



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:27 PM UTC

PDB ID : 1A02 / pdb_00001a02
Title : STRUCTURE OF THE DNA BINDING DOMAINS OF NFAT, FOS AND JUN BOUND TO DNA
Authors : Chen, L.; Glover, J.N.M.; Hogan, P.G.; Rao, A.; Harrison, S.C.
Deposited on : 1997-12-08
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

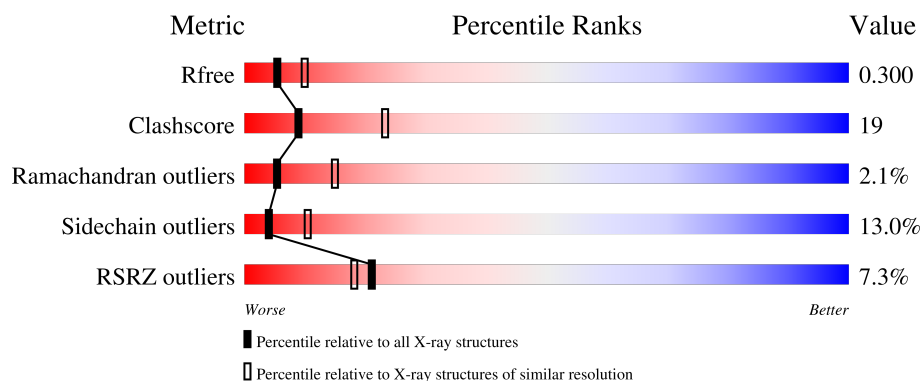
1 Overall quality at a glance

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	20	35% 65%
2	B	20	45% 45% 10%
3	N	301	8% 44% 41% 7% 7%
4	F	56	4% 68% 25% 5%
5	J	56	7% 64% 25% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3974 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(*DTP*DTP*DGP*DGP*DAP*DAP*DAP*DAP*DTP*DTP*DTP*DGP*DTP*DTP*DTP*DCP*DAP*DTP*DAP*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	20	Total	C	N	O	P	0	0	0
			410	199	71	121	19			

- Molecule 2 is a DNA chain called DNA (5'-D(*DAP*DAP*DCP*DTP*DAP*DTP*DGP*DAP*DAP*DAP*DCP*DAP*DAP*DAP*DTP*DTP*DTP*DTP*DCP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	P	0	0	0
			404	196	74	115	19			

- Molecule 3 is a protein called NUCLEAR FACTOR OF ACTIVATED T CELLS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	280	Total	C	N	O	S	0	0	0
			2204	1383	404	408	9			

- Molecule 4 is a protein called AP-1 FRAGMENT FOS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	53	Total	C	N	O	S	0	0	0
			442	262	92	87	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	138	MET	GLU	engineered mutation	UNP P01100
F	154	SER	CYS	engineered mutation	UNP P01100

- Molecule 5 is a protein called AP-1 FRAGMENT JUN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	52	Total	C	N	O	S	0	0	0
			426	257	92	75	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	263	MET	ILE	engineered mutation	UNP P05412
J	279	SER	CYS	engineered mutation	UNP P05412

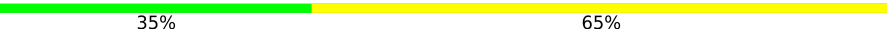
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	18	Total	O	0	0
			18	18		
6	N	46	Total	O	0	0
			46	46		
6	F	3	Total	O	0	0
			3	3		
6	J	1	Total	O	0	0
			1	1		

3 Residue-property plots

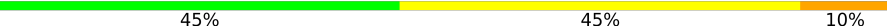
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

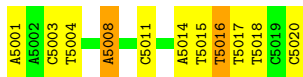
- Molecule 1: DNA (5'-D(*DTP*DTP*DGP*DGP*DAP*DAP*DAP*DAP*DTP*DTP*DTP*DGP*DTP*DTP*DTP*DCP*DAP*DTP*DAP*DG)-3')

Chain A: 

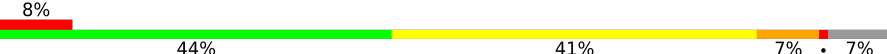


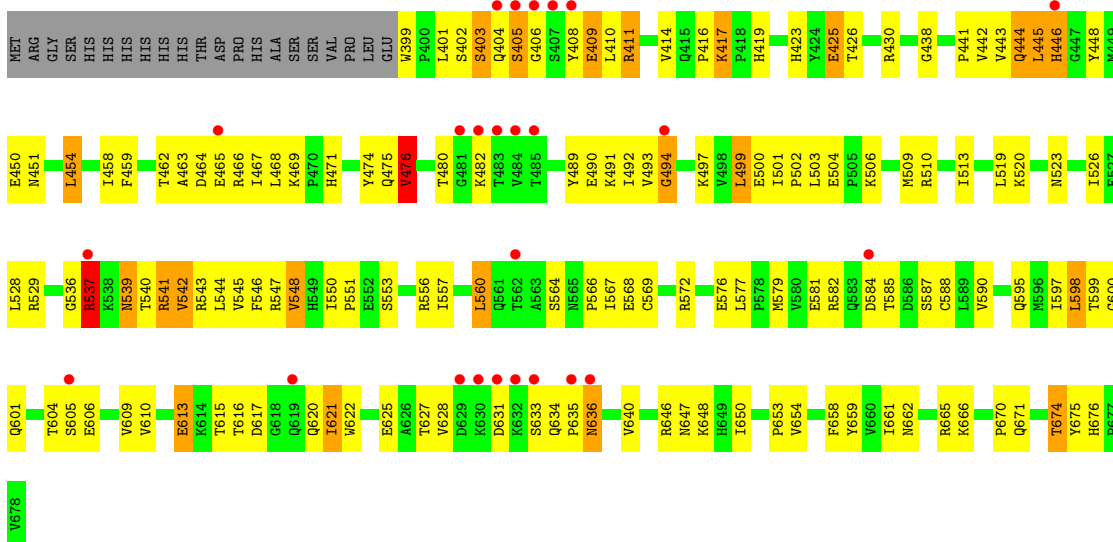
- Molecule 2: DNA (5'-D(*DAP*DAP*DCP*DTP*DAP*DTP*DGP*DAP*DAP*DAP*DCP*DAP*DAP*DAP*DTP*DTP*DTP*DTP*DCP*DC)-3')

Chain B: 



- Molecule 3: NUCLEAR FACTOR OF ACTIVATED T CELLS

Chain N: 



- Molecule 4: AP-1 FRAGMENT FOS



• Molecule 5: AP-1 FRAGMENT JUN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.66Å 85.46Å 83.37Å 90.00° 112.03° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 10.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.1 (10.00-2.70) 93.0 (10.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.71Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.246 , 0.303 0.254 , 0.300	Depositor DCC
R_{free} test set	1671 reflections (7.57%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3974	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.21% 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 [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	0.50	0/459	1.15	3/708 (0.4%)
2	B	0.46	0/453	1.10	4/696 (0.6%)
3	N	0.65	1/2253 (0.0%)	1.17	18/3050 (0.6%)
4	F	0.61	0/441	1.04	3/583 (0.5%)
5	J	0.63	0/425	0.92	2/558 (0.4%)
All	All	0.61	1/4031 (0.0%)	1.12	30/5595 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	627	THR	CA-CB	5.46	1.59	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	446	HIS	N-CA-C	11.20	125.06	111.40
3	N	417	LYS	CA-C-N	9.22	128.96	119.56
3	N	417	LYS	C-N-CA	9.22	128.96	119.56
3	N	438	GLY	N-CA-C	-8.86	103.40	114.92
3	N	606	GLU	N-CA-C	-8.39	102.31	112.54
3	N	476	VAL	CB-CA-C	-7.32	100.94	111.34
2	B	5011	DC	N1-C1'-C2'	7.00	124.01	113.50
3	N	576	GLU	N-CA-C	6.76	121.77	112.04
3	N	467	ILE	N-CA-C	-6.58	100.21	108.89
3	N	577	LEU	N-CA-C	6.58	117.93	109.65
5	J	310	MET	N-CA-C	-6.30	104.11	110.97
1	A	4020	DG	N9-C1'-C2'	6.26	122.88	113.50
4	F	148	LYS	N-CA-C	-6.17	104.24	110.97
4	F	152	ALA	N-CA-C	-5.94	104.44	111.03
3	N	444	GLN	N-CA-C	5.68	117.75	108.55
2	B	5008	DA	N9-C1'-C2'	5.66	122.00	113.50
3	N	403	SER	N-CA-C	-5.62	100.19	108.79
3	N	569	CYS	N-CA-C	5.45	118.93	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	539	ASN	N-CA-C	-5.44	102.04	109.71
3	N	425	GLU	N-CA-C	-5.39	106.65	113.18
1	A	4004	DG	N9-C1'-C2'	5.32	121.48	113.50
4	F	188	LYS	N-CA-C	-5.28	105.61	111.36
2	B	5020	DC	C2'-C3'-O3'	-5.26	103.61	111.50
1	A	4005	DA	N9-C1'-C2'	5.25	121.37	113.50
5	J	282	ARG	NE-CZ-NH2	5.24	123.92	119.20
3	N	411	ARG	NE-CZ-NH2	5.17	123.86	119.20
3	N	581	GLU	N-CA-C	-5.17	107.64	114.31
3	N	502	PRO	N-CA-C	5.08	119.28	111.21
2	B	5016	DT	N1-C1'-C2'	5.07	121.11	113.50
3	N	540	THR	N-CA-C	5.03	119.37	112.88

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	410	0	231	11	0
2	B	404	0	228	14	0
3	N	2204	0	2168	109	0
4	F	442	0	461	10	0
5	J	426	0	472	9	0
6	A	20	0	0	1	0
6	B	18	0	0	0	0
6	F	3	0	0	0	0
6	J	1	0	0	0	0
6	N	46	0	0	2	0
All	All	3974	0	3560	138	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 19.

All (138) 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:N:423:HIS:HB3	3:N:430:ARG:HG3	1.32	1.03
2:B:5003:DC:H2''	2:B:5004:DT:H71	1.42	1.02
1:A:4017:DA:H1'	1:A:4018:DT:H5'	1.40	1.01
3:N:613:GLU:HB2	3:N:622:TRP:HB3	1.42	0.99
3:N:474:TYR:CE1	3:N:520:LYS:HD3	2.09	0.88
2:B:5008:DA:H2'	5:J:280:ARG:HH22	1.39	0.88
3:N:399:TRP:HB3	3:N:547:ARG:HH22	1.39	0.87
3:N:584:ASP:HB2	3:N:597:ILE:H	1.40	0.87
3:N:490:GLU:HB3	3:N:500:GLU:HB3	1.56	0.86
3:N:410:LEU:HD22	3:N:548:VAL:HG22	1.56	0.84
3:N:600:GLY:O	3:N:636:ASN:HB2	1.79	0.82
3:N:401:LEU:HD22	4:F:180:GLN:HE22	1.45	0.81
1:A:4015:DT:H2''	1:A:4016:DC:H5'	1.63	0.79
3:N:406:GLY:HA3	3:N:560:LEU:HG	1.64	0.79
3:N:491:LYS:HE2	3:N:497:LYS:HD3	1.67	0.75
3:N:408:TYR:HB3	3:N:445:LEU:HD21	1.71	0.73
3:N:399:TRP:HB2	3:N:547:ARG:HH12	1.55	0.71
3:N:653:PRO:HB3	3:N:676:HIS:CD2	2.27	0.70
3:N:416:PRO:HG3	3:N:544:LEU:HD12	1.74	0.69
3:N:465:GLU:HG3	3:N:670:PRO:HG2	1.74	0.69
2:B:5008:DA:H2'	5:J:280:ARG:NH2	2.06	0.69
3:N:582:ARG:HB2	3:N:599:THR:HB	1.74	0.69
3:N:526:ILE:O	3:N:529:ARG:HG2	1.93	0.68
1:A:4017:DA:H2''	1:A:4018:DT:OP2	1.93	0.68
3:N:650:ILE:HD13	3:N:654:VAL:HG23	1.77	0.67
3:N:463:ALA:HA	3:N:543:ARG:HE	1.61	0.66
3:N:399:TRP:HB3	3:N:547:ARG:NH2	2.09	0.65
3:N:610:VAL:O	3:N:658:PHE:HA	1.95	0.65
3:N:441:PRO:HG2	3:N:513:ILE:HB	1.79	0.64
2:B:5003:DC:H2''	2:B:5004:DT:C7	2.23	0.63
3:N:408:TYR:CB	3:N:445:LEU:HD21	2.27	0.63
3:N:501:ILE:HG13	3:N:501:ILE:O	1.95	0.63
3:N:448:TYR:CE2	3:N:509:MET:HE2	2.34	0.62
3:N:401:LEU:HD22	4:F:180:GLN:NE2	2.13	0.61
3:N:584:ASP:CB	3:N:597:ILE:H	2.12	0.61
1:A:4012:DG:H5''	3:N:665:ARG:HH22	1.65	0.60
3:N:425:GLU:HG3	3:N:519:LEU:HD11	1.85	0.59
3:N:408:TYR:HB3	3:N:445:LEU:CD2	2.31	0.59
3:N:416:PRO:HG2	3:N:567:ILE:HD11	1.83	0.59
1:A:4017:DA:C1'	1:A:4018:DT:H5'	2.23	0.59
3:N:613:GLU:HB2	3:N:622:TRP:CB	2.25	0.58
3:N:462:THR:O	3:N:543:ARG:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5015:DT:H2''	2:B:5016:DT:OP2	2.04	0.58
1:A:4001:DT:H2''	1:A:4002:DT:O5'	2.03	0.57
1:A:4011:DT:H4'	3:N:537:ARG:NH1	2.18	0.57
4:F:162:THR:HG22	5:J:287:ILE:CG1	2.35	0.57
3:N:474:TYR:CZ	3:N:520:LYS:HD3	2.40	0.56
3:N:399:TRP:HB2	3:N:547:ARG:NH1	2.20	0.56
3:N:579:MET:O	3:N:600:GLY:HA3	2.04	0.56
3:N:419:HIS:HE1	3:N:601:GLN:HG3	1.70	0.56
5:J:300:GLN:O	5:J:304:LEU:HG	2.06	0.55
2:B:5015:DT:H2'	3:N:572:ARG:HH11	1.71	0.55
3:N:542:VAL:CG1	3:N:543:ARG:N	2.69	0.55
2:B:5008:DA:C2'	5:J:280:ARG:HH22	2.18	0.54
4:F:141:ARG:HH11	4:F:141:ARG:HG2	1.73	0.54
3:N:503:LEU:O	3:N:509:MET:SD	2.67	0.53
3:N:399:TRP:HE3	3:N:547:ARG:NH1	2.05	0.53
3:N:466:ARG:HB2	6:N:6086:HOH:O	2.08	0.53
2:B:5015:DT:H2'	3:N:572:ARG:NH1	2.23	0.53
3:N:408:TYR:CD2	3:N:550:ILE:HD12	2.44	0.53
3:N:584:ASP:HB2	3:N:597:ILE:N	2.18	0.53
2:B:5014:DA:H1'	2:B:5015:DT:H5'	1.90	0.52
3:N:476:VAL:HG23	3:N:497:LYS:HB3	1.91	0.52
3:N:560:LEU:HD12	3:N:560:LEU:N	2.24	0.52
3:N:542:VAL:O	3:N:566:PRO:HA	2.10	0.51
3:N:399:TRP:HE3	3:N:547:ARG:HH12	1.58	0.51
1:A:4014:DT:H3'	4:F:148:LYS:HE3	1.92	0.51
3:N:423:HIS:HB3	3:N:430:ARG:CG	2.23	0.51
3:N:404:GLN:HG2	3:N:405:SER:N	2.26	0.50
1:A:4017:DA:H1'	1:A:4018:DT:C5'	2.26	0.50
3:N:548:VAL:HG23	3:N:560:LEU:HD13	1.94	0.50
3:N:615:THR:HG23	3:N:621:ILE:HD12	1.94	0.50
2:B:5015:DT:H6	3:N:572:ARG:NH1	2.10	0.50
3:N:628:VAL:HG12	6:N:6005:HOH:O	2.11	0.49
3:N:419:HIS:CE1	3:N:601:GLN:HG3	2.46	0.49
2:B:5017:DT:H2''	2:B:5018:DT:H72	1.95	0.49
3:N:401:LEU:CD2	4:F:180:GLN:HE22	2.21	0.49
5:J:310:MET:HE2	5:J:314:GLN:HE21	1.78	0.49
1:A:4002:DT:H2''	1:A:4003:DG:C8	2.48	0.49
4:F:165:LEU:O	4:F:169:THR:HG23	2.14	0.48
3:N:443:VAL:HG21	3:N:546:PHE:CD2	2.49	0.47
3:N:634:GLN:C	3:N:636:ASN:H	2.21	0.47
3:N:463:ALA:O	3:N:466:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:468:LEU:HD13	3:N:469:LYS:N	2.30	0.47
3:N:475:GLN:HB3	3:N:497:LYS:HE3	1.96	0.47
3:N:587:SER:HB2	3:N:674:THR:HG23	1.97	0.47
3:N:662:ASN:O	3:N:666:LYS:HB2	2.16	0.46
3:N:426:THR:HG22	3:N:426:THR:O	2.16	0.46
3:N:445:LEU:HD11	3:N:550:ILE:HD11	1.96	0.46
3:N:489:TYR:HB2	3:N:499:LEU:HD22	1.96	0.46
3:N:504:GLU:HB3	3:N:506:LYS:HD2	1.96	0.46
3:N:408:TYR:CZ	3:N:550:ILE:HG21	2.50	0.46
3:N:523:ASN:ND2	3:N:536:GLY:HA3	2.31	0.46
3:N:419:HIS:CD2	3:N:568:GLU:HB3	2.51	0.46
3:N:459:PHE:CZ	3:N:545:VAL:HG11	2.51	0.46
3:N:468:LEU:HD23	3:N:543:ARG:CZ	2.45	0.46
3:N:454:LEU:H	3:N:509:MET:HE1	1.81	0.46
6:A:6020:HOH:O	5:J:276:ALA:HB2	2.16	0.45
3:N:406:GLY:CA	3:N:560:LEU:HG	2.41	0.45
3:N:458:ILE:N	3:N:499:LEU:O	2.50	0.45
3:N:493:VAL:HB	3:N:494:GLY:H	1.64	0.45
3:N:463:ALA:O	3:N:464:ASP:HB2	2.16	0.45
2:B:5001:DA:C8	2:B:5001:DA:O5'	2.69	0.45
3:N:414:VAL:HB	3:N:442:VAL:H	1.82	0.44
3:N:399:TRP:CB	3:N:547:ARG:HH12	2.26	0.44
3:N:444:GLN:HB2	3:N:510:ARG:HG3	1.99	0.44
3:N:551:PRO:HA	3:N:557:ILE:HD13	2.00	0.44
3:N:588:CYS:O	3:N:675:TYR:HA	2.17	0.44
3:N:653:PRO:HB3	3:N:676:HIS:HD2	1.79	0.44
3:N:548:VAL:HG23	3:N:560:LEU:HB2	2.00	0.44
3:N:646:ARG:HG3	3:N:647:ASN:H	1.81	0.43
4:F:179:LEU:O	4:F:182:GLU:HB3	2.19	0.43
3:N:448:TYR:CD2	3:N:509:MET:HE2	2.53	0.43
3:N:482:LYS:N	3:N:482:LYS:HD2	2.34	0.43
3:N:542:VAL:HG13	3:N:543:ARG:N	2.33	0.42
3:N:543:ARG:HG2	3:N:564:SER:O	2.18	0.42
4:F:176:LYS:O	4:F:180:GLN:HG3	2.20	0.42
2:B:5001:DA:O5'	2:B:5001:DA:H8	2.01	0.42
5:J:314:GLN:O	5:J:317:GLN:HG2	2.19	0.42
3:N:408:TYR:O	3:N:409:GLU:HB3	2.19	0.42
3:N:541:ARG:HE	3:N:541:ARG:HB2	1.61	0.42
3:N:503:LEU:HD23	3:N:503:LEU:HA	1.85	0.41
1:A:4002:DT:H2''	1:A:4003:DG:H8	1.85	0.41
3:N:598:LEU:HD22	3:N:640:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:182:GLU:OE2	5:J:308:ALA:HB1	2.21	0.41
3:N:414:VAL:HB	3:N:442:VAL:N	2.36	0.41
3:N:604:THR:OG1	3:N:605:SER:N	2.53	0.41
3:N:471:HIS:CE1	3:N:539:ASN:ND2	2.89	0.41
2:B:5014:DA:H2''	3:N:572:ARG:HH12	1.85	0.41
3:N:448:TYR:CE2	3:N:450:GLU:HB2	2.56	0.40
3:N:582:ARG:HG3	3:N:582:ARG:HH11	1.85	0.40
3:N:411:ARG:HE	3:N:446:HIS:HE1	1.70	0.40
3:N:650:ILE:CD1	3:N:654:VAL:HG23	2.49	0.40
3:N:409:GLU:O	3:N:409:GLU:CG	2.69	0.40
3:N:609:VAL:HA	3:N:659:TYR:O	2.20	0.40
3:N:646:ARG:CG	3:N:647:ASN:H	2.34	0.40
3:N:463:ALA:HA	3:N:543:ARG:NE	2.32	0.40
3:N:471:HIS:CE1	3:N:539:ASN:HD21	2.39	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	
3	N	278/301 (92%)	242 (87%)	28 (10%)	8 (3%)	3	9
4	F	51/56 (91%)	51 (100%)	0	0	100	100
5	J	50/56 (89%)	50 (100%)	0	0	100	100
All	All	379/413 (92%)	343 (90%)	28 (7%)	8 (2%)	5	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	590	VAL
3	N	633	SER
3	N	480	THR

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Mol	Chain	Res	Type
3	N	631	ASP
3	N	405	SER
3	N	494	GLY
3	N	537	ARG
3	N	635	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	
3	N	238/269 (88%)	206 (87%)	32 (13%)	4	9
4	F	47/50 (94%)	43 (92%)	4 (8%)	10	25
5	J	45/48 (94%)	38 (84%)	7 (16%)	2	7
All	All	330/367 (90%)	287 (87%)	43 (13%)	4	10

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	402	SER
3	N	403	SER
3	N	409	GLU
3	N	417	LYS
3	N	445	LEU
3	N	451	ASN
3	N	454	LEU
3	N	476	VAL
3	N	492	ILE
3	N	499	LEU
3	N	528	LEU
3	N	537	ARG
3	N	541	ARG
3	N	542	VAL
3	N	548	VAL
3	N	553	SER
3	N	556	ARG

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Mol	Chain	Res	Type
3	N	560	LEU
3	N	585	THR
3	N	595	GLN
3	N	598	LEU
3	N	613	GLU
3	N	616	THR
3	N	617	ASP
3	N	620	GLN
3	N	621	ILE
3	N	625	GLU
3	N	636	ASN
3	N	648	LYS
3	N	661	ILE
3	N	671	GLN
3	N	674	THR
4	F	142	ILE
4	F	171	GLN
4	F	177	SER
4	F	190	LYS
5	J	267	ARG
5	J	270	MET
5	J	272	ASN
5	J	282	ARG
5	J	286	ARG
5	J	296	THR
5	J	318	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
3	N	419	HIS
3	N	446	HIS
3	N	457	GLN
3	N	471	HIS
3	N	495	ASN
3	N	508	ASN
3	N	523	ASN
3	N	539	ASN
3	N	583	GLN
3	N	636	ASN
4	F	171	GLN
4	F	180	GLN

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Mol	Chain	Res	Type
5	J	317	GLN

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	20/20 (100%)	-0.06	0	100	100	28, 36, 61, 64	0
2	B	20/20 (100%)	-0.21	0	100	100	22, 37, 51, 52	0
3	N	280/301 (93%)	0.55	25 (8%)	15	13	23, 53, 90, 99	0
4	F	53/56 (94%)	0.32	2 (3%)	44	40	28, 49, 73, 90	0
5	J	52/56 (92%)	0.41	4 (7%)	19	17	35, 50, 95, 99	0
All	All	425/453 (93%)	0.44	31 (7%)	21	18	22, 50, 89, 99	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	483	THR	12.6
3	N	484	VAL	12.3
3	N	485	THR	10.0
3	N	406	GLY	7.9
3	N	481	GLY	7.1
3	N	632	LYS	6.0
3	N	633	SER	5.5
3	N	482	LYS	5.0
3	N	631	ASP	4.9
3	N	494	GLY	4.8
3	N	636	ASN	4.1
3	N	446	HIS	3.9
3	N	407	SER	3.9
3	N	404	GLN	3.5
3	N	405	SER	3.4
5	J	269	ARG	3.3
5	J	282	ARG	3.2
5	J	310	MET	3.0
3	N	629	ASP	2.9
3	N	408	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
3	N	562	THR	2.7
3	N	619	GLN	2.6
4	F	170	ASP	2.6
3	N	630	LYS	2.6
3	N	584	ASP	2.4
3	N	465	GLU	2.3
3	N	537	ARG	2.2
4	F	145	GLU	2.2
5	J	316	ALA	2.0
3	N	605	SER	2.0
3	N	635	PRO	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.