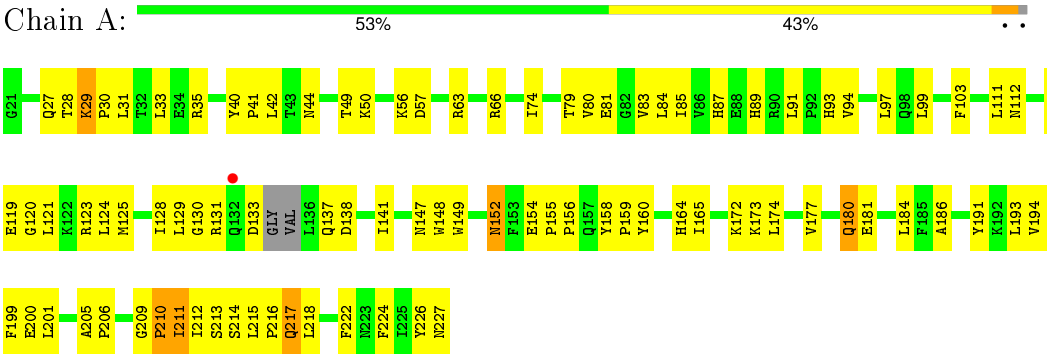
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			1	1		

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.

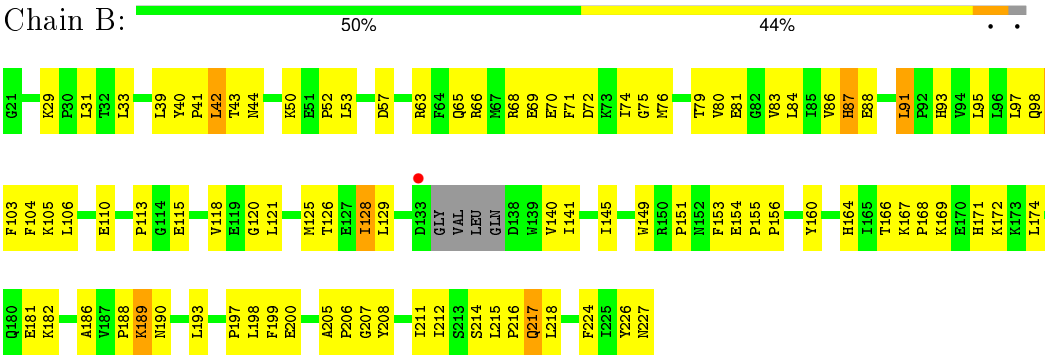
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

Chain A:



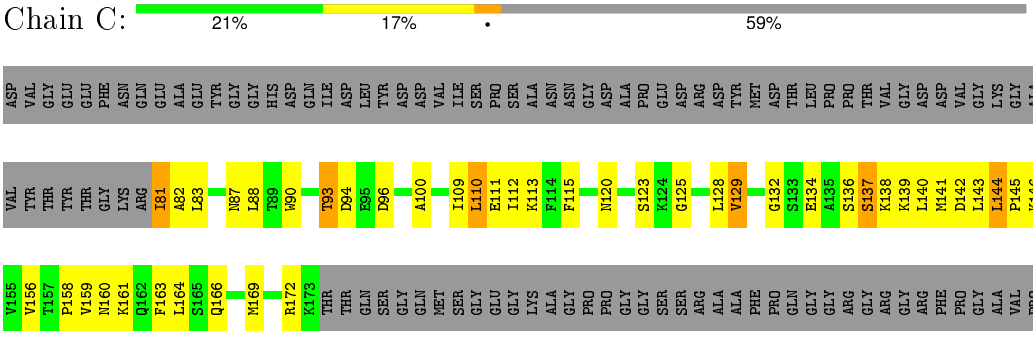
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

Chain B:

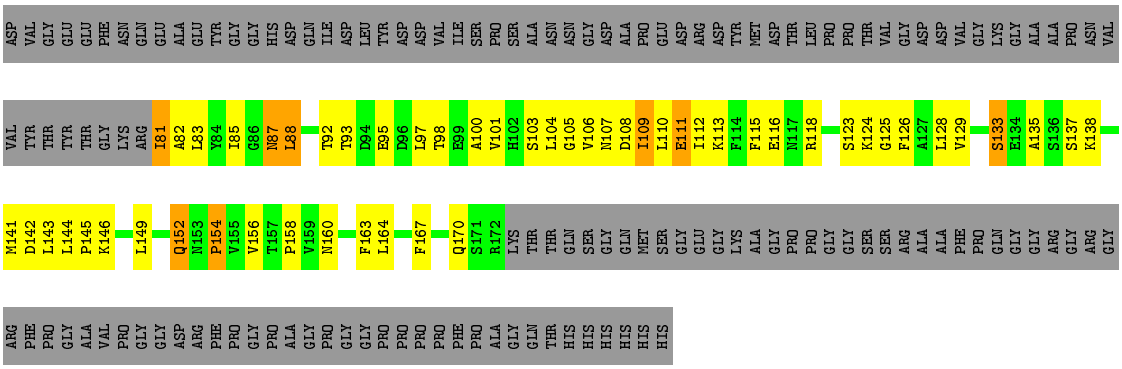


- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain C:

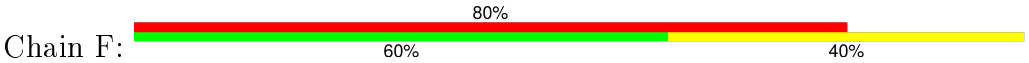


• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



• Molecule 3: RNA

• Molecule 3: RNA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	138.41Å 138.41Å 138.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.06 19.98 – 3.06	Depositor EDS
% Data completeness (in resolution range)	84.7 (19.98-3.06) 84.2 (19.98-3.06)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.04Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.211 , 0.286 0.214 , 0.296	Depositor DCC
R_{free} test set	716 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	69.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 50.3	EDS
Estimated twinning fraction	0.033 for l,-k,h 0.034 for l,-k,h	Xtriage
Reported twinning fraction	0.033 for l,-k,h	Depositor
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 16899 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5035	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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	0.35	0/1752	0.51	0/2376
1	B	0.35	0/1719	0.53	0/2331
2	C	0.31	0/745	0.49	0/1007
2	D	0.30	0/740	0.47	0/1000
3	E	0.30	0/113	0.80	0/174
3	F	0.33	0/113	0.84	1/174 (0.6%)
All	All	0.34	0/5182	0.53	1/7062 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2	U	O4'-C1'-N1	5.06	112.25	108.20

There are no chirality outliers.

There are no planarity outliers.

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	1699	0	1706	89	0
1	B	1672	0	1677	119	0
2	C	731	0	723	48	0
2	D	726	0	721	47	0
3	E	102	0	54	5	0
3	F	102	0	54	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	1	0
4	D	1	0	0	0	0
All	All	5035	0	4935	294	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 30.

All (294) 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:B:217:GLN:HE21	1:B:217:GLN:N	1.51	1.07
1:B:217:GLN:NE2	1:B:217:GLN:H	1.50	1.07
1:A:83:VAL:HG12	1:A:85:ILE:HD11	1.49	0.94
1:A:217:GLN:H	1:A:217:GLN:HE21	0.94	0.92
1:B:217:GLN:HE21	1:B:217:GLN:H	0.93	0.92
1:B:76:MET:HE2	1:B:171:HIS:HB2	1.53	0.89
1:B:128:ILE:HG23	1:B:129:LEU:HD13	1.54	0.88
1:A:217:GLN:N	1:A:217:GLN:HE21	1.73	0.86
1:A:164:HIS:CD2	2:D:123:SER:HB2	2.12	0.83
1:A:154:GLU:HB3	1:A:155:PRO:HD2	1.60	0.81
2:C:81:ILE:HG21	2:C:134:GLU:HG2	1.62	0.79
1:B:70:GLU:HB3	1:B:74:ILE:HD12	1.66	0.78
1:B:31:LEU:HD22	1:B:31:LEU:H	1.49	0.77
2:D:160:ASN:HB3	2:D:163:PHE:CD2	2.19	0.77
1:B:80:VAL:HG23	1:B:121:LEU:HD13	1.67	0.76
2:C:144:LEU:HD22	2:C:154:PRO:HG3	1.67	0.74
1:A:79:THR:HB	1:A:172:LYS:HG3	1.70	0.74
1:B:42:LEU:HD13	1:B:43:THR:HG23	1.68	0.74
1:B:98:GLN:NE2	1:B:101:THR:HA	2.04	0.72
1:B:86:VAL:HG23	1:B:93:HIS:HB2	1.72	0.72
1:A:84:LEU:HD12	1:A:84:LEU:H	1.54	0.71
2:C:136:SER:O	2:C:139:LYS:HB2	1.92	0.70
2:D:141:MET:HE1	2:D:158:PRO:HG3	1.73	0.70
1:A:56:LYS:HE3	1:A:66:ARG:NH2	2.06	0.69
1:A:99:LEU:HG	1:A:191:TYR:CE2	2.27	0.69
2:C:82:ALA:O	2:C:159:VAL:HG23	1.92	0.69
2:C:128:LEU:HD23	2:C:129:VAL:N	2.08	0.69
1:A:217:GLN:NE2	1:A:217:GLN:H	1.79	0.69
1:B:79:THR:HG22	1:B:172:LYS:HG3	1.74	0.69
1:A:180:GLN:NE2	1:A:180:GLN:H	1.91	0.68
2:D:160:ASN:HB3	2:D:163:PHE:HD2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:THR:HG21	2:D:149:LEU:HD13	1.76	0.67
1:A:83:VAL:CG1	1:A:85:ILE:HD11	2.24	0.67
1:A:85:ILE:HD12	1:A:94:VAL:HG22	1.75	0.67
1:B:99:LEU:CD1	1:B:103:PHE:HB3	2.25	0.67
1:B:205:ALA:N	1:B:206:PRO:HD2	2.11	0.66
1:B:84:LEU:HD23	1:B:179:LEU:HD21	1.75	0.66
1:A:103:PHE:CZ	3:E:3:G:C6	2.84	0.66
2:C:109:ILE:HD12	2:C:109:ILE:H	1.60	0.66
1:A:131:ARG:H	1:A:137:GLN:HE21	1.43	0.65
1:B:83:VAL:HG21	1:B:145:ILE:HD11	1.79	0.65
1:A:84:LEU:HD12	1:A:84:LEU:N	2.12	0.65
2:D:83:LEU:HD13	2:D:158:PRO:HA	1.79	0.64
2:C:88:LEU:HB2	2:C:125:GLY:O	1.96	0.64
1:A:84:LEU:C	1:A:85:ILE:HD13	2.16	0.64
2:C:81:ILE:CG2	2:C:134:GLU:HG2	2.28	0.64
1:B:128:ILE:O	1:B:129:LEU:HD12	1.98	0.64
1:A:199:PHE:HB2	2:C:120:ASN:HB2	1.78	0.64
1:A:215:LEU:HA	1:A:218:LEU:HD12	1.79	0.63
1:B:166:THR:HG23	2:C:93:THR:HB	1.81	0.63
1:B:214:SER:O	1:B:218:LEU:HG	1.98	0.63
1:B:50:LYS:HE2	1:B:186:ALA:CB	2.28	0.63
1:B:42:LEU:HD12	1:B:42:LEU:N	2.14	0.63
1:B:99:LEU:HD12	1:B:99:LEU:H	1.64	0.62
1:B:50:LYS:HE2	1:B:186:ALA:HB1	1.81	0.62
1:B:208:TYR:O	1:B:212:ILE:HB	1.99	0.62
2:D:141:MET:CE	2:D:158:PRO:HG3	2.29	0.62
1:B:164:HIS:ND1	2:C:123:SER:HB2	2.15	0.62
1:A:201:LEU:HD22	1:A:212:ILE:HG22	1.81	0.62
1:B:44:ASN:HB3	1:B:182:LYS:HB3	1.81	0.61
1:A:121:LEU:HD23	1:A:141:ILE:HD13	1.82	0.61
2:C:100:ALA:HB2	2:C:149:LEU:HD21	1.83	0.61
2:C:115:PHE:HE2	2:C:128:LEU:H	1.47	0.61
1:A:210:PRO:HG2	1:A:211:ILE:H	1.66	0.60
1:B:42:LEU:HD12	1:B:42:LEU:H	1.67	0.60
1:B:79:THR:HG21	1:B:172:LYS:HE2	1.83	0.60
1:B:95:LEU:HB3	1:B:193:LEU:HD11	1.83	0.60
1:A:205:ALA:N	1:A:206:PRO:HD2	2.16	0.60
2:D:82:ALA:O	2:D:83:LEU:HD22	2.02	0.59
1:B:115:GLU:OE2	1:B:120:GLY:HA2	1.99	0.59
1:B:97:LEU:O	1:B:104:PHE:HA	2.02	0.59
2:D:109:ILE:O	2:D:109:ILE:HG13	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:LEU:HD12	2:D:125:GLY:O	2.01	0.59
1:B:99:LEU:HD11	1:B:103:PHE:HD2	1.67	0.59
1:B:141:ILE:HG12	1:B:177:VAL:HG22	1.84	0.58
1:B:74:ILE:HG23	1:B:113:PRO:HG3	1.84	0.58
1:B:40:TYR:HE1	1:B:227:ASN:HD22	1.52	0.58
1:A:97:LEU:HD23	1:A:193:LEU:HD13	1.85	0.58
1:A:141:ILE:HG12	1:A:177:VAL:HG22	1.85	0.58
1:B:80:VAL:CG2	1:B:121:LEU:HD13	2.33	0.57
1:B:81:GLU:HB2	1:B:174:LEU:HD23	1.86	0.57
1:B:99:LEU:HD12	1:B:99:LEU:N	2.20	0.57
1:A:103:PHE:CE1	3:E:3:G:C5	2.92	0.56
1:A:131:ARG:H	1:A:137:GLN:NE2	2.02	0.56
2:C:141:MET:HA	2:C:156:VAL:HB	1.86	0.56
1:B:84:LEU:H	1:B:84:LEU:HD12	1.70	0.56
1:A:89:HIS:HD2	2:C:90:TRP:CH2	2.23	0.56
1:A:159:PRO:HG2	1:A:160:TYR:CD1	2.40	0.56
1:B:140:VAL:HG12	1:B:178:GLN:HG3	1.88	0.56
1:B:53:LEU:H	1:B:188:PRO:HB3	1.69	0.56
1:B:57:ASP:CG	1:B:63:ARG:HA	2.27	0.56
1:A:93:HIS:NE2	1:A:197:PRO:HB3	2.21	0.55
1:B:99:LEU:HD11	1:B:103:PHE:HB3	1.88	0.55
3:E:3:G:HO2'	3:E:4:U:H5	1.53	0.55
1:A:154:GLU:HB3	1:A:155:PRO:CD	2.33	0.55
1:A:31:LEU:HD22	1:A:31:LEU:H	1.70	0.55
1:A:112:ASN:O	1:A:115:GLU:HB2	2.06	0.55
1:A:131:ARG:NH1	1:A:133:ASP:HB2	2.21	0.55
1:A:159:PRO:HG2	1:A:160:TYR:HD1	1.70	0.55
1:B:197:PRO:HG2	1:B:200:GLU:HB2	1.89	0.55
2:D:167:PHE:O	2:D:170:GLN:HB2	2.06	0.55
2:D:97:LEU:HD23	2:D:97:LEU:C	2.26	0.54
1:B:81:GLU:HB2	1:B:174:LEU:CD2	2.37	0.54
1:A:197:PRO:O	1:A:200:GLU:HB3	2.08	0.54
2:C:140:LEU:HB2	2:C:156:VAL:HG11	1.88	0.54
1:B:71:PHE:HA	1:B:75:GLY:O	2.08	0.54
4:B:3:HOH:O	2:C:113:LYS:HG2	2.07	0.54
2:D:144:LEU:HB3	2:D:145:PRO:HD3	1.90	0.54
2:D:106:VAL:HG23	2:D:107:ASN:N	2.24	0.53
1:A:29:LYS:HG3	1:A:30:PRO:HD2	1.90	0.53
2:C:115:PHE:HE2	2:C:128:LEU:N	2.07	0.53
1:A:85:ILE:CD1	1:A:94:VAL:HG22	2.38	0.53
2:C:93:THR:HG23	2:C:96:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:OD1	1:A:66:ARG:HD3	2.10	0.52
1:B:76:MET:CE	1:B:171:HIS:HB2	2.35	0.52
1:B:93:HIS:NE2	1:B:197:PRO:HB3	2.24	0.52
3:E:3:G:H1'	3:E:4:U:C5	2.45	0.52
2:D:111:GLU:HG3	2:D:112:ILE:N	2.25	0.52
1:B:42:LEU:HG	1:B:88:GLU:HB2	1.91	0.52
1:B:164:HIS:CG	2:C:123:SER:HB2	2.45	0.52
1:B:53:LEU:HD23	1:B:188:PRO:HG3	1.93	0.51
1:B:63:ARG:HB3	1:B:63:ARG:NH1	2.25	0.51
2:D:164:LEU:HD23	2:D:164:LEU:C	2.31	0.51
1:B:154:GLU:HB2	1:B:156:PRO:HD2	1.91	0.51
1:B:42:LEU:HD13	1:B:43:THR:N	2.25	0.51
2:C:83:LEU:HD13	2:C:158:PRO:HA	1.93	0.51
2:D:116:GLU:HA	2:D:124:LYS:HG3	1.92	0.51
2:D:82:ALA:C	2:D:83:LEU:HD22	2.31	0.51
2:C:163:PHE:O	2:C:166:GLN:HB3	2.10	0.51
1:B:31:LEU:HD22	1:B:31:LEU:N	2.22	0.51
1:B:91:LEU:O	1:B:93:HIS:ND1	2.44	0.51
1:A:130:GLY:HA2	1:A:137:GLN:NE2	2.25	0.50
2:D:144:LEU:HG	2:D:154:PRO:HB2	1.93	0.50
2:D:83:LEU:CD1	2:D:158:PRO:HA	2.40	0.50
2:C:109:ILE:HD12	2:C:109:ILE:N	2.27	0.50
1:A:222:PHE:HB2	1:A:224:PHE:CZ	2.46	0.50
2:D:85:ILE:O	2:D:126:PHE:HB2	2.12	0.50
2:D:128:LEU:HD23	2:D:128:LEU:C	2.31	0.50
1:B:41:PRO:HA	1:B:87:HIS:O	2.12	0.50
1:B:154:GLU:HB3	1:B:155:PRO:HD2	1.94	0.49
1:B:42:LEU:HD11	1:B:88:GLU:OE2	2.12	0.49
2:D:144:LEU:HD23	2:D:156:VAL:HG21	1.93	0.49
2:D:101:VAL:HB	2:D:106:VAL:CG2	2.42	0.49
2:D:81:ILE:HD12	2:D:81:ILE:N	2.27	0.49
2:C:81:ILE:N	2:C:81:ILE:HD12	2.27	0.49
2:C:145:PRO:HD3	2:C:156:VAL:HG23	1.94	0.49
2:C:83:LEU:CD1	2:C:158:PRO:HA	2.42	0.49
1:B:98:GLN:HA	1:B:103:PHE:O	2.13	0.49
1:B:63:ARG:CZ	1:B:63:ARG:HB3	2.42	0.49
2:D:135:ALA:O	2:D:138:LYS:HB2	2.13	0.49
2:C:115:PHE:CE2	2:C:128:LEU:HB2	2.48	0.49
1:A:81:GLU:OE2	1:A:172:LYS:HE2	2.13	0.49
2:D:98:THR:O	2:D:101:VAL:HG22	2.12	0.49
1:A:81:GLU:HB2	1:A:174:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:GLN:HG2	1:B:99:LEU:N	2.28	0.48
1:B:205:ALA:N	1:B:206:PRO:CD	2.76	0.48
2:D:87:ASN:O	2:D:152:GLN:NE2	2.46	0.48
1:B:40:TYR:CD2	1:B:181:GLU:HA	2.49	0.48
2:C:132:GLY:O	2:C:134:GLU:HG3	2.14	0.48
1:B:189:LYS:HZ1	3:F:5:A:H2	1.61	0.48
1:B:189:LYS:NZ	3:F:5:A:H2	2.11	0.48
2:C:145:PRO:O	2:C:146:LYS:HB2	2.14	0.48
1:A:63:ARG:NH2	3:E:3:G:C6	2.81	0.48
2:D:101:VAL:O	2:D:105:GLY:N	2.47	0.48
1:A:31:LEU:HD22	1:A:31:LEU:N	2.28	0.48
2:C:142:ASP:HB2	2:C:143:LEU:CD1	2.44	0.48
1:B:149:TRP:CZ3	1:B:160:TYR:HA	2.49	0.48
1:A:83:VAL:HG12	1:A:85:ILE:CD1	2.32	0.48
2:C:137:SER:O	2:C:141:MET:HG2	2.14	0.48
2:D:87:ASN:O	2:D:152:GLN:HB3	2.14	0.48
1:B:128:ILE:HG23	1:B:129:LEU:CD1	2.36	0.47
1:A:87:HIS:CG	1:A:226:TYR:HD1	2.32	0.47
2:C:115:PHE:HE2	2:C:128:LEU:HB2	1.80	0.47
1:A:149:TRP:CZ3	1:A:160:TYR:HA	2.49	0.47
1:B:39:LEU:HD12	1:B:224:PHE:HB3	1.96	0.47
1:B:128:ILE:HD13	1:B:128:ILE:O	2.14	0.47
2:C:111:GLU:O	2:C:112:ILE:HG22	2.15	0.47
1:A:85:ILE:N	1:A:85:ILE:HD13	2.28	0.47
2:C:82:ALA:C	2:C:83:LEU:HD22	2.35	0.47
1:B:42:LEU:N	1:B:42:LEU:CD1	2.78	0.47
1:B:155:PRO:N	1:B:156:PRO:CD	2.78	0.47
1:B:40:TYR:CE1	1:B:227:ASN:ND2	2.83	0.47
1:A:209:GLY:O	1:A:213:SER:HB3	2.15	0.47
2:D:142:ASP:HB2	2:D:143:LEU:HG	1.97	0.47
1:B:99:LEU:HD11	1:B:103:PHE:CD2	2.49	0.46
1:B:40:TYR:HE1	1:B:227:ASN:ND2	2.13	0.46
1:B:207:GLY:C	1:B:208:TYR:CD2	2.89	0.46
1:A:49:THR:OG1	1:A:50:LYS:N	2.49	0.46
1:B:215:LEU:N	1:B:216:PRO:CD	2.79	0.46
2:D:106:VAL:HG23	2:D:107:ASN:H	1.79	0.46
1:A:131:ARG:HE	1:A:131:ARG:HB2	1.58	0.46
1:B:50:LYS:HG2	1:B:188:PRO:N	2.30	0.46
1:B:39:LEU:HD11	1:B:224:PHE:CD1	2.51	0.46
1:A:201:LEU:CD2	1:A:212:ILE:HG22	2.46	0.46
1:B:40:TYR:CE2	1:B:181:GLU:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASP:O	1:A:117:GLU:C	2.53	0.46
1:B:31:LEU:H	1:B:31:LEU:CD2	2.22	0.45
1:B:84:LEU:N	1:B:84:LEU:HD12	2.30	0.45
1:B:125:MET:HE2	1:B:177:VAL:HG21	1.97	0.45
1:A:125:MET:HA	1:A:128:ILE:HG22	1.97	0.45
1:B:189:LYS:HG2	1:B:190:ASN:N	2.31	0.45
1:A:84:LEU:HD21	1:A:125:MET:HE3	1.98	0.45
1:B:52:PRO:HA	1:B:188:PRO:HB3	1.99	0.45
1:B:167:LYS:HA	1:B:168:PRO:HD3	1.72	0.45
1:A:215:LEU:N	1:A:216:PRO:CD	2.80	0.45
1:B:214:SER:C	1:B:217:GLN:HE22	2.20	0.45
2:D:154:PRO:O	2:D:156:VAL:HG23	2.16	0.45
2:C:82:ALA:C	2:C:159:VAL:HG23	2.37	0.45
1:B:125:MET:CE	1:B:177:VAL:HG21	2.46	0.45
1:A:81:GLU:HB2	1:A:174:LEU:CD2	2.47	0.44
2:D:152:GLN:HB3	2:D:152:GLN:HE21	1.62	0.44
1:A:214:SER:O	1:A:218:LEU:HD12	2.18	0.44
2:D:118:ARG:HB3	2:D:118:ARG:NH1	2.33	0.44
1:A:148:TRP:CZ3	1:A:159:PRO:HD3	2.52	0.44
1:A:116:ASP:OD2	1:A:119:GLU:HG2	2.17	0.44
1:B:105:LYS:HG3	1:B:106:LEU:O	2.17	0.44
2:D:101:VAL:HB	2:D:106:VAL:HG22	2.00	0.44
1:B:68:ARG:HA	1:B:153:PHE:CE1	2.53	0.44
1:A:56:LYS:HE3	1:A:66:ARG:HH22	1.79	0.44
1:B:179:LEU:HD23	1:B:179:LEU:HA	1.79	0.44
1:B:39:LEU:HB3	1:B:87:HIS:HB3	2.00	0.44
1:B:91:LEU:CD1	1:B:198:LEU:H	2.30	0.44
1:B:40:TYR:CD1	1:B:227:ASN:HB2	2.53	0.44
1:A:91:LEU:O	1:A:93:HIS:ND1	2.51	0.43
2:D:83:LEU:HD11	2:D:141:MET:HE1	2.00	0.43
1:B:87:HIS:CE1	1:B:226:TYR:HB3	2.54	0.43
1:B:214:SER:C	1:B:217:GLN:NE2	2.72	0.43
1:B:178:GLN:H	1:B:178:GLN:HG2	1.55	0.43
1:A:152[A]:ASN:H	1:A:152[A]:ASN:ND2	2.16	0.43
1:A:211:ILE:O	1:A:212:ILE:C	2.57	0.43
1:B:29:LYS:HA	1:B:29:LYS:HD3	1.79	0.43
2:C:83:LEU:N	2:C:83:LEU:HD22	2.33	0.43
2:D:146:LYS:HD3	2:D:146:LYS:HA	1.67	0.43
1:A:128:ILE:O	1:A:128:ILE:HG13	2.19	0.42
2:C:128:LEU:C	2:C:128:LEU:HD23	2.39	0.42
1:B:164:HIS:O	2:C:93:THR:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD23	1:A:42:LEU:C	2.40	0.42
1:B:66:ARG:NH2	1:B:110:GLU:OE2	2.46	0.42
1:B:154:GLU:HB3	1:B:155:PRO:CD	2.48	0.42
1:A:124:LEU:O	1:A:128:ILE:HG22	2.19	0.42
2:D:137:SER:O	2:D:141:MET:HG2	2.20	0.42
1:A:194:VAL:HG22	1:A:195:ALA:N	2.35	0.42
1:A:210:PRO:CG	1:A:211:ILE:H	2.33	0.42
1:B:98:GLN:HE21	1:B:101:THR:HA	1.83	0.42
1:B:40:TYR:HD1	1:B:227:ASN:HB2	1.85	0.42
1:A:89:HIS:CD2	2:C:90:TRP:CH2	3.05	0.42
1:B:160:TYR:CD2	1:B:160:TYR:C	2.93	0.42
2:C:112:ILE:HG23	2:C:112:ILE:O	2.20	0.42
1:A:129:LEU:HA	1:A:186:ALA:O	2.19	0.42
1:B:214:SER:HA	1:B:217:GLN:HE22	1.85	0.42
1:A:80:VAL:HG23	1:A:121:LEU:HD13	2.02	0.42
2:D:98:THR:OG1	2:D:109:ILE:HD13	2.20	0.42
2:D:108:ASP:OD1	2:D:133:SER:HB3	2.20	0.42
1:B:104:PHE:N	1:B:104:PHE:CD2	2.88	0.42
1:B:190:ASN:N	1:B:190:ASN:OD1	2.52	0.42
1:B:50:LYS:HE2	1:B:186:ALA:HB3	2.00	0.41
1:B:155:PRO:HD2	1:B:156:PRO:HD3	2.02	0.41
2:C:160:ASN:HB3	2:C:163:PHE:CD2	2.55	0.41
1:B:216:PRO:HD2	1:B:217:GLN:HE22	1.85	0.41
1:B:166:THR:CG2	2:C:93:THR:HB	2.49	0.41
2:D:115:PHE:CD2	2:D:126:PHE:CE1	3.08	0.41
1:A:41:PRO:HD2	1:A:44:ASN:ND2	2.35	0.41
1:A:154:GLU:HB2	1:A:156:PRO:HD2	2.02	0.41
1:A:165:ILE:HD13	1:A:165:ILE:HA	1.94	0.41
1:B:99:LEU:HB2	1:B:100:GLY:H	1.70	0.41
1:A:40:TYR:CD2	1:A:181:GLU:HA	2.55	0.41
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.76	0.41
1:A:93:HIS:CD2	1:A:197:PRO:HB3	2.55	0.41
1:B:151:PRO:HD2	1:B:156:PRO:O	2.21	0.41
2:C:110:LEU:O	2:C:111:GLU:HB2	2.20	0.41
2:C:144:LEU:HD22	2:C:154:PRO:CG	2.45	0.41
2:D:108:ASP:O	2:D:110:LEU:HD12	2.21	0.41
1:A:147:ASN:OD1	1:A:173:LYS:HG3	2.20	0.41
1:B:91:LEU:HA	1:B:91:LEU:HD22	1.81	0.41
2:D:149:LEU:HD23	2:D:149:LEU:HA	1.89	0.41
2:D:97:LEU:O	2:D:100:ALA:N	2.52	0.41
1:A:42:LEU:O	1:A:42:LEU:HD23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:HIS:HE1	2:D:116:GLU:OE2	2.04	0.41
2:C:141:MET:CE	2:C:158:PRO:HG3	2.51	0.41
2:C:160:ASN:OD1	2:C:161:LYS:N	2.54	0.41
1:A:111:LEU:HD22	1:A:120:GLY:HA3	2.01	0.41
1:A:40:TYR:CD1	1:A:227:ASN:HB2	2.55	0.41
1:B:199:PHE:C	1:B:199:PHE:CD2	2.94	0.41
1:A:33:LEU:HD21	1:B:118:VAL:HG21	2.01	0.41
2:C:138:LYS:HG2	2:C:142:ASP:OD2	2.20	0.41
1:B:169:LYS:N	1:B:169:LYS:HD3	2.36	0.41
1:B:74:ILE:CG2	1:B:113:PRO:HG3	2.50	0.40
2:C:144:LEU:HD23	2:C:144:LEU:HA	1.89	0.40
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.72	0.40
1:A:199:PHE:CD2	1:A:199:PHE:C	2.94	0.40
2:D:87:ASN:HA	2:D:87:ASN:HD22	1.66	0.40
1:A:214:SER:C	1:A:218:LEU:HD12	2.42	0.40
1:A:158:TYR:C	1:A:160:TYR:H	2.24	0.40
1:B:65:GLN:O	1:B:69:GLU:HG3	2.21	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	203/207 (98%)	185 (91%)	16 (8%)	2 (1%)	19 56
1	B	199/207 (96%)	169 (85%)	28 (14%)	2 (1%)	19 56
2	C	91/229 (40%)	75 (82%)	16 (18%)	0	100 100
2	D	90/229 (39%)	78 (87%)	10 (11%)	2 (2%)	8 34
All	All	583/872 (67%)	507 (87%)	70 (12%)	6 (1%)	19 56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	ILE
2	D	154	PRO
1	B	101	THR
1	A	210	PRO
1	B	211	ILE
2	D	109	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	186/185 (100%)	174 (94%)	12 (6%)	21 54
1	B	182/185 (98%)	171 (94%)	11 (6%)	24 58
2	C	80/180 (44%)	69 (86%)	11 (14%)	4 18
2	D	80/180 (44%)	68 (85%)	12 (15%)	3 14
All	All	528/730 (72%)	482 (91%)	46 (9%)	13 42

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	28	THR
1	A	29	LYS
1	A	35	ARG
1	A	74	ILE
1	A	123	ARG
1	A	138	ASP
1	A	152[A]	ASN
1	A	152[B]	ASN
1	A	180	GLN
1	A	184	LEU
1	A	217	GLN
1	B	33	LEU
1	B	42	LEU
1	B	72	ASP
1	B	87	HIS

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Mol	Chain	Res	Type
1	B	91	LEU
1	B	99	LEU
1	B	126	THR
1	B	128	ILE
1	B	178	GLN
1	B	189	LYS
1	B	217	GLN
2	C	81	ILE
2	C	87	ASN
2	C	93	THR
2	C	94	ASP
2	C	110	LEU
2	C	129	VAL
2	C	137	SER
2	C	144	LEU
2	C	164	LEU
2	C	169	MET
2	C	172	ARG
2	D	81	ILE
2	D	87	ASN
2	D	88	LEU
2	D	93	THR
2	D	95	GLU
2	D	103	SER
2	D	104	LEU
2	D	111	GLU
2	D	113	LYS
2	D	129	VAL
2	D	133	SER
2	D	152	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	27	GLN
1	A	89	HIS
1	A	137	GLN
1	A	164	HIS
1	A	180	GLN
1	A	217	GLN
1	A	223	ASN

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Mol	Chain	Res	Type
1	B	22	ASN
1	B	98	GLN
1	B	217	GLN
2	C	87	ASN
2	C	166	GLN
2	D	87	ASN
2	D	152	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	4/5 (80%)	2 (50%)	0
3	F	4/5 (80%)	0	0
All	All	8/10 (80%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	3	G
3	E	5	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	205/207 (99%)	-0.68	1 (0%) 91 81	35, 54, 85, 100	13 (6%)
1	B	203/207 (98%)	-0.63	1 (0%) 91 81	33, 56, 92, 115	11 (5%)
2	C	93/229 (40%)	-0.54	0 100 100	44, 68, 92, 104	6 (6%)
2	D	92/229 (40%)	-0.48	0 100 100	54, 75, 92, 98	9 (9%)
3	E	5/5 (100%)	1.26	1 (20%) 1 0	83, 100, 113, 114	2 (40%)
3	F	5/5 (100%)	2.29	4 (80%) 0 0	91, 111, 127, 142	2 (40%)
All	All	603/882 (68%)	-0.57	7 (1%) 81 61	33, 61, 92, 142	43 (7%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	3	G	3.1
3	F	5	A	2.9
3	E	5	A	2.6
1	B	133	ASP	2.4
3	F	1	U	2.3
1	A	132	GLN	2.3
3	F	4	U	2.0

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

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

6.3 Carbohydrates

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.