Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:32 PM EDT

PDB ID	:	4AWL
Title	:	The NF-Y transcription factor is structurally and functionally a sequence specific histone
Authors	:	Nardini, M.; Gnesutta, N.; Donati, G.; Gatta, R.; Forni, C.; Fossati, A.; Vonrhein, C.; Moras, D.; Romier, C.; Mantovani, R.; Bolognesi, M.
Deposited on	:	2012-06-04
Resolution	:	3.08 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 (i) 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 (1)) were used in the production of this report:

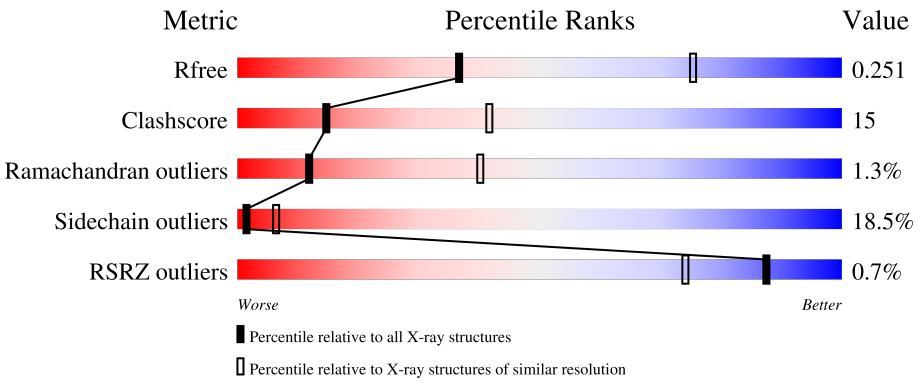
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	78	% 33% 29% 15% • 21%
2	B	94	% 68% 24% 5% •
3	C	94	54% 23% 6% • 15%
4	I	25	40% 36% 24%
5	J	25	20% 56% 24%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2949 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 NUCLEAR TRANSCRIPTION FACTOR Y SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	62	530	330	114	84	2	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	MET	-	expression tag	UNP P23511
A	304	GLY	-	expression tag	UNP P23511
A	305	SER	-	expression tag	UNP P23511
A	306	LEU	-	expression tag	UNP P23511
A	307	VAL	-	expression tag	UNP P23511
A	308	PRO	-	expression tag	UNP P23511
A	309	ARG	-	expression tag	UNP P23511

- Molecule 2 is a protein called NUCLEAR TRANSCRIPTION FACTOR Y SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	92	745	473	125	142	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	48	MET	-	expression tag	UNP P25208

- Molecule 3 is a protein called NUCLEAR TRANSCRIPTION FACTOR Y SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	80	653	423	111	116	3	0	0	0

- Molecule 4 is a DNA chain called HSP70 PROMOTER FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	I	25	505	242	91	148	24	0	0	0

- Molecule 5 is a DNA chain called HSP70 PROMOTER FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	J	25	514	245	97	148	24	0	0	0

- Molecule 6 is water.

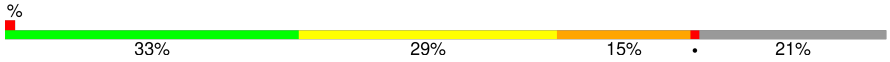
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	B	1	1	1	0	0
			Total	O		
6	I	1	1	1	0	0

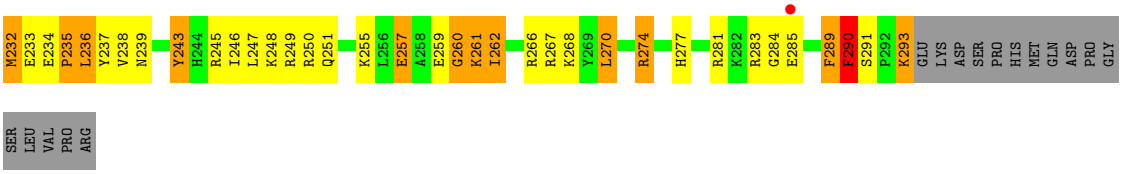
3 Residue-property plots (i)

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: NUCLEAR TRANSCRIPTION FACTOR Y SUBUNIT ALPHA

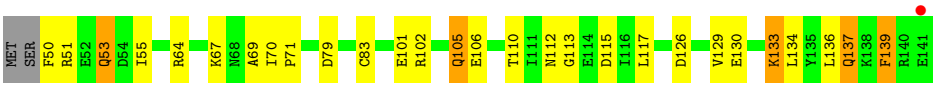
Chain A:





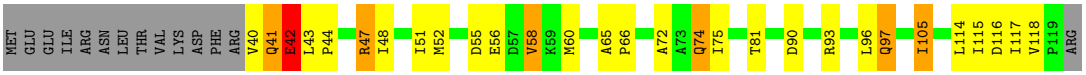
• Molecule 2: NUCLEAR TRANSCRIPTION FACTOR Y SUBUNIT BETA

Chain B:



• Molecule 3: NUCLEAR TRANSCRIPTION FACTOR Y SUBUNIT GAMMA

Chain C:

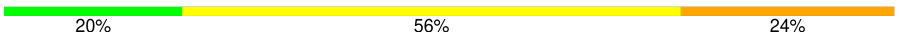


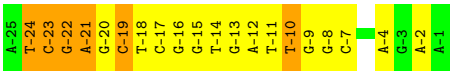
• Molecule 4: HSP70 PROMOTER FRAGMENT

Chain I:

• Molecule 5: HSP70 PROMOTER FRAGMENT

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	54.70Å 62.56Å 139.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.46 – 3.08 35.46 – 3.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.46-3.08) 94.9 (35.46-3.08)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.191 , 0.250 0.199 , 0.251	Depositor DCC
R_{free} test set	418 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å^2)	76.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2949	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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	0.58	0/541	1.02	3/714 (0.4%)
2	B	0.71	0/757	0.72	1/1014 (0.1%)
3	C	0.64	0/663	0.83	2/894 (0.2%)
4	I	1.04	0/565	1.84	20/869 (2.3%)
5	J	1.10	1/577 (0.2%)	2.01	25/890 (2.8%)
All	All	0.83	1/3103 (0.0%)	1.39	51/4381 (1.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	-4	DA	C3'-O3'	-5.44	1.36	1.44

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	290	PHE	CB-CA-C	14.63	139.67	110.40
5	J	-12	DA	O4'-C1'-N9	-13.21	98.75	108.00
5	J	-21	DA	O4'-C1'-N9	-10.76	100.47	108.00
1	A	289	PHE	CB-CA-C	9.56	129.53	110.40
4	I	23	DG	P-O3'-C3'	9.20	130.74	119.70
5	J	-24	DT	O4'-C1'-N1	8.70	114.09	108.00
5	J	-8	DG	C8-N9-C4	-8.33	103.07	106.40
5	J	-13	DG	O4'-C1'-N9	-7.95	102.43	108.00
5	J	-14	DT	O4'-C1'-N1	-7.93	102.45	108.00
3	C	58	VAL	CB-CA-C	-7.92	96.35	111.40
5	J	-16	DG	P-O3'-C3'	7.85	129.12	119.70
5	J	-9	DG	O4'-C1'-N9	-7.74	102.58	108.00
4	I	6	DA	O4'-C1'-N9	-7.73	102.59	108.00
5	J	-7	DC	O4'-C1'-N1	-7.60	102.68	108.00
4	I	11	DA	O4'-C1'-N9	-7.51	102.75	108.00
4	I	20	DC	O4'-C1'-N1	7.25	113.07	108.00
5	J	-11	DT	O4'-C1'-N1	-7.04	103.07	108.00
4	I	8	DC	O4'-C1'-N1	-7.02	103.08	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	42	GLU	CB-CA-C	6.67	123.75	110.40
5	J	-19	DC	O4'-C1'-N1	6.45	112.52	108.00
5	J	-9	DG	O4'-C4'-C3'	-6.45	101.92	104.50
5	J	-16	DG	O4'-C1'-N9	6.33	112.43	108.00
4	I	15	DC	P-O3'-C3'	6.33	127.29	119.70
4	I	18	DA	O4'-C1'-N9	-6.32	103.58	108.00
5	J	-8	DG	P-O3'-C3'	5.99	126.89	119.70
4	I	16	DC	O4'-C1'-N1	-5.93	103.85	108.00
5	J	-15	DG	O4'-C1'-N9	-5.93	103.85	108.00
5	J	-22	DG	O5'-P-OP2	-5.87	100.42	105.70
4	I	14	DA	O4'-C1'-N9	-5.83	103.92	108.00
4	I	3	DC	O4'-C1'-N1	-5.82	103.93	108.00
2	B	105	GLN	CB-CA-C	-5.79	98.82	110.40
5	J	-10	DT	C6-C5-C7	-5.78	119.43	122.90
4	I	4	DT	C5-C4-O4	-5.75	120.87	124.90
5	J	-20	DG	O4'-C1'-C2'	-5.71	101.33	105.90
4	I	5	DG	P-O3'-C3'	5.52	126.32	119.70
4	I	3	DC	O4'-C4'-C3'	-5.42	102.33	104.50
5	J	-10	DT	C4-C5-C7	5.42	122.25	119.00
1	A	290	PHE	N-CA-C	-5.41	96.40	111.00
4	I	4	DT	N3-C4-O4	5.40	123.14	119.90
4	I	5	DG	N1-C6-O6	-5.32	116.71	119.90
4	I	3	DC	C3'-C2'-C1'	-5.30	96.14	102.50
5	J	-23	DC	P-O3'-C3'	5.29	126.05	119.70
5	J	-8	DG	N7-C8-N9	5.22	115.71	113.10
4	I	12	DT	N3-C4-O4	5.19	123.01	119.90
5	J	-17	DC	O4'-C1'-C2'	-5.18	101.75	105.90
5	J	-10	DT	C1'-O4'-C4'	-5.17	104.93	110.10
4	I	12	DT	C5-C4-O4	-5.17	121.28	124.90
5	J	-23	DC	C3'-C2'-C1'	-5.09	96.40	102.50
4	I	3	DC	N1-C1'-C2'	5.08	122.26	112.60
4	I	13	DC	N1-C2-O2	5.06	121.94	118.90
5	J	-2	DA	O4'-C1'-N9	-5.02	104.49	108.00

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	530	0	549	34	0
2	B	745	0	747	20	0
3	C	653	0	686	23	0
4	I	505	0	283	10	0
5	J	514	0	283	10	0
6	B	1	0	0	0	0
6	I	1	0	0	0	0
All	All	2949	0	2548	84	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 15.

All (84) 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:42:GLU:HA	3:C:42:GLU:OE1	1.47	1.08
1:A:259:GLU:CG	1:A:260:GLY:H	1.72	1.02
1:A:259:GLU:HG3	1:A:260:GLY:H	1.31	0.92
1:A:259:GLU:HG3	1:A:260:GLY:N	1.85	0.92
1:A:261:LYS:HG2	2:B:50:PHE:N	1.99	0.78
3:C:58:VAL:O	3:C:58:VAL:HG12	1.83	0.76
3:C:42:GLU:OE1	3:C:42:GLU:CA	2.30	0.74
1:A:274:ARG:HB3	5:J:-10:DT:H5'	1.70	0.73
1:A:243:TYR:C	1:A:243:TYR:HD1	1.93	0.71
2:B:129:VAL:O	2:B:133:LYS:HG3	1.90	0.70
1:A:259:GLU:HG2	1:A:260:GLY:H	1.56	0.68
1:A:232:MET:HB3	1:A:250:ARG:HH22	1.56	0.68
1:A:234:GLU:HG2	1:A:235:PRO:HD2	1.76	0.67
1:A:243:TYR:C	1:A:243:TYR:CD1	2.67	0.67
3:C:44:PRO:HB3	4:I:16:DC:H5"	1.78	0.65
1:A:289:PHE:O	1:A:290:PHE:CB	2.43	0.65
4:I:19:DG:H1	5:J:-19:DC:H42	1.45	0.64
1:A:281:ARG:NH2	4:I:11:DA:H5'	2.14	0.63
5:J:-23:DC:H2'	5:J:-23:DC:OP2	2.01	0.60
3:C:115:ILE:HD12	3:C:116:ASP:H	1.66	0.60
1:A:237:TYR:O	1:A:237:TYR:CD1	2.56	0.59
3:C:115:ILE:HD12	3:C:116:ASP:N	2.19	0.58
1:A:237:TYR:O	1:A:237:TYR:HD1	1.87	0.57
1:A:232:MET:HB3	1:A:250:ARG:NH2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:ILE:O	3:C:52:MET:HG3	2.04	0.57
1:A:261:LYS:CG	2:B:50:PHE:N	2.68	0.56
3:C:40:VAL:HG13	3:C:41:GLN:N	2.20	0.56
2:B:136:LEU:O	2:B:136:LEU:HG	2.05	0.56
2:B:112:ASN:O	2:B:115:ASP:HB2	2.06	0.55
2:B:70:ILE:HB	2:B:71:PRO:HD2	1.89	0.55
1:A:283:ARG:HA	1:A:289:PHE:O	2.06	0.55
1:A:289:PHE:O	1:A:290:PHE:HB3	2.05	0.55
2:B:113:GLY:O	2:B:117:LEU:HD12	2.07	0.54
4:I:19:DG:H2'	4:I:20:DC:H6	1.73	0.54
5:J:-24:DT:H6	5:J:-24:DT:OP2	1.90	0.54
5:J:-19:DC:H2"	5:J:-18:DT:H5'	1.90	0.53
3:C:105:ILE:HD13	3:C:118:VAL:HG21	1.91	0.52
2:B:137:GLN:OE1	2:B:137:GLN:HA	2.09	0.52
3:C:65:ALA:HB3	3:C:66:PRO:HD3	1.92	0.52
1:A:232:MET:O	1:A:233:GLU:HB2	2.09	0.52
3:C:72:ALA:HA	3:C:75:ILE:HD12	1.92	0.52
2:B:112:ASN:OD1	2:B:112:ASN:C	2.47	0.51
1:A:257:GLU:HA	1:A:262:ILE:HD11	1.92	0.51
1:A:274:ARG:NH2	4:I:13:DC:O2	2.45	0.50
2:B:102:ARG:O	2:B:106:GLU:HG2	2.12	0.50
4:I:15:DC:H2"	4:I:16:DC:C6	2.47	0.49
1:A:259:GLU:O	1:A:260:GLY:O	2.30	0.49
3:C:47:ARG:O	3:C:51:ILE:HG13	2.12	0.48
3:C:93:ARG:NH1	3:C:97:GLN:HG3	2.27	0.48
4:I:19:DG:H2'	4:I:20:DC:C6	2.47	0.48
1:A:248:LYS:O	1:A:251:GLN:HB2	2.13	0.48
3:C:55:ASP:HB3	3:C:58:VAL:HG23	1.96	0.48
1:A:255:LYS:HE3	1:A:259:GLU:OE1	2.14	0.47
5:J:-19:DC:C2'	5:J:-18:DT:H5'	2.45	0.46
2:B:129:VAL:O	2:B:133:LYS:CG	2.61	0.46
1:A:245:ARG:O	1:A:246:ILE:C	2.54	0.46
2:B:133:LYS:O	2:B:136:LEU:HB3	2.16	0.46
2:B:83:CYS:SG	3:C:118:VAL:HG11	2.56	0.45
1:A:234:GLU:CG	1:A:235:PRO:HD2	2.46	0.45
1:A:255:LYS:HA	1:A:255:LYS:HD2	1.85	0.45
3:C:60:MET:HG2	5:J:-21:DA:H5'	1.98	0.45
5:J:-22:DG:H2"	5:J:-21:DA:C8	2.53	0.44
1:A:284:GLY:N	1:A:289:PHE:O	2.51	0.43
3:C:44:PRO:HB3	4:I:16:DC:C5'	2.45	0.43
3:C:117:ILE:HG22	3:C:118:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:LEU:HD22	2:B:133:LYS:HE3	2.01	0.43
1:A:243:TYR:HA	1:A:246:ILE:HD12	1.99	0.43
2:B:69:ALA:HB3	3:C:81:THR:HG21	1.99	0.43
3:C:114:LEU:O	3:C:117:ILE:HB	2.19	0.42
3:C:74:GLN:HE21	3:C:74:GLN:HB2	1.56	0.42
2:B:110:THR:HG21	5:J:-22:DG:H5"	2.02	0.42
1:A:277:HIS:O	1:A:281:ARG:HG3	2.19	0.42
1:A:293:LYS:HE2	1:A:293:LYS:H	1.84	0.42
4:I:18:DA:H1'	4:I:19:DG:H5"	2.02	0.41
2:B:126:ASP:OD1	2:B:126:ASP:N	2.53	0.41
2:B:70:ILE:HB	2:B:71:PRO:CD	2.50	0.41
2:B:130:GLU:HA	2:B:133:LYS:HG3	2.02	0.41
2:B:53:GLN:NE2	2:B:53:GLN:H	2.19	0.41
1:A:235:PRO:HB2	1:A:236:LEU:H	1.63	0.41
1:A:270:LEU:HB2	5:J:-10:DT:OP2	2.21	0.41
3:C:41:GLN:O	3:C:42:GLU:HB2	2.20	0.41
4:I:15:DC:H2"	4:I:16:DC:OP2	2.21	0.41
3:C:43:LEU:HD23	3:C:44:PRO:HD2	2.04	0.40
1:A:238:VAL:O	1:A:239:ASN:C	2.60	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	60/78 (77%)	47 (78%)	11 (18%)	2 (3%)	4 19
2	B	90/94 (96%)	83 (92%)	6 (7%)	1 (1%)	14 44
3	C	78/94 (83%)	74 (95%)	4 (5%)	0	100 100
All	All	228/266 (86%)	204 (90%)	21 (9%)	3 (1%)	12 40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	GLY
1	A	235	PRO
2	B	139	PHE

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	52/67 (78%)	35 (67%)	17 (33%)	0 0
2	B	82/84 (98%)	70 (85%)	12 (15%)	3 13
3	C	71/85 (84%)	62 (87%)	9 (13%)	4 17
All	All	205/236 (87%)	167 (82%)	38 (18%)	1 6

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	MET
1	A	236	LEU
1	A	243	TYR
1	A	247	LEU
1	A	249	ARG
1	A	257	GLU
1	A	261	LYS
1	A	262	ILE
1	A	266	ARG
1	A	267	ARG
1	A	268	LYS
1	A	270	LEU
1	A	274	ARG
1	A	285	GLU
1	A	290	PHE
1	A	291	SER
1	A	293	LYS
2	B	51	ARG
2	B	53	GLN
2	B	55	ILE

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Mol	Chain	Res	Type
2	B	64	ARG
2	B	67	LYS
2	B	79	ASP
2	B	101	GLU
2	B	105	GLN
2	B	133	LYS
2	B	134	LEU
2	B	137	GLN
2	B	139	PHE
3	C	41	GLN
3	C	42	GLU
3	C	47	ARG
3	C	56	GLU
3	C	74	GLN
3	C	90	ASP
3	C	96	LEU
3	C	97	GLN
3	C	105	ILE

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

Mol	Chain	Res	Type
2	B	53	GLN
3	C	74	GLN
3	C	87	HIS
3	C	91	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	62/78 (79%)	-0.02	1 (1%)	72	51	55, 85, 123, 132	0
2	B	92/94 (97%)	-0.28	1 (1%)	80	62	39, 78, 132, 171	0
3	C	80/94 (85%)	-0.34	0	100	100	40, 74, 105, 123	0
4	I	25/25 (100%)	-0.60	0	100	100	54, 72, 108, 116	0
5	J	25/25 (100%)	-0.53	0	100	100	48, 68, 90, 91	0
All	All	284/316 (89%)	-0.29	2 (0%)	87	74	39, 77, 123, 171	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	141	GLU	2.8
1	A	285	GLU	2.1

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 monosaccharides 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.