



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:44 AM UTC

PDB ID : 5GNJ / pdb_00005gnj
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 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:

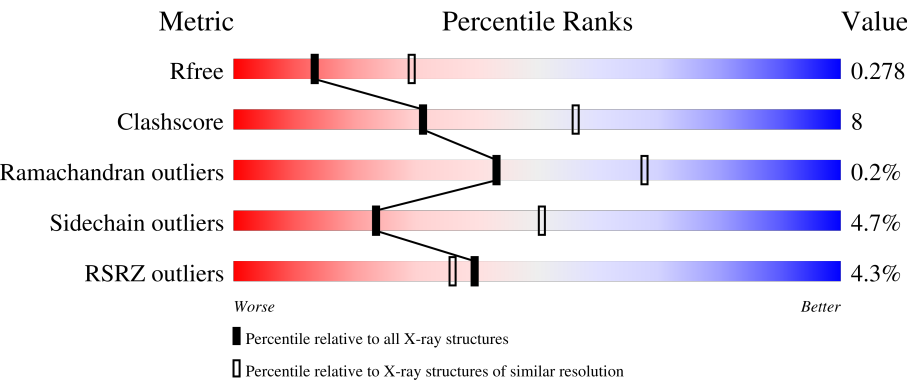
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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 $\leq 5\%$. 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	4% 71% 10% • 17%
1	B	89	4% 61% 22% •• 13%
1	E	89	2% 60% 19% • 18%
1	F	89	% 70% 12% 18%
1	G	89	% 69% 13% 18%

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Mol	Chain	Length	Quality of chain
1	I	89	
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

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

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
2	K	14	Total	C	N	O	P	0	0	0
			285	136	59	77	13			
2	C	14	Total	C	N	O	P	0	0	0
			285	136	59	77	13			
2	H	14	Total	C	N	O	P	0	0	0
			285	136	59	77	13			
2	O	13	Total	C	N	O	P	0	0	0
			268	126	54	75	13			

- 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
3	L	14	Total	C	N	O	P	0	0	0
			282	134	50	85	13			
3	D	14	Total	C	N	O	P	0	0	0
			282	134	50	85	13			
3	J	13	Total	C	N	O	P	0	0	0
			263	124	45	81	13			

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

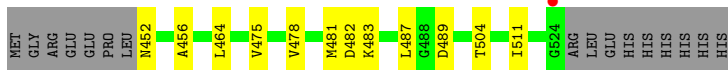
- Molecule 4 is water.

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

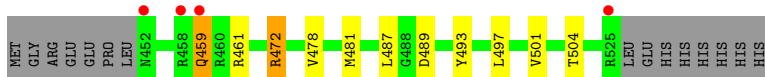
- Molecule 1: Transcription factor MYC2



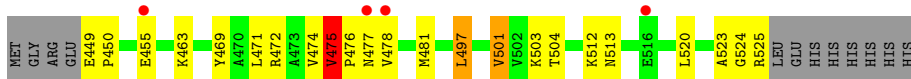
- Molecule 1: Transcription factor MYC2



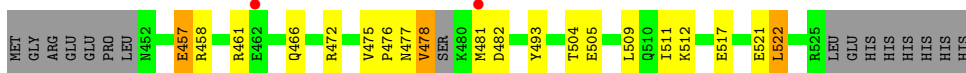
- Molecule 1: Transcription factor MYC2



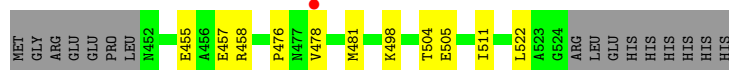
- Molecule 1: Transcription factor MYC2



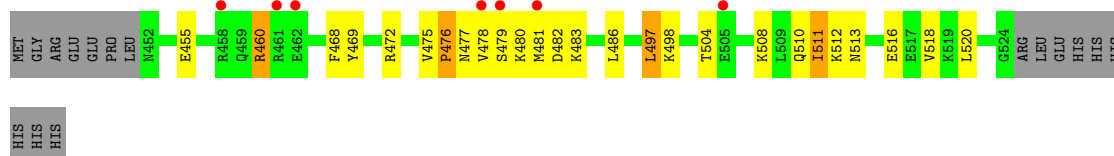
- Molecule 1: Transcription factor MYC2



- Molecule 1: Transcription factor MYC2



- Molecule 1: Transcription factor MYC2



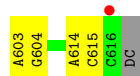
- Molecule 1: Transcription factor MYC2



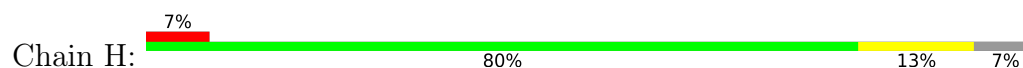
- Molecule 2: DNA (5'-D(*AP*GP*GP*AP*AP*CP*AP*CP*GP*TP*GP*AP*CP*CP*C)-3')



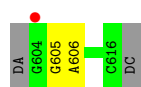
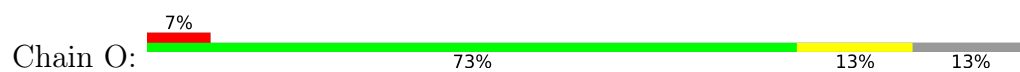
- Molecule 2: DNA (5'-D(*AP*GP*GP*AP*AP*CP*AP*CP*GP*TP*GP*AP*CP*CP*C)-3')



- 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')



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



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



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



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)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.206 , 0.273 0.220 , 0.278	Depositor DCC
R_{free} test set	1613 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	63.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 82.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.75	0/589	1.02	0/790
1	B	0.83	0/612	1.17	4/821 (0.5%)
1	E	0.75	0/571	1.09	2/765 (0.3%)
1	F	0.71	0/575	1.00	1/770 (0.1%)
1	G	0.70	0/574	1.03	1/771 (0.1%)
1	I	0.73	0/592	1.20	7/796 (0.9%)
1	M	0.70	0/574	1.18	2/770 (0.3%)
1	N	0.75	0/588	1.12	3/787 (0.4%)
2	C	0.45	0/321	0.64	0/494
2	H	0.35	0/321	0.59	0/494
2	K	0.55	0/321	0.74	0/494
2	O	0.29	0/301	0.50	0/462
3	D	0.44	0/315	0.55	0/484
3	J	0.39	0/293	0.59	0/449
3	L	0.45	0/315	0.58	0/484
3	P	0.37	0/268	0.52	0/412
All	All	0.65	0/7130	0.95	20/10043 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	477	ASN	N-CA-C	11.45	126.82	109.41
1	B	481	MET	N-CA-C	10.35	124.53	112.93
1	I	480	LYS	N-CA-C	-10.13	92.94	109.96
1	I	477	ASN	N-CA-C	9.17	124.12	111.74
1	B	477	ASN	N-CA-C	7.32	121.56	111.90
1	F	476	PRO	N-CA-C	6.70	122.23	113.86
1	M	476	PRO	N-CA-C	6.14	121.54	113.86
1	I	451	LEU	N-CA-C	6.09	117.91	111.28
1	B	475	VAL	N-CA-C	5.86	114.96	108.05
1	I	474	VAL	CA-C-N	-5.76	118.44	122.59
1	I	474	VAL	C-N-CA	-5.76	118.44	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	478	VAL	N-CA-C	5.74	115.56	106.32
1	E	476	PRO	N-CA-C	5.65	119.13	111.22
1	N	477	ASN	N-CA-C	5.64	119.93	112.25
1	N	453	HIS	N-CA-C	-5.43	106.82	113.50
1	G	475	VAL	N-CA-C	5.39	114.41	108.05
1	E	481	MET	N-CA-C	5.17	117.20	110.43
1	N	476	PRO	N-CA-C	5.15	123.07	112.47
1	I	453	HIS	N-CA-C	-5.10	107.19	113.41
1	I	479	SER	N-CA-C	5.07	120.85	114.31

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	9	0
1	B	607	0	627	13	0
1	E	568	0	582	18	0
1	F	571	0	595	13	0
1	G	570	0	581	8	0
1	I	587	0	607	8	0
1	M	570	0	586	34	0
1	N	584	0	607	16	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	101	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 (101) 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:CG2	1:M:481:MET:HE3	1.63	1.27
1:M:478:VAL:HG21	1:M:481:MET:HE3	1.14	1.05
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:M:478:VAL:CG2	1:M:481:MET:CE	2.38	0.81
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:HG23	1:M:481:MET:HE3	1.67	0.74
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:HG3	1:M:460:ARG:NH2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:481:MET:HE1	1:G:489:ASP:OD2	2.08	0.53
1:M:472:ARG:HH21	1:M:486:LEU:HD22	1.73	0.53
1:G:504:THR:HG22	1:I:504:THR:HG22	1.89	0.53
2:C:603:DA:H2''	2:C:604:DG:O5'	2.08	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:A:481:MET:HE1	1:A:489:ASP:OD2	2.11	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:OE1	1:A:459:GLN:HA	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:N:522:LEU:C	1:N:524:GLY:H	2.24	0.45
1:A:493:TYR:O	1:A:497:LEU:HB2	2.16	0.45
1:M:455:GLU:H	1:M:455:GLU:HG3	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:N:481:MET:HE3	1:N:485:SER:HB3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:E:509:LEU:HA	1.72	0.43
1:B:524:GLY:HA2	1:B:525:ARG:HA	1.72	0.43
1:I:463:LYS:HB2	1:I:463:LYS:HE2	1.80	0.42
1:B:512:LYS:HE2	1:B:512:LYS:HB2	1.77	0.42
1:M:460:ARG:HH22	3:P:807:DT:C2'	2.31	0.42
1:M:478:VAL:O	1:M:478:VAL:HG13	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
2:K:604:DG:H2''	2:K:605:DG:C8	2.54	0.42
1:B:469:TYR:O	1:B:472:ARG:HG2	2.20	0.42
2:C:614:DA:H2''	2:C:615:DC:C6	2.54	0.42
1:I:516:GLU:HG2	1:M:516:GLU:HB3	2.01	0.42
1:B:503:LYS:HE3	1:B:503:LYS:HB3	1.91	0.42
1:A:501:VAL:HG23	1:B:501:VAL:HG23	2.00	0.42
1:F:481:MET:HE2	1:F:481:MET:HB3	1.87	0.41
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:I:522:LEU:HD12	1:I:522:LEU:HA	1.93	0.41
1:E:458:ARG:NH2	2:H:611:DG:OP1	2.53	0.41
1:N:455:GLU:OE2	1:N:458:ARG:NH1	2.43	0.41
1:G:478:VAL:O	1:G:478:VAL:HG23	2.20	0.41
1:B:471:LEU:O	1:B:474:VAL:HG12	2.21	0.41
1:I:468:PHE:HD1	1:I:486:LEU:HD23	1.84	0.41
1:E:512:LYS:HE2	1:F:511:ILE:HD13	2.03	0.41
1:F:478:VAL:O	1:F:478:VAL:HG12	2.20	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:N:522:LEU:C	1:N:524:GLY:N	2.79	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

5.3.1 Protein backbone

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
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%)	9	23
All	All	573/712 (80%)	557 (97%)	15 (3%)	1 (0%)	43	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	476	PRO

5.3.2 Protein sidechains

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%)	60 (97%)	2 (3%)	34	64
1	B	64/79 (81%)	59 (92%)	5 (8%)	11	29
1	E	58/79 (73%)	52 (90%)	6 (10%)	7	18
1	F	59/79 (75%)	58 (98%)	1 (2%)	53	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	59/79 (75%)	59 (100%)	0	100	100
1	I	61/79 (77%)	58 (95%)	3 (5%)	22	49
1	M	60/79 (76%)	56 (93%)	4 (7%)	15	36
1	N	63/79 (80%)	61 (97%)	2 (3%)	34	64
All	All	486/632 (77%)	463 (95%)	23 (5%)	23	51

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	451	LEU
1	I	455	GLU
1	I	510	GLN
1	A	459	GLN
1	A	472	ARG
1	B	455	GLU
1	B	475	VAL
1	B	497	LEU
1	B	501	VAL
1	B	513	ASN
1	E	457	GLU
1	E	466	GLN
1	E	475	VAL
1	E	478	VAL
1	E	505	GLU
1	E	522	LEU
1	F	457	GLU
1	M	460	ARG
1	M	497	LEU
1	M	510	GLN
1	M	511	ILE
1	N	466	GLN
1	N	497	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	453	HIS
1	I	510	GLN
1	A	514	GLN
1	B	466	GLN

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Mol	Chain	Res	Type
1	F	459	GLN
1	F	466	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 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, 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%)	0.16	4 (5%) 31 27	30, 62, 96, 141	0
1	B	77/89 (86%)	0.19	4 (5%) 33 29	43, 63, 107, 122	0
1	E	73/89 (82%)	0.22	2 (2%) 56 53	49, 65, 103, 134	0
1	F	73/89 (82%)	0.27	1 (1%) 73 72	53, 69, 103, 132	0
1	G	73/89 (82%)	-0.05	1 (1%) 73 72	44, 62, 89, 101	0
1	I	75/89 (84%)	0.05	2 (2%) 56 53	46, 62, 99, 135	0
1	M	73/89 (82%)	0.41	7 (9%) 13 11	46, 69, 121, 142	0
1	N	73/89 (82%)	0.38	5 (6%) 23 20	30, 71, 110, 137	0
2	C	14/15 (93%)	0.24	1 (7%) 22 19	60, 73, 153, 191	0
2	H	14/15 (93%)	0.65	1 (7%) 22 19	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%)	0.92	1 (7%) 19 17	84, 112, 199, 220	0
3	D	14/15 (93%)	0.11	0 100 100	59, 76, 131, 158	0
3	J	13/15 (86%)	0.37	0 100 100	64, 87, 162, 169	0
3	L	14/15 (93%)	-0.08	0 100 100	51, 71, 132, 151	0
3	P	12/15 (80%)	0.77	1 (8%) 17 14	90, 110, 176, 190	0
All	All	699/832 (84%)	0.23	30 (4%) 40 36	30, 68, 125, 232	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	524	GLY	5.7
1	M	458	ARG	4.1
1	F	478	VAL	3.8
1	B	477	ASN	3.6
1	B	516	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	N	523	ALA	3.5
1	I	523	ALA	3.2
1	A	525	ARG	3.1
1	M	478	VAL	3.1
1	A	452	ASN	3.0
1	N	479	SER	2.8
1	E	462	GLU	2.7
3	P	816	DC	2.7
1	G	524	GLY	2.7
1	A	459	GLN	2.6
1	M	461	ARG	2.6
2	H	603	DA	2.4
1	M	481	MET	2.3
1	A	458	ARG	2.3
2	C	616	DC	2.2
1	M	479	SER	2.2
1	B	478	VAL	2.1
1	E	481	MET	2.1
1	N	456	ALA	2.1
1	B	455	GLU	2.1
1	N	452	ASN	2.1
2	O	604	DG	2.1
1	M	505	GLU	2.1
1	I	449	GLU	2.0
1	M	462	GLU	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.