Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:16 am BST

PDB ID	:	5X07
Title	:	Crystal structure of FOXA2 DNA binding domain bound to a full consensus DNA site
Authors	:	Li, J.; Guo, M.; Zhou, Z.; Jiang, L.; Chen, X.; Qu, L.; Wu, D.; Chen, Z.; Chen, L.; Chen, Y.
Deposited on	:	2017-01-20
Resolution	:	2.80 Å(reported)

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

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

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

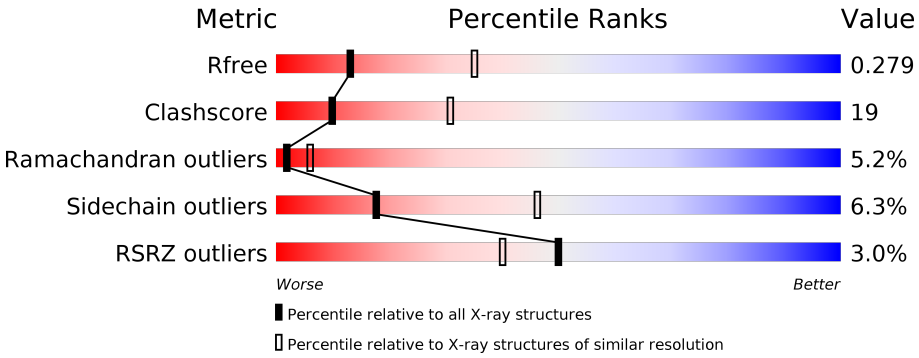
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	16	56% 38% 6%
1	D	16	50% 44% 6%
1	G	16	6% 31% 69%
1	J	16	38% 63%
2	B	16	56% 44%
2	E	16	38% 63%

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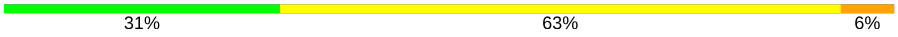
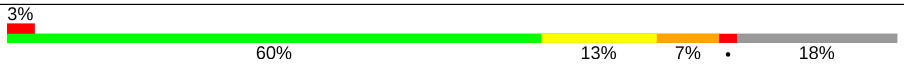
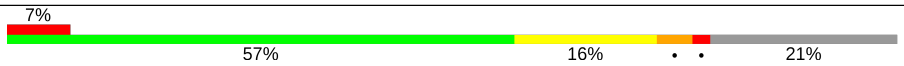
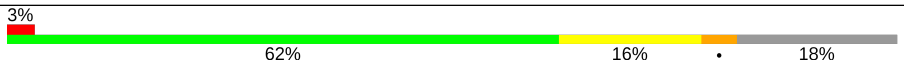
Mol	Chain	Length	Quality of chain
2	H	16	
2	K	16	
3	C	104	
3	F	104	
3	I	104	
3	L	104	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5405 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 DNA chain called DNA (5'-D(*TP*CP*TP*TP*GP*TP*TP*TP*AP*CP*AP*TP*TP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	16	Total	C	N	O	P	0	0	0
			321	158	46	102	15			
1	A	16	Total	C	N	O	P	0	0	0
			321	158	46	102	15			
1	G	16	Total	C	N	O	P	0	0	0
			321	158	46	102	15			
1	J	16	Total	C	N	O	P	0	0	0
			321	158	46	102	15			

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*AP*AP*AP*AP*TP*GP*TP*AP*AP*AP*CP*AP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	16	Total	C	N	O	P	0	0	0
			329	158	70	86	15			
2	B	16	Total	C	N	O	P	0	0	0
			329	158	70	86	15			
2	H	16	Total	C	N	O	P	0	0	0
			329	158	70	86	15			
2	K	16	Total	C	N	O	P	0	0	0
			329	158	70	86	15			

- Molecule 3 is a protein called Hepatocyte nuclear factor 3-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	85	Total	C	N	O	S	0	0	0
			707	458	122	123	4			
3	C	84	Total	C	N	O	S	0	0	0
			701	455	121	121	4			
3	I	82	Total	C	N	O	S	0	0	0
			690	448	119	119	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	85	Total	C	N	O	S	0	0	0
			707	458	122	123	4			

There are 8 discrepancies between the modelled and reference sequences:

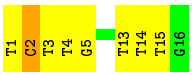
Chain	Residue	Modelled	Actual	Comment	Reference
F	155	GLY	-	expression tag	UNP Q9Y261
F	156	PRO	-	expression tag	UNP Q9Y261
C	155	GLY	-	expression tag	UNP Q9Y261
C	156	PRO	-	expression tag	UNP Q9Y261
I	155	GLY	-	expression tag	UNP Q9Y261
I	156	PRO	-	expression tag	UNP Q9Y261
L	155	GLY	-	expression tag	UNP Q9Y261
L	156	PRO	-	expression tag	UNP Q9Y261

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 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.

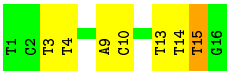
• Molecule 1: DNA (5'-D(*TP*CP*TP*TP*GP*TP*TP*TP*AP*CP*AP*TP*TP*TP*TP*G)-3')

Chain D:



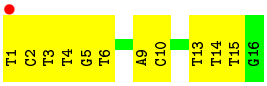
• Molecule 1: DNA (5'-D(*TP*CP*TP*TP*GP*TP*TP*TP*AP*CP*AP*TP*TP*TP*TP*G)-3')

Chain A:



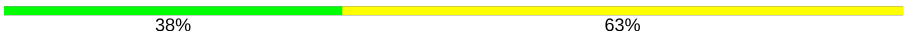
• Molecule 1: DNA (5'-D(*TP*CP*TP*TP*GP*TP*TP*TP*AP*CP*AP*TP*TP*TP*TP*G)-3')

Chain G:



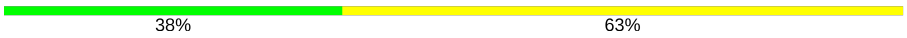
• Molecule 1: DNA (5'-D(*TP*CP*TP*TP*GP*TP*TP*TP*AP*CP*AP*TP*TP*TP*TP*G)-3')

Chain J:



• Molecule 2: DNA (5'-D(*CP*AP*AP*AP*AP*TP*GP*TP*AP*AP*AP*CP*AP*AP*GP*A)-3')

Chain E:



• Molecule 2: DNA (5'-D(*CP*AP*AP*AP*AP*TP*GP*TP*AP*AP*AP*CP*AP*AP*GP*A)-3')

Chain B:

• Molecule 2: DNA (5'-D(*CP*AP*AP*AP*AP*TP*GP*TP*AP*AP*AP*CP*AP*AP*GP*A)-3')

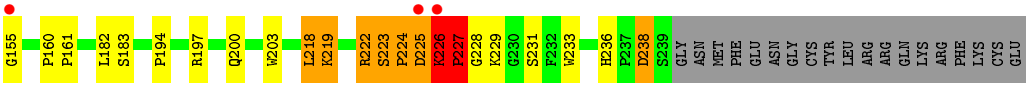
Chain H:

• Molecule 2: DNA (5'-D(*CP*AP*AP*AP*AP*TP*GP*TP*AP*AP*AP*CP*AP*AP*GP*A)-3')

Chain K:

• Molecule 3: Hepatocyte nuclear factor 3-beta

Chain F:

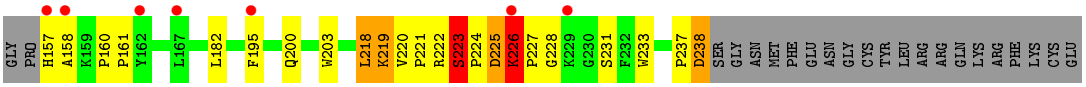


• Molecule 3: Hepatocyte nuclear factor 3-beta

Chain C:

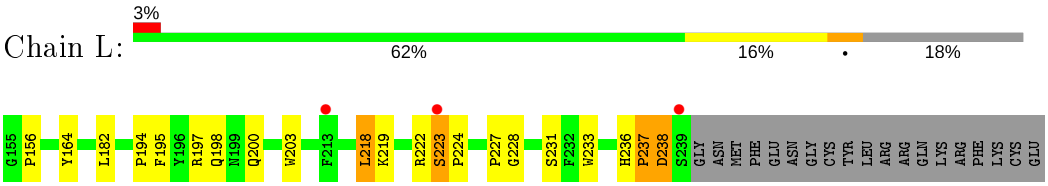
• Molecule 3: Hepatocyte nuclear factor 3-beta

Chain I:



• Molecule 3: Hepatocyte nuclear factor 3-beta

Chain L:


3%
62%
16%
18%
G155
P156
Y164
L182
P194
F195
Y196
R197
Q198
N199
Q200
W203
F213
L218
K219
R222
S223
P224
P227
G228
S231
F232
W233
H236
P237
D238
S239
GLY
ASN
MET
PHE
GLU
ASN
GLY
CYS
TYR
LEU
ARG
ARG
GLN
LYS
ARG
PHE
LYS
CYS
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	195.13Å 71.93Å 72.16Å 90.00° 103.14° 90.00°	Depositor
Resolution (Å)	33.64 – 2.80 33.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (33.64-2.80) 96.6 (33.64-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.240 , 0.279 0.247 , 0.279	Depositor DCC
R_{free} test set	1994 reflections (8.49%)	wwPDB-VP
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5405	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.53	0/356	1.18	1/548 (0.2%)
1	D	0.62	1/356 (0.3%)	1.13	0/548
1	G	0.59	0/356	1.13	0/548
1	J	0.56	0/356	1.19	0/548
2	B	0.49	0/372	0.85	0/572
2	E	0.62	0/372	0.82	0/572
2	H	0.60	1/372 (0.3%)	0.79	0/572
2	K	0.54	0/372	0.88	0/572
3	C	0.56	0/727	0.77	5/988 (0.5%)
3	F	0.46	2/733 (0.3%)	0.63	1/996 (0.1%)
3	I	0.31	0/715	0.60	1/971 (0.1%)
3	L	0.24	0/733	0.52	0/996
All	All	0.50	4/5820 (0.1%)	0.85	8/8431 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2	DC	O3'-P	-5.67	1.54	1.61
3	F	224	PRO	N-CD	5.43	1.55	1.47
2	H	15	DG	O3'-P	-5.09	1.55	1.61
3	F	227	PRO	N-CD	5.04	1.54	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	223	SER	C-N-CD	6.73	142.53	128.40
3	C	236	HIS	C-N-CD	6.14	141.30	128.40
3	C	175	SER	C-N-CD	6.04	141.08	128.40
3	F	226	LYS	C-N-CD	5.93	140.86	128.40
3	C	224	PRO	CA-N-CD	-5.48	103.83	111.50
3	C	227	PRO	CA-N-CD	-5.31	104.06	111.50
1	A	15	DT	O4'-C4'-C3'	-5.20	102.42	104.50
3	I	223	SER	C-N-CD	-5.17	109.22	120.60

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	321	0	188	5	0
1	D	321	0	188	9	44
1	G	321	0	188	18	44
1	J	321	0	188	8	0
2	B	329	0	180	4	0
2	E	329	0	180	6	46
2	H	329	0	180	9	46
2	K	329	0	180	7	0
3	C	701	0	682	40	0
3	F	707	0	687	37	0
3	I	690	0	672	36	0
3	L	707	0	687	18	0
All	All	5405	0	4200	178	90

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 (178) 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)
3:C:222:ARG:HG3	3:C:232:PHE:CE2	1.65	1.30
3:I:237:PRO:C	3:I:238:ASP:OD1	1.76	1.22
3:F:222:ARG:CZ	3:F:229:LYS:H	1.60	1.13
3:I:223:SER:H	3:I:224:PRO:HD3	1.02	1.09
3:I:223:SER:H	3:I:224:PRO:CD	1.69	1.05
3:I:158:ALA:O	3:I:195:PHE:HB2	1.56	1.03
3:C:222:ARG:HB3	3:C:223:SER:HA	1.38	1.02
3:F:222:ARG:NH1	3:F:229:LYS:H	1.57	0.99
3:F:222:ARG:HB3	3:F:223:SER:HA	1.45	0.98
3:C:222:ARG:H	3:C:223:SER:HB2	1.28	0.97
3:I:237:PRO:O	3:I:238:ASP:OD1	1.82	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:222:ARG:HG3	3:C:232:PHE:CD2	2.00	0.96
3:C:223:SER:H	3:C:224:PRO:HD3	1.31	0.95
3:F:222:ARG:CD	3:F:228:GLY:HA2	1.97	0.94
3:I:225:ASP:C	3:I:227:PRO:HD3	1.88	0.94
1:D:1:DT:H2'	1:D:2:DC:C6	2.05	0.91
3:I:223:SER:N	3:I:224:PRO:HD3	1.85	0.90
3:F:222:ARG:CB	3:F:223:SER:HA	2.01	0.89
3:F:222:ARG:NE	3:F:229:LYS:N	2.22	0.88
3:I:157:HIS:O	3:I:195:PHE:HD1	1.59	0.85
1:D:2:DC:H42	2:E:15:DG:H1	1.24	0.85
3:F:222:ARG:CZ	3:F:229:LYS:N	2.41	0.84
3:F:223:SER:HB3	3:F:224:PRO:HD3	1.61	0.83
3:C:222:ARG:CG	3:C:232:PHE:CE2	2.57	0.82
1:G:1:DT:H2'	1:G:2:DC:C6	2.16	0.81
3:C:218:LEU:HA	3:C:219:LYS:HB2	1.62	0.81
3:C:223:SER:H	3:C:224:PRO:CD	1.93	0.80
3:F:222:ARG:NH1	3:F:229:LYS:N	2.29	0.80
3:F:222:ARG:NE	3:F:229:LYS:H	1.76	0.80
3:C:222:ARG:N	3:C:223:SER:HB2	1.97	0.80
3:C:224:PRO:HD2	3:C:225:ASP:H	1.46	0.80
3:C:222:ARG:HB3	3:C:223:SER:CA	2.11	0.79
1:G:1:DT:H3'	1:G:2:DC:C5	2.19	0.78
3:I:223:SER:N	3:I:224:PRO:CD	2.41	0.77
3:L:218:LEU:HA	3:L:219:LYS:HB2	1.65	0.77
3:I:157:HIS:HA	1:J:8:DT:OP1	1.85	0.77
3:F:225:ASP:O	3:F:227:PRO:HD3	1.87	0.75
3:I:224:PRO:HG2	3:I:225:ASP:OD2	1.85	0.75
3:F:222:ARG:N	3:F:223:SER:HB2	2.02	0.75
3:F:218:LEU:HA	3:F:219:LYS:HB2	1.69	0.74
3:I:218:LEU:HA	3:I:219:LYS:HB2	1.68	0.74
1:G:1:DT:H3	2:H:16:DA:H61	1.32	0.74
1:G:1:DT:H3'	1:G:2:DC:C6	2.24	0.72
1:D:1:DT:H2"	1:D:2:DC:O4'	1.90	0.71
3:F:222:ARG:HH11	3:F:229:LYS:CA	2.03	0.71
3:F:222:ARG:HE	3:F:229:LYS:N	1.88	0.71
3:I:158:ALA:O	3:I:195:PHE:CB	2.38	0.69
1:G:1:DT:H2'	1:G:2:DC:C5	2.27	0.68
3:I:238:ASP:OD1	3:I:238:ASP:N	2.22	0.67
3:C:176:PRO:HD2	3:C:177:ASN:H	1.59	0.67
3:F:222:ARG:NE	3:F:228:GLY:HA2	2.10	0.66
3:I:224:PRO:CG	3:I:225:ASP:H	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:DG:OP1	3:L:231:SER:N	2.29	0.65
1:D:2:DC:N4	2:E:15:DG:H1	1.95	0.65
3:C:170:MET:O	3:C:174:GLN:HG2	1.95	0.65
3:L:195:PHE:O	3:L:198:GLN:NE2	2.31	0.64
1:G:1:DT:H3	2:H:16:DA:N6	1.96	0.64
3:F:222:ARG:CB	3:F:223:SER:CA	2.74	0.63
3:C:172:ILE:O	3:C:175:SER:OG	2.17	0.63
3:I:225:ASP:C	3:I:226:LYS:HG2	2.20	0.61
3:C:224:PRO:CD	3:C:225:ASP:H	2.13	0.61
3:C:236:HIS:HD2	3:C:237:PRO:O	1.84	0.61
1:A:3:DT:H1'	1:A:4:DT:H5'	1.82	0.61
3:I:225:ASP:C	3:I:227:PRO:CD	2.68	0.60
3:F:223:SER:HB3	3:F:224:PRO:CD	2.31	0.60
1:A:4:DT:H5"	3:C:229:LYS:HG3	1.82	0.60
1:G:1:DT:C3'	1:G:2:DC:C5	2.85	0.60
3:C:170:MET:O	3:C:174:GLN:CG	2.50	0.59
1:G:1:DT:C2'	1:G:2:DC:C6	2.85	0.59
3:I:224:PRO:HG2	3:I:225:ASP:H	1.68	0.59
3:F:222:ARG:HD3	3:F:228:GLY:HA2	1.83	0.59
3:C:224:PRO:HD2	3:C:225:ASP:N	2.15	0.58
3:F:222:ARG:HD2	3:F:228:GLY:HA2	1.84	0.58
3:C:218:LEU:CA	3:C:219:LYS:HB2	2.35	0.57
3:F:222:ARG:HH11	3:F:229:LYS:C	2.07	0.56
3:C:176:PRO:CD	3:C:177:ASN:H	2.18	0.56
3:L:194:PRO:HA	3:L:197:ARG:HG3	1.88	0.56
3:F:222:ARG:H	3:F:223:SER:HB2	1.71	0.56
1:D:1:DT:C2'	1:D:2:DC:C6	2.85	0.56
1:G:1:DT:C3'	1:G:2:DC:C6	2.89	0.55
3:C:238:ASP:N	3:C:238:ASP:OD2	2.40	0.55
3:L:200:GLN:HA	3:L:203:TRP:NE1	2.21	0.55
2:B:12:DC:H4'	3:L:156:PRO:HG3	1.87	0.54
3:F:222:ARG:HH11	3:F:229:LYS:N	1.98	0.54
3:C:223:SER:N	3:C:224:PRO:HD3	2.13	0.54
1:G:1:DT:C2'	1:G:2:DC:C5	2.90	0.53
2:B:5:DA:H2"	2:B:6:DT:H5'	1.90	0.53
1:G:13:DT:H1'	1:G:14:DT:H5'	1.91	0.53
3:F:222:ARG:NH1	3:F:229:LYS:HB3	2.23	0.53
1:D:13:DT:H1'	1:D:14:DT:H5'	1.91	0.53
3:I:224:PRO:CD	3:I:225:ASP:H	2.22	0.53
3:C:222:ARG:H	3:C:223:SER:CB	2.11	0.52
3:F:236:HIS:ND1	3:F:238:ASP:HB3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:218:LEU:O	3:C:234:THR:N	2.22	0.52
3:I:157:HIS:O	3:I:195:PHE:CD1	2.51	0.52
3:C:222:ARG:CA	3:C:223:SER:HB2	2.40	0.52
3:F:194:PRO:HA	3:F:197:ARG:HG3	1.92	0.51
3:C:224:PRO:CD	3:C:225:ASP:N	2.72	0.51
3:F:155:GLY:HA2	2:H:11:DA:H1'	1.93	0.51
3:F:219:LYS:H	3:F:233:TRP:HA	1.76	0.51
3:F:222:ARG:NH1	3:F:229:LYS:O	2.42	0.50
3:I:224:PRO:CG	3:I:225:ASP:N	2.73	0.50
3:I:226:LYS:N	3:I:227:PRO:CD	2.75	0.50
3:I:226:LYS:N	3:I:227:PRO:HD3	2.27	0.49
2:B:3:DA:H1'	2:B:4:DA:H5'	1.94	0.49
3:L:222:ARG:HD3	3:L:228:GLY:HA3	1.94	0.49
2:E:5:DA:H2"	2:E:6:DT:H5'	1.95	0.49
2:E:8:DT:H1'	2:E:9:DA:H5'	1.95	0.49
3:I:224:PRO:CD	3:I:225:ASP:N	2.77	0.48
1:D:5:DG:OP1	3:F:231:SER:N	2.42	0.48
3:C:222:ARG:N	3:C:223:SER:CB	2.72	0.47
3:L:219:LYS:H	3:L:233:TRP:HA	1.79	0.47
3:F:200:GLN:HA	3:F:203:TRP:NE1	2.29	0.47
1:G:3:DT:H1'	1:G:4:DT:H5'	1.96	0.47
2:H:5:DA:H2"	2:H:6:DT:H5'	1.96	0.47
3:I:158:ALA:O	3:I:195:PHE:CD1	2.68	0.47
3:C:223:SER:N	3:C:224:PRO:CD	2.72	0.47
2:E:1:DC:H2'	2:E:2:DA:C8	2.49	0.47
3:I:158:ALA:C	3:I:195:PHE:CD1	2.89	0.46
2:K:7:DG:H3'	3:L:164:TYR:HE2	1.80	0.46
1:A:14:DT:H1'	1:A:15:DT:H5'	1.97	0.46
3:I:200:GLN:HA	3:I:203:TRP:NE1	2.30	0.46
2:K:5:DA:H2"	2:K:6:DT:H5'	1.96	0.46
1:G:2:DC:H42	2:H:15:DG:H1	1.63	0.46
3:I:219:LYS:HD3	3:I:219:LYS:HA	1.63	0.46
2:K:7:DG:H3'	3:L:164:TYR:CE2	2.51	0.46
3:C:194:PRO:HA	3:C:197:ARG:HG3	1.98	0.46
3:C:222:ARG:CB	3:C:223:SER:HB2	2.45	0.46
2:E:3:DA:H1'	2:E:4:DA:H5'	1.97	0.46
1:G:6:DT:OP1	3:I:219:LYS:NZ	2.34	0.46
2:H:3:DA:H1'	2:H:4:DA:H5'	1.98	0.46
1:D:3:DT:H1'	1:D:4:DT:H5'	1.99	0.45
3:I:160:PRO:HA	3:I:161:PRO:HD3	1.75	0.45
1:J:9:DA:H1'	1:J:10:DC:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:LYS:H	3:C:233:TRP:HA	1.81	0.45
3:I:222:ARG:HD3	3:I:228:GLY:HA3	1.99	0.45
3:L:238:ASP:OD1	3:L:238:ASP:N	2.49	0.45
2:H:1:DC:H2'	2:H:2:DA:C8	2.52	0.45
2:H:8:DT:H1'	2:H:9:DA:H5'	1.97	0.44
1:J:14:DT:H1'	1:J:15:DT:H5'	1.97	0.44
3:C:227:PRO:HA	3:C:228:GLY:HA3	1.77	0.44
3:C:237:PRO:HD2	3:C:237:PRO:O	2.17	0.44
3:F:219:LYS:HA	3:F:219:LYS:HD3	1.67	0.44
3:F:225:ASP:CG	3:F:226:LYS:HG2	2.38	0.44
3:F:222:ARG:NH1	3:F:229:LYS:CA	2.75	0.44
2:B:8:DT:H1'	2:B:9:DA:H5'	1.99	0.44
1:G:14:DT:H1'	1:G:15:DT:H5'	2.00	0.44
1:J:16:DG:H1	2:K:1:DC:H42	1.66	0.44
1:J:4:DT:H2"	1:J:5:DG:H5"	2.00	0.44
1:J:6:DT:OP1	3:L:219:LYS:NZ	2.32	0.44
3:L:223:SER:H	3:L:224:PRO:HD2	1.83	0.44
1:G:9:DA:H1'	1:G:10:DC:H5'	1.99	0.44
3:F:222:ARG:HH11	3:F:229:LYS:CB	2.30	0.43
2:K:1:DC:H2'	2:K:2:DA:C8	2.53	0.43
3:L:227:PRO:HA	3:L:228:GLY:HA3	1.67	0.43
1:G:5:DG:OP1	3:I:231:SER:N	2.52	0.43
2:K:9:DA:H1'	2:K:10:DA:H5'	2.01	0.43
3:F:160:PRO:HA	3:F:161:PRO:HD3	1.74	0.43
3:C:160:PRO:HA	3:C:161:PRO:HD3	1.78	0.43
3:C:219:LYS:HD3	3:C:219:LYS:HA	1.77	0.42
1:J:3:DT:H1'	1:J:4:DT:H5'	2.01	0.42
3:C:218:LEU:HD21	3:C:236:HIS:ND1	2.33	0.42
3:F:222:ARG:HB3	3:F:223:SER:CA	2.25	0.42
1:A:13:DT:H1'	1:A:14:DT:H5'	2.01	0.41
3:C:176:PRO:CD	3:C:177:ASN:N	2.82	0.41
1:D:14:DT:H1'	1:D:15:DT:H5'	2.01	0.41
3:I:227:PRO:HA	3:I:228:GLY:HA3	1.68	0.41
3:C:218:LEU:HD21	3:C:236:HIS:CG	2.56	0.41
3:L:219:LYS:HD3	3:L:219:LYS:HA	1.65	0.41
3:I:158:ALA:O	3:I:195:PHE:CG	2.73	0.41
3:I:220:VAL:HA	3:I:221:PRO:HD2	1.82	0.41
1:G:1:DT:N3	2:H:16:DA:N6	2.66	0.40
3:I:219:LYS:H	3:I:233:TRP:HA	1.86	0.40
2:K:16:DA:H4'	3:L:228:GLY:O	2.20	0.40
3:L:236:HIS:HA	3:L:237:PRO:HD3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:222:ARG:HH22	3:C:228:GLY:HA2	1.87	0.40
3:L:219:LYS:HG2	3:L:233:TRP:CH2	2.57	0.40
1:A:9:DA:H1'	1:A:10:DC:H5'	2.03	0.40

All (90) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:DT:C2	2:H:16:DA:C2[4_7410]	0.32	1.88
2:E:16:DA:C6	1:G:1:DT:O4[4_7410]	0.35	1.85
1:D:1:DT:O4	2:H:16:DA:N7[4_7410]	0.45	1.75
2:E:16:DA:C8	1:G:1:DT:C7[4_7410]	0.47	1.73
2:E:16:DA:O3'	1:G:1:DT:O5'[4_7410]	0.49	1.71
1:D:1:DT:C4	2:H:16:DA:C5[4_7410]	0.53	1.67
2:E:16:DA:C2	1:G:1:DT:N3[4_7410]	0.67	1.53
2:E:16:DA:N3	1:G:1:DT:N3[4_7410]	0.69	1.51
1:D:1:DT:C5	2:H:16:DA:C4[4_7410]	0.70	1.50
2:E:16:DA:C4	1:G:1:DT:C5[4_7410]	0.77	1.43
1:D:1:DT:C7	2:H:16:DA:N9[4_7410]	0.79	1.41
2:E:16:DA:N9	1:G:1:DT:C5[4_7410]	0.82	1.38
1:D:1:DT:C7	2:H:16:DA:C1'[4_7410]	0.83	1.37
1:D:1:DT:C6	2:H:16:DA:N3[4_7410]	0.84	1.36
1:D:1:DT:N1	2:H:16:DA:N3[4_7410]	0.84	1.36
2:E:16:DA:N9	1:G:1:DT:C6[4_7410]	0.85	1.35
2:E:16:DA:N7	1:G:1:DT:C7[4_7410]	0.85	1.35
1:D:1:DT:C5	2:H:16:DA:N9[4_7410]	0.87	1.33
1:D:1:DT:C4	2:H:16:DA:C4[4_7410]	0.88	1.32
1:D:1:DT:N3	2:H:16:DA:C6[4_7410]	0.89	1.31
2:E:16:DA:C4	1:G:1:DT:C4[4_7410]	0.91	1.29
2:E:16:DA:C5	1:G:1:DT:C4[4_7410]	0.97	1.23
2:E:16:DA:N3	1:G:1:DT:C2[4_7410]	0.97	1.23
1:D:1:DT:O4	2:H:16:DA:C5[4_7410]	1.01	1.19
1:D:1:DT:C2	2:H:16:DA:N1[4_7410]	1.03	1.17
1:D:1:DT:N1	2:H:16:DA:C2[4_7410]	1.07	1.13
2:E:16:DA:C5	1:G:1:DT:O4[4_7410]	1.08	1.12
1:D:1:DT:N3	2:H:16:DA:N1[4_7410]	1.11	1.09
2:E:16:DA:O3'	1:G:1:DT:C5'[4_7410]	1.11	1.09
2:E:16:DA:C1'	1:G:1:DT:C6[4_7410]	1.12	1.08
2:E:16:DA:N1	2:H:16:DA:N6[4_7410]	1.12	1.08
1:D:1:DT:N3	2:H:16:DA:C5[4_7410]	1.27	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:DT:O2	2:H:16:DA:N1[4_7410]	1.29	0.91
2:E:16:DA:C3'	1:G:1:DT:O5'[4_7410]	1.29	0.91
2:E:16:DA:C5	1:G:1:DT:C5[4_7410]	1.39	0.81
1:D:1:DT:O2	2:H:16:DA:C2[4_7410]	1.40	0.80
2:E:16:DA:C8	1:G:1:DT:C5[4_7410]	1.44	0.76
2:E:16:DA:N1	1:G:1:DT:O4[4_7410]	1.49	0.71
2:E:16:DA:C4	1:G:1:DT:C6[4_7410]	1.49	0.71
2:E:16:DA:C6	1:G:1:DT:C4[4_7410]	1.50	0.70
1:D:1:DT:C6	2:H:16:DA:C4[4_7410]	1.52	0.68
2:E:16:DA:N3	1:G:1:DT:C4[4_7410]	1.52	0.68
1:D:1:DT:O4	2:H:16:DA:C8[4_7410]	1.53	0.67
1:D:1:DT:N3	2:H:16:DA:C2[4_7410]	1.54	0.66
1:D:1:DT:C4	2:H:16:DA:N7[4_7410]	1.56	0.64
1:D:1:DT:C2	2:H:16:DA:N3[4_7410]	1.57	0.63
1:D:1:DT:C5	2:H:16:DA:N3[4_7410]	1.57	0.63
2:E:16:DA:N6	1:G:1:DT:O4[4_7410]	1.58	0.62
2:E:16:DA:C4	1:G:1:DT:N3[4_7410]	1.62	0.58
2:E:16:DA:N3	1:G:1:DT:N1[4_7410]	1.65	0.55
2:E:16:DA:N9	1:G:1:DT:C7[4_7410]	1.67	0.53
1:D:1:DT:N3	2:H:16:DA:C4[4_7410]	1.68	0.52
1:D:1:DT:C7	2:H:16:DA:C8[4_7410]	1.69	0.51
1:D:1:DT:C7	2:H:16:DA:O4'[4_7410]	1.71	0.49
2:E:16:DA:C2	1:G:1:DT:C4[4_7410]	1.72	0.48
1:D:1:DT:C4	2:H:16:DA:N9[4_7410]	1.74	0.46
2:E:16:DA:N1	1:G:1:DT:N3[4_7410]	1.76	0.44
2:E:16:DA:N7	1:G:1:DT:C5[4_7410]	1.76	0.44
1:D:1:DT:C4	2:H:16:DA:C6[4_7410]	1.77	0.43
2:E:16:DA:N1	1:G:1:DT:C4[4_7410]	1.81	0.39
1:D:1:DT:C7	2:H:16:DA:C2'[4_7410]	1.82	0.38
2:E:16:DA:C2	1:G:1:DT:C2[4_7410]	1.83	0.37
2:E:16:DA:C5	1:G:1:DT:C7[4_7410]	1.84	0.36
1:D:1:DT:C5	2:H:16:DA:C1'[4_7410]	1.85	0.35
1:D:1:DT:C4	2:H:16:DA:C8[4_7410]	1.94	0.26
1:D:1:DT:N3	2:H:16:DA:N3[4_7410]	1.94	0.26
2:E:16:DA:C1'	1:G:1:DT:N1[4_7410]	1.95	0.25
1:D:1:DT:C5	2:H:16:DA:C5[4_7410]	1.96	0.24
2:E:16:DA:O3'	1:G:1:DT:C4'[4_7410]	1.97	0.23
2:E:16:DA:O4'	1:G:1:DT:C6[4_7410]	2.00	0.20
1:D:1:DT:O4	2:H:16:DA:C4[4_7410]	2.02	0.18
2:E:16:DA:C1'	1:G:1:DT:O4'[4_7410]	2.02	0.18
1:D:1:DT:C5	2:H:16:DA:C8[4_7410]	2.05	0.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:DT:C4	2:H:16:DA:N3[4_7410]	2.05	0.15
2:E:16:DA:C2	2:H:16:DA:N6[4_7410]	2.06	0.14
1:D:1:DT:C2	2:H:16:DA:C6[4_7410]	2.07	0.13
2:E:16:DA:C4	1:G:1:DT:O4[4_7410]	2.07	0.13
2:E:16:DA:N3	1:G:1:DT:C5[4_7410]	2.07	0.13
2:E:16:DA:N3	1:G:1:DT:C6[4_7410]	2.07	0.13
2:E:16:DA:C4	1:G:1:DT:N1[4_7410]	2.08	0.12
2:E:16:DA:N3	1:G:1:DT:O2[4_7410]	2.10	0.10
1:D:1:DT:C7	2:H:16:DA:C4[4_7410]	2.11	0.09
1:D:1:DT:C6	2:H:16:DA:N9[4_7410]	2.12	0.08
2:E:16:DA:O3'	1:G:1:DT:O4'[4_7410]	2.13	0.07
1:D:1:DT:C6	2:H:16:DA:C2[4_7410]	2.14	0.06
1:D:1:DT:N1	2:H:16:DA:C4[4_7410]	2.15	0.05
1:D:1:DT:O4	2:H:16:DA:C6[4_7410]	2.17	0.03
2:E:16:DA:N9	1:G:1:DT:N1[4_7410]	2.18	0.02
1:D:1:DT:C1'	2:H:16:DA:C2[4_7410]	2.18	0.02
2:E:16:DA:C4	1:G:1:DT:C2[4_7410]	2.19	0.01

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
3	C	82/104 (79%)	68 (83%)	5 (6%)	9 (11%)	0 1
3	F	83/104 (80%)	73 (88%)	6 (7%)	4 (5%)	2 7
3	I	80/104 (77%)	72 (90%)	6 (8%)	2 (2%)	5 19
3	L	83/104 (80%)	76 (92%)	5 (6%)	2 (2%)	6 20
All	All	328/416 (79%)	289 (88%)	22 (7%)	17 (5%)	2 6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	223	SER

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Mol	Chain	Res	Type
3	C	223	SER
3	C	224	PRO
3	C	225	ASP
3	C	226	LYS
3	I	226	LYS
3	F	225	ASP
3	C	176	PRO
3	I	223	SER
3	L	223	SER
3	F	222	ARG
3	C	219	LYS
3	C	227	PRO
3	F	226	LYS
3	L	237	PRO
3	C	175	SER
3	C	228	GLY

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
3	C	79/97 (81%)	74 (94%)	5 (6%)	18 46
3	F	80/97 (82%)	74 (92%)	6 (8%)	13 37
3	I	78/97 (80%)	72 (92%)	6 (8%)	13 35
3	L	80/97 (82%)	77 (96%)	3 (4%)	33 67
All	All	317/388 (82%)	297 (94%)	20 (6%)	18 46

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	182	LEU
3	F	183	SER
3	F	218	LEU
3	F	219	LYS
3	F	227	PRO

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Mol	Chain	Res	Type
3	F	238	ASP
3	C	174	GLN
3	C	182	LEU
3	C	218	LEU
3	C	222	ARG
3	C	238	ASP
3	I	182	LEU
3	I	218	LEU
3	I	219	LYS
3	I	225	ASP
3	I	226	LYS
3	I	238	ASP
3	L	182	LEU
3	L	218	LEU
3	L	238	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	236	HIS

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

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	16/16 (100%)	-0.44	0 100 100	48, 63, 76, 81	0
1	D	16/16 (100%)	-0.45	0 100 100	39, 51, 80, 188	0
1	G	16/16 (100%)	-0.19	1 (6%) 20 12	47, 74, 99, 249	0
1	J	16/16 (100%)	0.09	0 100 100	61, 87, 124, 145	0
2	B	16/16 (100%)	-0.49	0 100 100	44, 70, 91, 94	0
2	E	16/16 (100%)	-0.33	0 100 100	41, 57, 88, 90	0
2	H	16/16 (100%)	-0.30	0 100 100	54, 74, 96, 129	0
2	K	16/16 (100%)	-0.20	0 100 100	66, 84, 101, 104	0
3	C	84/104 (80%)	0.19	0 100 100	39, 57, 106, 140	0
3	F	85/104 (81%)	0.22	3 (3%) 44 34	38, 51, 130, 165	0
3	I	82/104 (78%)	0.55	7 (8%) 10 5	44, 68, 131, 189	0
3	L	85/104 (81%)	0.41	3 (3%) 44 34	48, 74, 116, 141	0
All	All	464/544 (85%)	0.17	14 (3%) 50 40	38, 67, 124, 249	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	195	PHE	4.1
3	I	157	HIS	3.8
1	G	1	DT	3.6
3	F	155	GLY	3.4
3	I	158	ALA	3.2
3	F	225	ASP	2.9
3	I	162	TYR	2.9
3	I	226	LYS	2.7
3	L	223	SER	2.5
3	F	226	LYS	2.3
3	I	229	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	L	213	PHE	2.2
3	I	167	LEU	2.1
3	L	239	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.