Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:51 AM UTC

PDB ID	:	4F02 / pdb_00004f02
Title	:	Crystal structure of the PABP-binding site of eIF4G in complex with RRM1-2 of PABP and poly(A)
Authors	:	Safaee, N.; Kozlov, G.; Gehring, K.B.
Deposited on	:	2012-05-03
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

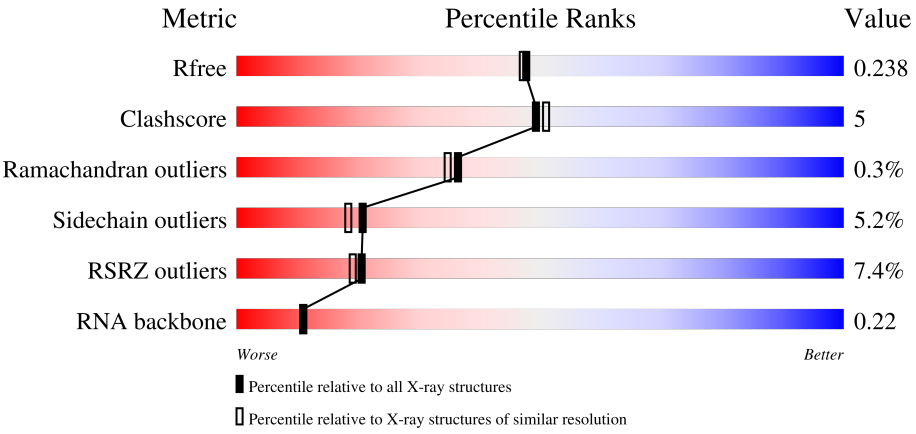
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)
RNA backbone	3983	1000 (2.36-1.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	213	3% 72% 9% 18%
1	D	213	3% 71% 8% • 18%
2	B	11	9% 36% 9% 27% 9% 18%
2	E	11	9% 27% 27% 27% 18%

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Mol	Chain	Length	Quality of chain
3	C	27	
3	F	27	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3663 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 Polyadenylate-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1376	868	244	255	9			
1	D	174	Total	C	N	O	S	0	2	0
			1392	877	249	256	10			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P11940
A	-3	PRO	-	expression tag	UNP P11940
A	-2	LEU	-	expression tag	UNP P11940
A	-1	GLY	-	expression tag	UNP P11940
A	0	SER	-	expression tag	UNP P11940
A	191	TYR	-	expression tag	UNP P11940
A	192	PRO	-	expression tag	UNP P11940
A	193	TYR	-	expression tag	UNP P11940
A	194	ASP	-	expression tag	UNP P11940
A	195	VAL	-	expression tag	UNP P11940
A	196	PRO	-	expression tag	UNP P11940
A	197	ASP	-	expression tag	UNP P11940
A	198	TYR	-	expression tag	UNP P11940
A	199	ALA	-	expression tag	UNP P11940
A	200	GLY	-	expression tag	UNP P11940
A	201	SER	-	expression tag	UNP P11940
A	202	SER	-	expression tag	UNP P11940
A	203	GLY	-	expression tag	UNP P11940
A	204	ARG	-	expression tag	UNP P11940
A	205	ILE	-	expression tag	UNP P11940
A	206	VAL	-	expression tag	UNP P11940
A	207	THR	-	expression tag	UNP P11940
A	208	ASP	-	expression tag	UNP P11940
D	-4	GLY	-	expression tag	UNP P11940
D	-3	PRO	-	expression tag	UNP P11940

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	LEU	-	expression tag	UNP P11940
D	-1	GLY	-	expression tag	UNP P11940
D	0	SER	-	expression tag	UNP P11940
D	191	TYR	-	expression tag	UNP P11940
D	192	PRO	-	expression tag	UNP P11940
D	193	TYR	-	expression tag	UNP P11940
D	194	ASP	-	expression tag	UNP P11940
D	195	VAL	-	expression tag	UNP P11940
D	196	PRO	-	expression tag	UNP P11940
D	197	ASP	-	expression tag	UNP P11940
D	198	TYR	-	expression tag	UNP P11940
D	199	ALA	-	expression tag	UNP P11940
D	200	GLY	-	expression tag	UNP P11940
D	201	SER	-	expression tag	UNP P11940
D	202	SER	-	expression tag	UNP P11940
D	203	GLY	-	expression tag	UNP P11940
D	204	ARG	-	expression tag	UNP P11940
D	205	ILE	-	expression tag	UNP P11940
D	206	VAL	-	expression tag	UNP P11940
D	207	THR	-	expression tag	UNP P11940
D	208	ASP	-	expression tag	UNP P11940

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	18	0	0
			195	90	45	52	8			
2	E	9	Total	C	N	O	P	0	0	0
			198	90	45	54	9			

- Molecule 3 is a protein called Eukaryotic translation initiation factor 4 gamma 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	20	Total	C	N	O	S	0	0	0
			149	90	29	29	1			
3	F	20	Total	C	N	O	S	0	0	0
			157	94	29	33	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	204	TYR	-	expression tag	UNP Q04637
F	204	TYR	-	expression tag	UNP Q04637

- Molecule 4 is water.

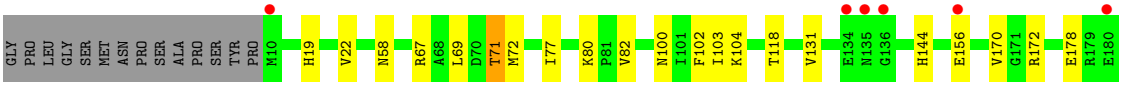
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	88	Total O 88 88	0	0
4	B	20	Total O 20 20	0	0
4	C	2	Total O 2 2	0	0
4	D	73	Total O 73 73	0	0
4	E	13	Total O 13 13	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

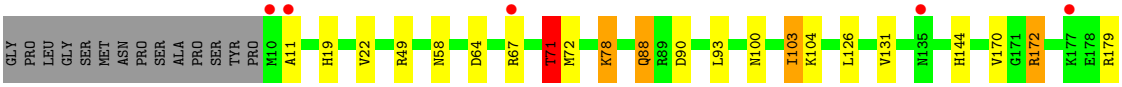
• Molecule 1: Polyadenylate-binding protein 1

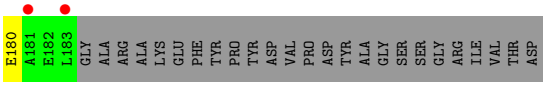
Chain A:



• Molecule 1: Polyadenylate-binding protein 1

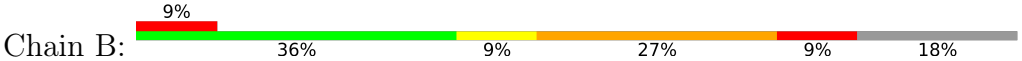
Chain D:

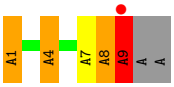




• Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

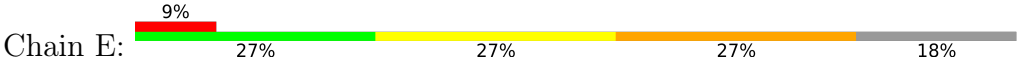
Chain B:





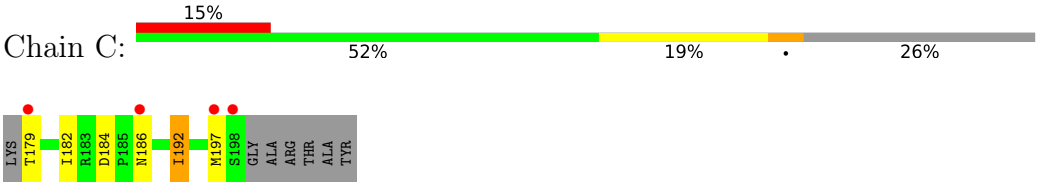
• Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain E:



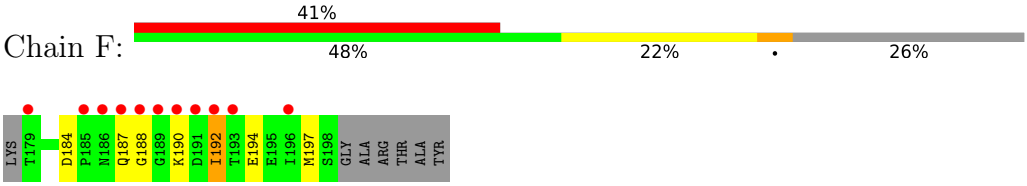
• Molecule 3: Eukaryotic translation initiation factor 4 gamma 1

Chain C:



• Molecule 3: Eukaryotic translation initiation factor 4 gamma 1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	130.19Å 130.19Å 86.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.11 – 2.00 36.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (36.11-2.00) 97.8 (36.11-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.87 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.230 0.215 , 0.238	Depositor DCC
R_{free} test set	2596 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3663	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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 (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	1.00	0/1401	0.97	0/1883
1	D	0.97	1/1423 (0.1%)	1.04	5/1910 (0.3%)
2	B	1.57	4/221 (1.8%)	1.73	9/343 (2.6%)
2	E	1.09	1/224 (0.4%)	1.75	8/347 (2.3%)
3	C	0.81	0/149	1.06	0/199
3	F	1.51	3/157 (1.9%)	1.12	0/209
All	All	1.06	9/3575 (0.3%)	1.14	22/4891 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	188	GLY	C-N	8.91	1.46	1.33
3	F	190	LYS	N-CA	6.70	1.54	1.46
2	B	7	A	P-OP2	-6.60	1.35	1.49
2	E	9	A	O5'-C5'	5.96	1.51	1.42
2	B	8	A	P-OP1	-5.47	1.38	1.49
2	B	7	A	P-OP1	-5.46	1.38	1.49
2	B	8	A	C3'-O3'	-5.42	1.35	1.43
1	D	88	GLN	CA-CB	5.12	1.59	1.52
3	F	187	GLN	C-N	5.08	1.40	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	A	C2'-C3'-O3'	-12.99	94.22	113.70
2	E	9	A	O4'-C1'-N9	10.77	124.65	108.50
2	E	9	A	O4'-C4'-C3'	-9.57	94.43	104.00
1	D	11	ALA	N-CA-C	-8.51	100.37	110.41
1	D	49	ARG	NE-CZ-NH2	-8.17	111.84	119.20
2	B	4	A	N9-C1'-C2'	8.00	124.00	112.00
2	E	9	A	O5'-C5'-C4'	7.56	122.83	111.50
2	B	9	A	O4'-C4'-C3'	-7.20	96.80	104.00
2	E	4	A	N9-C1'-C2'	7.09	122.64	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	9	A	O4'-C1'-N9	6.91	118.87	108.50
2	E	8	A	O3'-P-O5'	-6.54	94.19	104.00
2	E	9	A	C5'-C4'-O4'	6.48	119.52	109.80
2	B	1	A	O5'-C5'-C4'	5.93	120.39	111.50
2	B	9	A	O5'-C5'-C4'	5.77	120.16	111.50
2	B	9	A	C4'-C3'-C2'	-5.75	96.85	102.60
2	B	9	A	C5'-C4'-O4'	5.70	118.34	109.80
1	D	49	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	D	71	THR	N-CA-CB	-5.39	103.18	110.67
2	E	7	A	O3'-P-O5'	-5.36	95.97	104.00
2	E	6	A	O4'-C1'-C2'	-5.28	100.52	105.80
1	D	49	ARG	CD-NE-CZ	5.25	131.75	124.40
2	B	1	A	O4'-C1'-C2'	-5.12	102.48	107.60

There are no chirality outliers.

There are no planarity outliers.

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	1376	0	1363	13	0
1	D	1392	0	1388	17	0
2	B	195	0	101	4	0
2	E	198	0	100	4	0
3	C	149	0	149	3	0
3	F	157	0	157	1	0
4	A	88	0	0	3	0
4	B	20	0	0	0	0
4	C	2	0	0	0	0
4	D	73	0	0	5	0
4	E	13	0	0	0	0
All	All	3663	0	3258	36	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (36) 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:178:GLU:OE2	4:A:380:HOH:O	1.56	1.18
2:B:8:A:O2'	2:B:9:A:H5"	1.45	1.17
1:D:172[A]:ARG:NH1	4:D:370:HOH:O	1.81	1.13
1:D:172[A]:ARG:CD	4:D:369:HOH:O	2.04	1.05
1:A:178:GLU:OE1	4:A:379:HOH:O	1.84	0.95
1:D:58:ASN:HD21	2:E:8:A:H61	1.15	0.90
1:D:172[A]:ARG:HD3	4:D:369:HOH:O	1.70	0.85
1:A:58:ASN:HD21	2:B:8:A:H61	1.27	0.81
1:A:67:ARG:O	1:A:71:THR:HB	1.84	0.78
1:D:172[A]:ARG:NE	4:D:369:HOH:O	2.14	0.74
1:A:71:THR:HG22	1:A:72:MET:HG3	1.71	0.72
1:D:67:ARG:O	1:D:71:THR:HB	1.90	0.70
1:D:88:GLN:HE21	1:D:90:ASP:H	1.39	0.69
1:D:64:ASP:OD1	1:D:67:ARG:NH2	2.30	0.64
2:B:8:A:O2'	2:B:9:A:C5'	2.35	0.64
1:D:172[A]:ARG:CZ	4:D:369:HOH:O	2.44	0.62
3:C:184:ASP:HB2	3:C:192:ILE:HD12	1.82	0.62
3:C:182:ILE:HG22	3:C:192:ILE:HD11	1.87	0.56
1:D:58:ASN:ND2	2:E:8:A:H61	1.97	0.50
1:D:104:LYS:HD3	2:E:2:A:N7	2.28	0.48
2:B:8:A:C2'	2:B:9:A:H5"	2.38	0.48
1:A:172:ARG:NE	4:A:378:HOH:O	2.24	0.47
1:A:102:PHE:CE2	1:A:104:LYS:HB2	2.49	0.47
1:D:71:THR:HG22	1:D:72:MET:HG3	1.96	0.46
1:A:118:THR:HG23	3:C:197:MET:HE1	1.99	0.45
1:D:19:HIS:HB3	1:D:22:VAL:HG23	2.00	0.44
1:D:78:LYS:HB3	1:D:78:LYS:HE3	1.68	0.44
1:A:103:ILE:HD13	1:A:170:VAL:HG13	1.99	0.44
3:F:184:ASP:HB2	3:F:192:ILE:HD12	2.01	0.43
1:D:103:ILE:HD13	1:D:170:VAL:HG13	2.00	0.43
1:A:100:ASN:HA	1:A:144:HIS:HA	2.02	0.42
1:A:19:HIS:HB3	1:A:22:VAL:HG23	2.00	0.42
1:D:100:ASN:HA	1:D:144:HIS:HA	2.02	0.41
1:D:179:ARG:NH2	2:E:2:A:OP1	2.54	0.40
1:A:80:LYS:HE2	1:A:80:LYS:HB3	1.96	0.40
1:A:77:ILE:HD12	1:A:82:VAL:HG11	2.03	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	173/213 (81%)	171 (99%)	2 (1%)	0	100	100
1	D	174/213 (82%)	171 (98%)	3 (2%)	0	100	100
3	C	18/27 (67%)	17 (94%)	1 (6%)	0	100	100
3	F	18/27 (67%)	17 (94%)	0	1 (6%)	1	0
All	All	383/480 (80%)	376 (98%)	6 (2%)	1 (0%)	36	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	197	MET

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	146/179 (82%)	142 (97%)	4 (3%)	39	42
1	D	149/179 (83%)	140 (94%)	9 (6%)	17	14
3	C	16/22 (73%)	13 (81%)	3 (19%)	1	1
3	F	18/22 (82%)	16 (89%)	2 (11%)	6	3
All	All	329/402 (82%)	311 (94%)	18 (6%)	21	17

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	71	THR
1	A	131	VAL
1	A	156	GLU
3	C	179	THR
3	C	186	ASN
3	C	192	ILE
1	D	71	THR
1	D	78	LYS
1	D	93	LEU
1	D	103	ILE
1	D	126	LEU
1	D	131	VAL
1	D	172[A]	ARG
1	D	172[B]	ARG
1	D	180	GLU
3	F	192	ILE
3	F	194	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	D	58	ASN
1	D	60	GLN
1	D	88	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	9/11 (81%)	2 (22%)	1 (11%)
2	E	8/11 (72%)	2 (25%)	0
All	All	17/22 (77%)	4 (23%)	1 (5%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	4	A
2	B	9	A
2	E	4	A
2	E	9	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1	A

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 oligosaccharides 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

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	175/213 (82%)	0.14	6 (3%) 48 47	21, 32, 51, 64	0
1	D	174/213 (81%)	0.26	7 (4%) 42 41	14, 34, 58, 89	2 (1%)
2	B	9/11 (81%)	-0.38	1 (11%) 10 9	4, 24, 59, 61	1 (11%)
2	E	9/11 (81%)	-0.07	1 (11%) 10 9	24, 30, 70, 71	0
3	C	20/27 (74%)	1.36	4 (20%) 3 2	40, 63, 75, 89	0
3	F	20/27 (74%)	2.36	11 (55%) 0 0	43, 84, 105, 106	0
All	All	407/502 (81%)	0.34	30 (7%) 20 19	4, 35, 72, 106	3 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	183	LEU	4.4
3	F	186	ASN	4.4
3	F	188	GLY	4.3
3	C	198	SER	4.3
1	D	10	MET	4.2
3	F	187	GLN	4.1
3	F	179	THR	3.9
1	D	181	ALA	3.7
3	F	190	LYS	3.7
2	B	9	A	3.7
3	F	189	GLY	3.4
1	A	135	ASN	3.2
1	A	10	MET	3.0
3	F	192	ILE	2.8
3	C	186	ASN	2.8
3	F	196	ILE	2.8
1	D	67	ARG	2.7
3	F	185	PRO	2.7
3	C	179	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	193	THR	2.4
1	D	135	ASN	2.4
2	E	9	A	2.3
1	D	11	ALA	2.3
1	A	134	GLU	2.1
1	A	156	GLU	2.1
1	A	136	GLY	2.1
1	D	177	LYS	2.1
1	A	180	GLU	2.1
3	C	197	MET	2.0
3	F	191	ASP	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 oligosaccharides 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.