



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:30 am BST

PDB ID : 5GNJ
Title : Structure of a transcription factor and DNA complex
Authors : Lian, T.; Xu, Y.; Su, X.
Deposited on : 2016-07-21
Resolution : 2.70 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

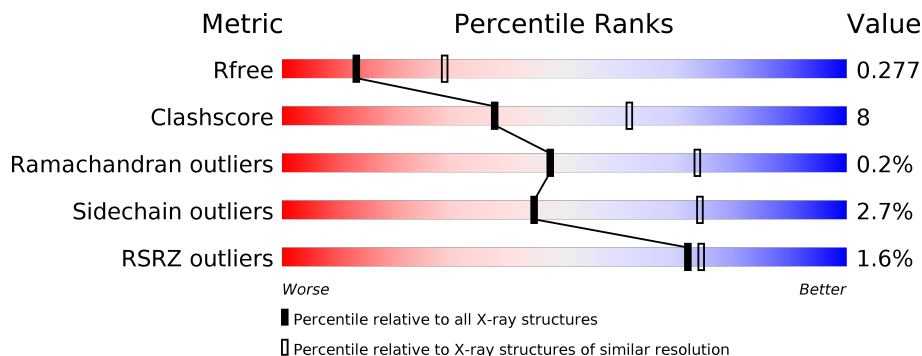
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. 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	89	 72% 10% 17%
1	B	89	 64% 21% 13%
1	E	89	 62% 18% 18%
1	F	89	 72% 10% 18%
1	G	89	 72% 10% 18%
1	I	89	 73% 11% 16%

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Mol	Chain	Length	Quality of chain
1	M	89	
1	N	89	
2	C	15	
2	H	15	
2	K	15	
2	O	15	
3	D	15	
3	J	15	
3	L	15	
3	P	15	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6894 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 Transcription factor MYC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	73	Total 570	C 357	N 105	O 107	S 1	0	0	0
1	I	75	Total 587	C 371	N 108	O 107	S 1	0	0	0
1	A	74	Total 585	C 365	N 107	O 112	S 1	0	0	0
1	B	77	Total 607	C 382	N 110	O 114	S 1	0	0	0
1	E	73	Total 568	C 357	N 106	O 105		0	0	0
1	F	73	Total 571	C 360	N 106	O 104	S 1	0	0	0
1	M	73	Total 570	C 358	N 103	O 108	S 1	0	0	0
1	N	73	Total 584	C 365	N 107	O 111	S 1	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	445	MET	-	expression tag	UNP Q39204
G	526	LEU	-	expression tag	UNP Q39204
G	527	GLU	-	expression tag	UNP Q39204
G	528	HIS	-	expression tag	UNP Q39204
G	529	HIS	-	expression tag	UNP Q39204
G	530	HIS	-	expression tag	UNP Q39204
G	531	HIS	-	expression tag	UNP Q39204
G	532	HIS	-	expression tag	UNP Q39204
G	533	HIS	-	expression tag	UNP Q39204
I	445	MET	-	expression tag	UNP Q39204
I	526	LEU	-	expression tag	UNP Q39204
I	527	GLU	-	expression tag	UNP Q39204
I	528	HIS	-	expression tag	UNP Q39204

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Chain	Residue	Modelled	Actual	Comment	Reference
I	529	HIS	-	expression tag	UNP Q39204
I	530	HIS	-	expression tag	UNP Q39204
I	531	HIS	-	expression tag	UNP Q39204
I	532	HIS	-	expression tag	UNP Q39204
I	533	HIS	-	expression tag	UNP Q39204
A	445	MET	-	expression tag	UNP Q39204
A	526	LEU	-	expression tag	UNP Q39204
A	527	GLU	-	expression tag	UNP Q39204
A	528	HIS	-	expression tag	UNP Q39204
A	529	HIS	-	expression tag	UNP Q39204
A	530	HIS	-	expression tag	UNP Q39204
A	531	HIS	-	expression tag	UNP Q39204
A	532	HIS	-	expression tag	UNP Q39204
A	533	HIS	-	expression tag	UNP Q39204
B	445	MET	-	expression tag	UNP Q39204
B	526	LEU	-	expression tag	UNP Q39204
B	527	GLU	-	expression tag	UNP Q39204
B	528	HIS	-	expression tag	UNP Q39204
B	529	HIS	-	expression tag	UNP Q39204
B	530	HIS	-	expression tag	UNP Q39204
B	531	HIS	-	expression tag	UNP Q39204
B	532	HIS	-	expression tag	UNP Q39204
B	533	HIS	-	expression tag	UNP Q39204
E	445	MET	-	expression tag	UNP Q39204
E	526	LEU	-	expression tag	UNP Q39204
E	527	GLU	-	expression tag	UNP Q39204
E	528	HIS	-	expression tag	UNP Q39204
E	529	HIS	-	expression tag	UNP Q39204
E	530	HIS	-	expression tag	UNP Q39204
E	531	HIS	-	expression tag	UNP Q39204
E	532	HIS	-	expression tag	UNP Q39204
E	533	HIS	-	expression tag	UNP Q39204
F	445	MET	-	expression tag	UNP Q39204
F	526	LEU	-	expression tag	UNP Q39204
F	527	GLU	-	expression tag	UNP Q39204
F	528	HIS	-	expression tag	UNP Q39204
F	529	HIS	-	expression tag	UNP Q39204
F	530	HIS	-	expression tag	UNP Q39204
F	531	HIS	-	expression tag	UNP Q39204
F	532	HIS	-	expression tag	UNP Q39204
F	533	HIS	-	expression tag	UNP Q39204
M	445	MET	-	expression tag	UNP Q39204

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Chain	Residue	Modelled	Actual	Comment	Reference
M	526	LEU	-	expression tag	UNP Q39204
M	527	GLU	-	expression tag	UNP Q39204
M	528	HIS	-	expression tag	UNP Q39204
M	529	HIS	-	expression tag	UNP Q39204
M	530	HIS	-	expression tag	UNP Q39204
M	531	HIS	-	expression tag	UNP Q39204
M	532	HIS	-	expression tag	UNP Q39204
M	533	HIS	-	expression tag	UNP Q39204
N	445	MET	-	expression tag	UNP Q39204
N	526	LEU	-	expression tag	UNP Q39204
N	527	GLU	-	expression tag	UNP Q39204
N	528	HIS	-	expression tag	UNP Q39204
N	529	HIS	-	expression tag	UNP Q39204
N	530	HIS	-	expression tag	UNP Q39204
N	531	HIS	-	expression tag	UNP Q39204
N	532	HIS	-	expression tag	UNP Q39204
N	533	HIS	-	expression tag	UNP Q39204

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	K	14	Total 285	C 136	N 59	O 77	P 13	0	0	0
2	C	14	Total 285	C 136	N 59	O 77	P 13	0	0	0
2	H	14	Total 285	C 136	N 59	O 77	P 13	0	0	0
2	O	13	Total 268	C 126	N 54	O 75	P 13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	L	14	Total 282	C 134	N 50	O 85	P 13	0	0	0
3	D	14	Total 282	C 134	N 50	O 85	P 13	0	0	0
3	J	13	Total 263	C 124	N 45	O 81	P 13	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	12	Total	C	N	O	P	0	0	0
			240	115	42	72	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	5	Total	O	0	0
			5	5		
4	I	9	Total	O	0	0
			9	9		
4	K	6	Total	O	0	0
			6	6		
4	L	5	Total	O	0	0
			5	5		
4	A	8	Total	O	0	0
			8	8		
4	B	4	Total	O	0	0
			4	4		
4	C	2	Total	O	0	0
			2	2		
4	D	5	Total	O	0	0
			5	5		
4	E	3	Total	O	0	0
			3	3		
4	F	2	Total	O	0	0
			2	2		
4	H	3	Total	O	0	0
			3	3		
4	J	5	Total	O	0	0
			5	5		
4	M	2	Total	O	0	0
			2	2		
4	N	1	Total	O	0	0
			1	1		
4	O	1	Total	O	0	0
			1	1		
4	P	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 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: Transcription factor MYC2

Chain G: 



- Molecule 1: Transcription factor MYC2

Chain I: 



- Molecule 1: Transcription factor MYC2

Chain A: 



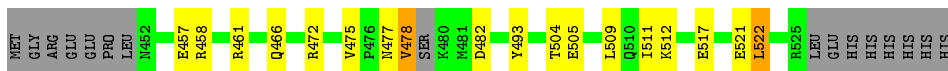
- Molecule 1: Transcription factor MYC2

Chain B: 



- Molecule 1: Transcription factor MYC2

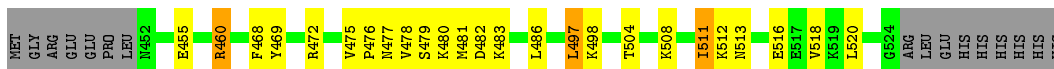
Chain E: 



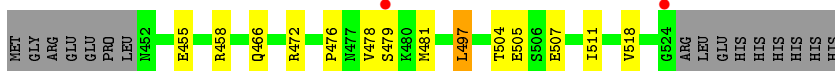
- Molecule 1: Transcription factor MYC2



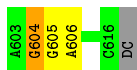
- Molecule 1: Transcription factor MYC2



- Molecule 1: Transcription factor MYC2



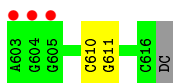
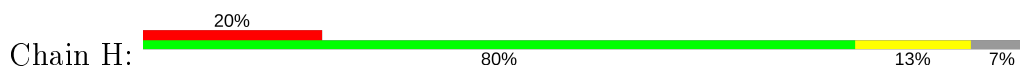
- Molecule 2: DNA (5'-D(*AP*GP*GP*AP*AP*CP*AP*CP*GP*TP*GP*AP*CP*CP*C)-3')



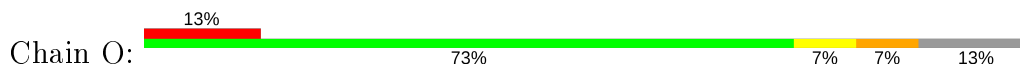
- Molecule 2: DNA (5'-D(*AP*GP*GP*AP*AP*CP*AP*CP*GP*TP*GP*AP*CP*CP*C)-3')

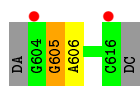


- Molecule 2: DNA (5'-D(*AP*GP*GP*AP*AP*CP*AP*CP*GP*TP*GP*AP*CP*CP*C)-3')



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





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

Chain L: 93% 7%



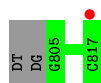
- Molecule 3: DNA (5'-D(*TP*GP*GP*GP*TP*CP*AP*CP*GP*TP*GP*TP*TP*CP*C)-3')

Chain D: 80% 13% 7%



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

Chain J: 7% 87% 13%



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

Chain P: 67% 13% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.10Å 79.70Å 102.80Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	49.65 – 2.70 49.65 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.65-2.70) 95.7 (49.65-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.206 , 0.273 0.217 , 0.277	Depositor DCC
R_{free} test set	1613 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	63.9	Xtrriage
Anisotropy	0.279	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6894	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.54	0/589	0.74	1/790 (0.1%)
1	B	0.61	0/612	0.79	1/821 (0.1%)
1	E	0.55	0/571	0.72	0/765
1	F	0.54	0/575	0.77	0/770
1	G	0.49	0/574	0.71	0/771
1	I	0.56	0/592	0.79	1/796 (0.1%)
1	M	0.51	0/574	0.81	1/770 (0.1%)
1	N	0.55	0/588	0.85	0/787
2	C	1.00	1/321 (0.3%)	0.95	0/494
2	H	0.85	0/321	0.91	0/494
2	K	1.17	1/321 (0.3%)	1.02	0/494
2	O	0.73	0/301	0.88	1/462 (0.2%)
3	D	1.01	1/315 (0.3%)	0.96	0/484
3	J	0.94	0/293	1.04	0/449
3	L	1.04	0/315	1.00	0/484
3	P	0.83	0/268	1.01	1/412 (0.2%)
All	All	0.71	3/7130 (0.0%)	0.85	6/10043 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	604	DG	C3'-O3'	-8.31	1.33	1.44
2	C	604	DG	C3'-O3'	-5.92	1.36	1.44
3	D	815	DT	C1'-N1	5.03	1.55	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	480	LYS	N-CA-C	-6.69	92.94	111.00
1	M	477	ASN	N-CA-C	5.86	126.82	111.00
1	A	464	LEU	CA-CB-CG	5.47	127.88	115.30
3	P	814	DT	N3-C4-O4	5.30	123.08	119.90
2	O	605	DG	O4'-C1'-N9	5.17	111.62	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	MET	N-CA-C	5.01	124.53	111.00

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	585	0	598	8	0
1	B	607	0	627	13	0
1	E	568	0	582	18	0
1	F	571	0	595	12	0
1	G	570	0	581	7	0
1	I	587	0	607	8	0
1	M	570	0	586	34	0
1	N	584	0	607	13	0
2	C	285	0	154	2	0
2	H	285	0	154	2	0
2	K	285	0	154	2	0
2	O	268	0	145	1	0
3	D	282	0	154	1	0
3	J	263	0	142	0	0
3	L	282	0	154	0	0
3	P	240	0	129	2	0
4	A	8	0	0	1	0
4	B	4	0	0	0	0
4	C	2	0	0	0	0
4	D	5	0	0	1	0
4	E	3	0	0	1	0
4	F	2	0	0	0	0
4	G	5	0	0	0	0
4	H	3	0	0	0	0
4	I	9	0	0	0	0
4	J	5	0	0	0	0
4	K	6	0	0	0	0
4	L	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	2	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
All	All	6894	0	5969	95	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 8.

All (95) 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:M:478:VAL:HG21	1:M:481:MET:CE	1.59	1.30
1:M:478:VAL:HG21	1:M:481:MET:HE3	1.26	1.10
1:M:478:VAL:CG2	1:M:481:MET:CE	2.38	1.01
1:E:522:LEU:HD12	1:F:522:LEU:HD13	1.47	0.97
1:M:460:ARG:HH21	1:M:460:ARG:HG3	1.36	0.91
1:M:478:VAL:HG21	1:M:481:MET:SD	2.15	0.86
1:E:457:GLU:OE1	4:E:601:HOH:O	2.00	0.79
1:E:522:LEU:CD1	1:F:522:LEU:HD13	2.15	0.77
1:M:478:VAL:CG2	1:M:481:MET:HE2	2.17	0.75
1:M:512:LYS:HG3	1:N:511:ILE:HD12	1.71	0.72
1:M:478:VAL:CG2	1:M:481:MET:SD	2.78	0.70
1:M:460:ARG:NH2	1:M:460:ARG:HG3	2.00	0.69
3:D:811:DG:O6	4:D:901:HOH:O	2.09	0.69
1:I:513:ASN:OD1	1:M:513:ASN:ND2	2.27	0.67
1:E:461:ARG:NH1	2:H:610:DC:OP2	2.28	0.66
1:M:478:VAL:CG2	1:M:481:MET:HE3	2.14	0.65
1:E:477:ASN:O	1:E:478:VAL:HG12	1.97	0.64
1:M:497:LEU:HB3	1:N:497:LEU:HD22	1.79	0.64
1:E:511:ILE:HG22	1:F:511:ILE:HG22	1.82	0.60
1:M:478:VAL:HG22	1:M:478:VAL:O	2.02	0.58
1:M:478:VAL:HG22	1:M:481:MET:HG3	1.84	0.58
1:A:461:ARG:NH1	4:A:601:HOH:O	2.24	0.57
1:M:498:LYS:HG2	1:N:497:LEU:HD11	1.85	0.57
1:N:479:SER:HB3	1:N:481:MET:HB2	1.87	0.56
1:F:478:VAL:HG13	1:F:481:MET:SD	2.47	0.55
1:F:455:GLU:OE2	1:F:458:ARG:NH1	2.40	0.54
1:N:478:VAL:HB	1:N:479:SER:OG	2.07	0.54
1:G:452:ASN:N	1:G:456:ALA:H	2.05	0.53
1:M:472:ARG:HH21	1:M:486:LEU:HD22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:603:DA:H2''	2:C:604:DG:O5'	2.08	0.53
1:G:504:THR:HG22	1:I:504:THR:HG22	1.89	0.53
1:N:479:SER:HB3	1:N:481:MET:N	2.23	0.52
1:G:482:ASP:OD1	1:G:483:LYS:N	2.42	0.52
2:K:605:DG:H2''	2:K:606:DA:H5'	1.91	0.51
1:E:504:THR:CG2	1:F:505:GLU:HG3	2.41	0.50
1:M:460:ARG:HH22	3:P:807:DT:H2'	1.77	0.50
1:B:520:LEU:O	1:B:523:ALA:HB3	2.12	0.49
1:E:482:ASP:OD1	1:E:482:ASP:N	2.44	0.49
1:M:518:VAL:HG12	1:N:518:VAL:HG12	1.95	0.49
1:A:459:GLN:HA	1:A:459:GLN:OE1	2.11	0.48
1:E:504:THR:HG21	1:F:505:GLU:HG3	1.95	0.48
1:G:511:ILE:HG22	1:I:511:ILE:HG22	1.94	0.48
2:O:605:DG:H2''	2:O:606:DA:OP2	2.13	0.48
1:M:469:TYR:O	1:M:472:ARG:HG2	2.15	0.47
1:N:504:THR:O	1:N:507:GLU:HG2	2.15	0.47
1:B:475:VAL:HA	1:B:476:PRO:HD3	1.76	0.46
1:M:482:ASP:OD1	1:M:483:LYS:N	2.49	0.45
1:M:511:ILE:CG2	1:N:511:ILE:HG13	2.47	0.45
1:A:493:TYR:O	1:A:497:LEU:HB2	2.16	0.45
1:M:455:GLU:HG3	1:M:455:GLU:H	1.49	0.45
1:A:487:LEU:HD22	1:B:471:LEU:HD22	1.99	0.45
1:B:449:GLU:HA	1:B:450:PRO:HD3	1.78	0.44
1:B:463:LYS:HB2	1:B:463:LYS:HE2	1.88	0.44
1:E:504:THR:HG22	1:F:504:THR:HG22	2.00	0.44
1:I:520:LEU:HD13	1:M:520:LEU:HG	1.98	0.44
1:M:504:THR:HG21	1:N:505:GLU:HG3	1.99	0.44
1:E:493:TYR:OH	1:F:498:LYS:HE2	2.18	0.44
1:M:460:ARG:HH21	1:M:460:ARG:CG	2.13	0.43
1:M:468:PHE:CD2	1:M:483:LYS:HE2	2.52	0.43
1:E:472:ARG:HH12	1:E:478:VAL:HG13	1.83	0.43
1:A:497:LEU:HB3	1:B:497:LEU:HD22	2.00	0.43
1:E:509:LEU:HA	1:E:509:LEU:HD23	1.72	0.43
1:B:524:GLY:HA2	1:B:525:ARG:HA	1.72	0.43
1:B:512:LYS:HE2	1:B:512:LYS:HB2	1.77	0.42
1:I:463:LYS:HE2	1:I:463:LYS:HB2	1.80	0.42
1:M:460:ARG:HH22	3:P:807:DT:C2'	2.31	0.42
1:M:478:VAL:HG13	1:M:478:VAL:O	2.18	0.42
1:A:472:ARG:HG3	1:A:478:VAL:HG23	2.01	0.42
1:E:511:ILE:CG2	1:F:511:ILE:HG22	2.48	0.42
1:B:469:TYR:O	1:B:472:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:604:DG:H2''	2:K:605:DG:C8	2.54	0.42
2:C:614:DA:H2''	2:C:615:DC:C6	2.54	0.42
1:B:503:LYS:HE3	1:B:503:LYS:HB3	1.91	0.42
1:I:516:GLU:HG2	1:M:516:GLU:HB3	2.01	0.42
1:A:501:VAL:HG23	1:B:501:VAL:HG23	2.00	0.42
1:M:475:VAL:HA	1:M:476:PRO:HD3	1.89	0.41
1:M:508:LYS:HE2	1:M:512:LYS:NZ	2.35	0.41
1:E:458:ARG:HG2	1:E:461:ARG:HH12	1.86	0.41
1:E:458:ARG:NH2	2:H:611:DG:OP1	2.53	0.41
1:I:522:LEU:HA	1:I:522:LEU:HD12	1.93	0.41
1:N:455:GLU:OE2	1:N:458:ARG:NH1	2.43	0.41
1:B:471:LEU:O	1:B:474:VAL:HG12	2.21	0.41
1:G:478:VAL:HG23	1:G:478:VAL:O	2.20	0.41
1:F:478:VAL:O	1:F:478:VAL:HG12	2.20	0.41
1:E:512:LYS:HE2	1:F:511:ILE:HD13	2.03	0.41
1:I:468:PHE:HD1	1:I:486:LEU:HD23	1.84	0.41
1:E:517:GLU:O	1:E:521:GLU:HG3	2.21	0.41
1:N:472:ARG:NH1	1:N:479:SER:HB2	2.36	0.41
1:A:504:THR:HG22	1:B:504:THR:HG22	2.02	0.40
1:M:478:VAL:HG22	1:M:481:MET:SD	2.60	0.40
1:M:478:VAL:HG22	1:M:481:MET:CG	2.50	0.40
1:N:472:ARG:HH11	1:N:479:SER:HB2	1.86	0.40
1:G:487:LEU:HA	1:G:487:LEU:HD23	1.90	0.40
1:G:464:LEU:HA	1:G:464:LEU:HD12	1.83	0.40
1:M:479:SER:O	1:M:480:LYS:CB	2.70	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	72/89 (81%)	72 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	75/89 (84%)	73 (97%)	2 (3%)	0	100	100
1	E	69/89 (78%)	68 (99%)	1 (1%)	0	100	100
1	F	71/89 (80%)	67 (94%)	4 (6%)	0	100	100
1	G	71/89 (80%)	70 (99%)	1 (1%)	0	100	100
1	I	73/89 (82%)	71 (97%)	2 (3%)	0	100	100
1	M	71/89 (80%)	68 (96%)	3 (4%)	0	100	100
1	N	71/89 (80%)	68 (96%)	2 (3%)	1 (1%)	11	28
All	All	573/712 (80%)	557 (97%)	15 (3%)	1 (0%)	47	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	476	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	62/79 (78%)	61 (98%)	1 (2%)	62	85
1	B	64/79 (81%)	62 (97%)	2 (3%)	40	69
1	E	58/79 (73%)	53 (91%)	5 (9%)	10	24
1	F	59/79 (75%)	59 (100%)	0	100	100
1	G	59/79 (75%)	59 (100%)	0	100	100
1	I	61/79 (77%)	61 (100%)	0	100	100
1	M	60/79 (76%)	57 (95%)	3 (5%)	24	51
1	N	63/79 (80%)	61 (97%)	2 (3%)	39	68
All	All	486/632 (77%)	473 (97%)	13 (3%)	44	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	459	GLN
1	B	497	LEU
1	B	513	ASN
1	E	466	GLN
1	E	475	VAL
1	E	478	VAL
1	E	505	GLU
1	E	522	LEU
1	M	460	ARG
1	M	497	LEU
1	M	511	ILE
1	N	466	GLN
1	N	497	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	510	GLN
1	M	513	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 carbohydrates 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

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	74/89 (83%)	-0.12	1 (1%) 75 77	30, 62, 96, 141	0
1	B	77/89 (86%)	-0.22	0 100 100	43, 63, 107, 122	0
1	E	73/89 (82%)	-0.19	0 100 100	49, 65, 103, 134	0
1	F	73/89 (82%)	-0.22	1 (1%) 75 77	53, 69, 103, 132	0
1	G	73/89 (82%)	-0.20	0 100 100	44, 62, 89, 101	0
1	I	75/89 (84%)	-0.16	1 (1%) 77 78	46, 62, 99, 135	0
1	M	73/89 (82%)	-0.01	0 100 100	46, 69, 121, 142	0
1	N	73/89 (82%)	-0.00	2 (2%) 54 55	30, 71, 110, 137	0
2	C	14/15 (93%)	-0.07	0 100 100	60, 73, 153, 191	0
2	H	14/15 (93%)	0.76	3 (21%) 0 0	76, 97, 172, 232	0
2	K	14/15 (93%)	0.10	0 100 100	53, 71, 114, 145	0
2	O	13/15 (86%)	0.40	2 (15%) 2 1	84, 112, 199, 221	0
3	D	14/15 (93%)	-0.22	0 100 100	59, 76, 131, 158	0
3	J	13/15 (86%)	0.06	1 (7%) 13 11	64, 87, 162, 169	0
3	L	14/15 (93%)	-0.21	0 100 100	51, 71, 132, 151	0
3	P	12/15 (80%)	0.29	0 100 100	90, 110, 176, 190	0
All	All	699/832 (84%)	-0.10	11 (1%) 72 74	30, 68, 125, 232	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	603	DA	5.5
2	O	604	DG	4.9
1	A	452	ASN	3.4
1	N	524	GLY	3.3
1	F	478	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	604	DG	2.6
1	N	479	SER	2.4
2	H	605	DG	2.4
2	O	616	DC	2.2
1	I	523	ALA	2.1
3	J	817	DC	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 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.