



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 11:45 pm BST

PDB ID : 1OWR
Title : CRYSTAL STRUCTURE OF HUMAN NFAT1 BOUND MONOMERICALLY TO DNA
Authors : Stroud, J.C.; Chen, L.
Deposited on : 2003-03-29
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

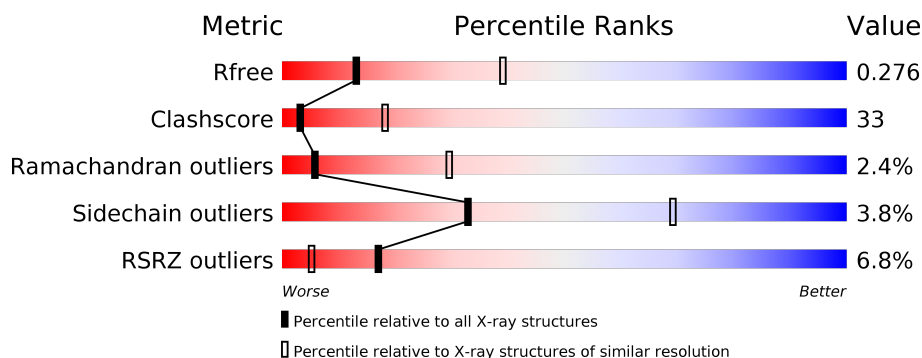
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	15	<div> <div>7%</div> <div>13%</div> <div>87%</div> </div>
1	C	15	<div> <div>100%</div> </div>
1	E	15	<div> <div>80%</div> <div>20%</div> </div>
1	G	15	<div> <div>7%</div> <div>7%</div> <div>93%</div> </div>
2	B	15	<div> <div>93%</div> <div>7%</div> </div>
2	D	15	<div> <div>93%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	15	<div><div></div><div>7%87%7%</div></div>
2	H	15	<div><div></div><div>93%7%</div></div>
3	M	284	<div><div></div><div>11%51%48%. </div></div>
3	N	284	<div><div></div><div>15%51%44%5% </div></div>
3	P	284	<div><div></div><div>2%56%41%. </div></div>
3	Q	284	<div><div></div><div>%50%49%. </div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11436 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 NFAT1 Monomeric Binding Site, Plus Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			
1	C	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			
1	E	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			
1	G	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			

- Molecule 2 is a DNA chain called NFAT1 Monomeric Binding Site, Minus Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			
2	D	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			
2	F	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			
2	H	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			

- Molecule 3 is a protein called Nuclear factor of activated T-cells, cytoplasmic 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	284	Total	C	N	O	S	0	0	0
			2250	1414	411	416	9			
3	N	284	Total	C	N	O	S	0	0	0
			2250	1414	411	416	9			
3	P	284	Total	C	N	O	S	0	0	0
			2250	1414	411	416	9			
3	Q	284	Total	C	N	O	S	0	0	0
			2250	1414	411	416	9			

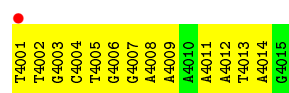
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	395	VAL	-	CLONING ARTIFACT	UNP Q13469
N	395	VAL	-	CLONING ARTIFACT	UNP Q13469
P	395	VAL	-	CLONING ARTIFACT	UNP Q13469
Q	395	VAL	-	CLONING ARTIFACT	UNP Q13469

3 Residue-property plots

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.

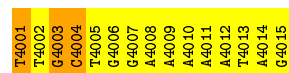
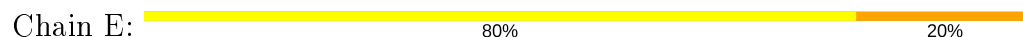
- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



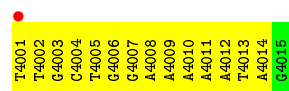
- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



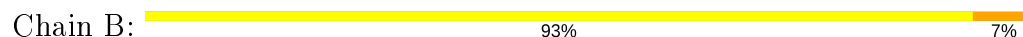
- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



- Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand



- Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand

Chain D:  93% 7%

A5001
A5002
C5003
T5004
A5005
T5006
T5007
T5008
T5009
T5010
C5011
C5012
A5013
G5014
C5015

- Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand

Chain F:  7% 87% 7%

A5001
A5002
C5003
T5004
A5005
T5006
T5007
T5008
T5009
T5010
C5011
C5012
A5013
G5014
C5015

- Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand

Chain H:  93% 7%

A5001
A5002
C5003
T5004
A5005
T5006
T5007
T5008
T5009
T5010
C5011
C5012
A5013
G5014
C5015

- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain M:  11% 51% 48% .

Y595
P396
L397
W399
S403
Q404
S405
R411
I412
E413
V414
Q415
P416
K417
P418
H419
H420
R421
A422
H423
Y424
E425
T426
E427
G428
S429
R430
G431
A432
V433
K434
A435
P436
T437
G438
G439
H440
P441
V442
V443
Q444
E450
N451
G455
L456
Q457
I458
F459
I460
G461
T462
A463
D464
E465
R466

I467
L468
K469
P470
H471
A472
F473
Y474
Q475
I479
V484
T485
T486
T487
S488
Y489
V493
L499
E500
H501
I501
Y502
P502
L503
E504
P505
M509
R510
D514
C515
I518
L519
K520
L521
R522
N523
A524
I525
E526
E527
R529
E532
T533
D534
G536
N539
R543
L544
V545
F546

R547
E552
S553
S554
G555
R556
L557
L560
Q561
N565
C569
S570
R571
R572
S573
A574
E575
E576
L577
K578
M579
V580
E581
R582
Q583
D584
S587
G588
Y591
G594
N595
N596
L597
L598
T599
G600
Q601
N602
T604
S605
E606
S607
T612
G613
K614
T615
T616
D617
G618
Q619
Q620

L621
W622
T627
V628
D629
K630
D631
K632
S633
Q634
P635
N636
K637
L638
I642
P643
E644
T645
R646
N647
K648
H649
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R651
V656
Y659
V660
L661
N662
G663
K664
R665
Q671
T674
Y678

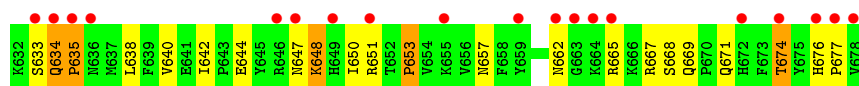
- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain N:  15% 51% 44% 5%

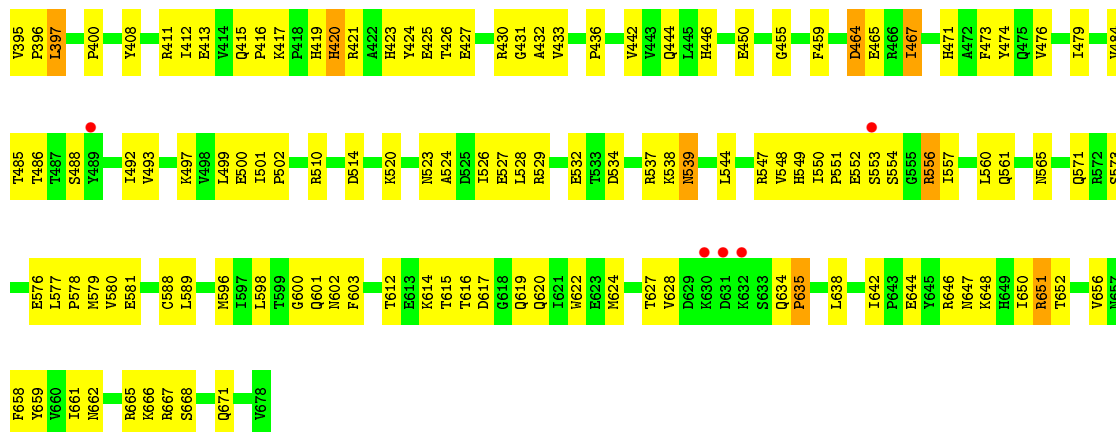
Y595
P396
L397
P400
S403
Y408
R411
I412
E413
V414
Q415
P416
K417
P418
H419
H420
R421
A422
H423
Y424
E425
T426
E427
G430
G431
A432
V433
K434
A435
P436
H440
P441
V442
Y448
H449
E450
N451
L456
Q457
I458
F459
I460
A463
I467
L468
H471
A472
F473

I479
T480
G481
K482
T483
T485
T486
Y487
S488
Y489
I492
V493
L499
E500
I501
P502
L503
E504
P505
R510
A511
D514
K520
G521
L521
R522
N523
A524
I525
E526
E527
T528
L529
R537
K538
N539
V542
R543
L544
V545
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I550
P551
E552
S553
S554
G555
R556
A572
F557
V558

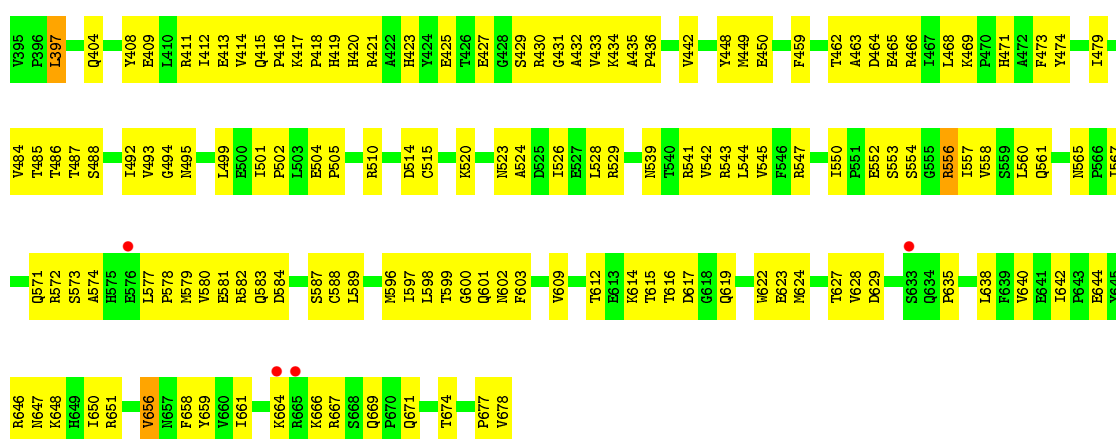
S559
L560
Q561
N565
P566
S570
Q571
R572
S573
A574
H575
E576
L577
P578
M579
V580
E581
R582
Q583
D584
T585
D586
S587
C588
Y591
G592
Q593
G594
Q595
N596
L597
L598
T599
G600
Q601
N602
T604
S605
E613
K614
T615
T616
D617
G618
Q619
Q620
T621
E623
T627
V628
D629
K630
D631



- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2



- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.65Å 94.85Å 112.79Å 90.00° 104.34° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.01 – 2.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.00) 91.5 (20.01-2.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.273 0.251 , 0.276	Depositor DCC
R_{free} test set	3538 reflections (8.91%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.697	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11436	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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	0.71	0/349	0.89	0/538
1	C	0.63	0/349	0.78	0/538
1	E	0.78	0/349	1.10	3/538 (0.6%)
1	G	0.55	0/349	0.78	0/538
2	B	0.79	0/333	0.99	1/511 (0.2%)
2	D	0.88	1/333 (0.3%)	1.02	1/511 (0.2%)
2	F	0.70	0/333	0.87	0/511
2	H	0.64	0/333	0.81	1/511 (0.2%)
3	M	0.52	0/2300	0.76	0/3115
3	N	0.51	0/2300	0.79	0/3115
3	P	0.49	0/2300	0.74	0/3115
3	Q	0.47	0/2300	0.72	1/3115 (0.0%)
All	All	0.55	1/11928 (0.0%)	0.79	7/16656 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
2	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5001	DA	N9-C4	-7.20	1.33	1.37

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4004	DC	O5'-P-OP2	-6.38	99.96	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5004	DT	OP2-P-O3'	6.15	118.73	105.20
1	E	4004	DC	O4'-C4'-C3'	-5.32	102.37	104.50
2	H	5008	DT	N1-C1'-C2'	5.16	122.40	112.60
2	D	5003	DC	O5'-P-OP2	5.12	116.85	110.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	4001	DT	Sidechain
2	F	5002	DA	Sidechain

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	310	0	171	33	0
1	C	310	0	171	36	0
1	E	310	0	171	24	0
1	G	310	0	171	36	0
2	B	299	0	173	23	0
2	D	299	0	173	16	0
2	F	299	0	173	23	0
2	H	299	0	173	17	0
3	M	2250	0	2238	142	0
3	N	2250	0	2238	135	0
3	P	2250	0	2238	121	0
3	Q	2250	0	2238	143	0
All	All	11436	0	10328	724	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 33.

The worst 5 of 724 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4008:DA:OP1	3:M:665:ARG:HB3	1.37	1.17
1:C:4003:DG:H2''	1:C:4004:DC:H5'	1.20	1.16
3:M:421:ARG:HD2	3:M:571:GLN:HB2	1.27	1.12
1:G:4003:DG:H2''	1:G:4004:DC:H5'	1.21	1.11
1:A:4004:DC:H2''	1:A:4005:DT:H5''	1.16	1.09

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	
3	M	282/284 (99%)	252 (89%)	24 (8%)	6 (2%)	7	33
3	N	282/284 (99%)	251 (89%)	21 (7%)	10 (4%)	3	20
3	P	282/284 (99%)	254 (90%)	21 (7%)	7 (2%)	5	28
3	Q	282/284 (99%)	251 (89%)	27 (10%)	4 (1%)	11	43
All	All	1128/1136 (99%)	1008 (89%)	93 (8%)	27 (2%)	6	29

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	635	PRO
3	N	426	THR
3	N	482	LYS
3	P	635	PRO
3	Q	635	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	
3	M	247/254 (97%)	240 (97%)	7 (3%)	43	77
3	N	247/254 (97%)	230 (93%)	17 (7%)	15	48
3	P	247/254 (97%)	240 (97%)	7 (3%)	43	77
3	Q	247/254 (97%)	240 (97%)	7 (3%)	43	77
All	All	988/1016 (97%)	950 (96%)	38 (4%)	33	69

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	620	GLN
3	N	653	PRO
3	Q	651	ARG
3	N	627	THR
3	N	667	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	602	ASN
3	P	507	ASN
3	Q	657	ASN
3	P	415	GLN
3	P	446	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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 [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	15/15 (100%)	-0.32	1 (6%) 17 5	34, 44, 84, 95	0
1	C	15/15 (100%)	-0.47	0 100 100	33, 42, 77, 87	0
1	E	15/15 (100%)	-0.11	0 100 100	47, 57, 103, 112	0
1	G	15/15 (100%)	0.09	1 (6%) 17 5	44, 55, 96, 103	0
2	B	15/15 (100%)	-0.22	0 100 100	18, 48, 79, 80	0
2	D	15/15 (100%)	-0.39	0 100 100	27, 45, 62, 63	0
2	F	15/15 (100%)	-0.19	0 100 100	35, 67, 101, 117	0
2	H	15/15 (100%)	-0.17	0 100 100	38, 62, 83, 96	0
3	M	284/284 (100%)	0.35	31 (10%) 5 2	16, 65, 120, 142	0
3	N	284/284 (100%)	0.52	44 (15%) 2 1	17, 76, 124, 141	0
3	P	284/284 (100%)	-0.19	5 (1%) 68 40	22, 54, 94, 130	0
3	Q	284/284 (100%)	-0.12	4 (1%) 75 49	25, 62, 101, 126	0
All	All	1256/1256 (100%)	0.11	86 (6%) 17 5	16, 62, 114, 142	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	576	GLU	6.0
3	M	664	LYS	6.0
3	M	633	SER	5.9
3	M	637	MET	5.3
3	M	665	ARG	5.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.