



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 07:43 AM UTC

PDB ID : 1MDJ / pdb_00001mdj
Title : HIGH RESOLUTION SOLUTION NMR STRUCTURE OF MIXED DISULFIDE INTERMEDIATE BETWEEN HUMAN THIOREDOXIN (C35A, C62A, C69A, C73A) MUTANT AND A 13 RESIDUE PEPTIDE COMPRISING ITS TARGET SITE IN HUMAN NFkB (RESIDUES 56-68 OF THE P50 SUBUNIT OF NFkB)
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Deposited on : 1995-02-27

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

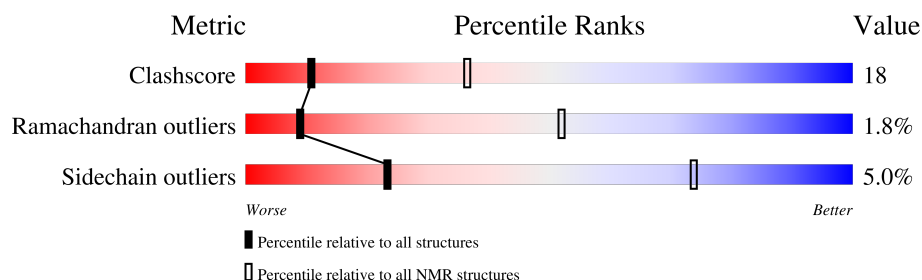
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	105	
2	B	13	

2 Ensemble composition and analysis

This entry contains 30 models. Model 2 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:104, B:3-B:11 (112)	0.20	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	5, 7, 8, 9, 12, 16, 17, 21, 22, 25, 30
2	2, 3, 6, 13, 15, 18, 19, 24, 28
3	1, 14, 20, 23
4	27, 29
Single-model clusters	4; 10; 11; 26

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1851 atoms, of which 919 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called THIOREDOXIN.

Mol	Chain	Residues	Atoms						Trace
1	A	105	Total	C	H	N	O	S	0
			1624	524	808	128	161	3	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	ALA	CYS	conflict	UNP P10599
A	62	ALA	CYS	conflict	UNP P10599
A	69	ALA	CYS	conflict	UNP P10599
A	73	ALA	CYS	conflict	UNP P10599
A	74	THR	MET	conflict	UNP P10599

- Molecule 2 is a protein called TARGET SITE IN HUMAN NFKB.

Mol	Chain	Residues	Atoms						Trace
2	B	13	Total	C	H	N	O	S	0
			209	70	99	21	18	1	

- Molecule 3 is water.

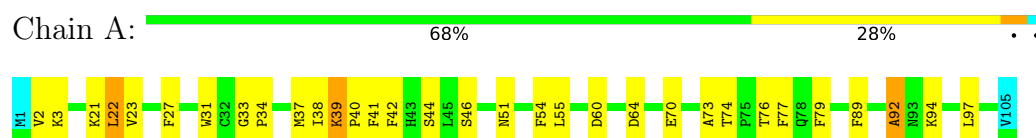
Mol	Chain	Residues	Atoms		
3	A	6	Total	H	O
			18	12	6

4 Residue-property plots [i](#)

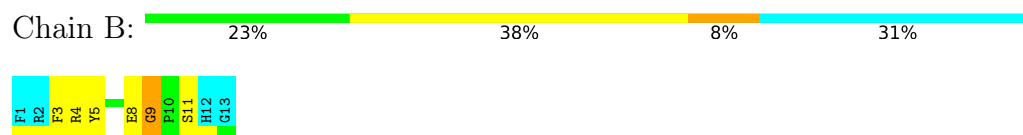
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: THIOREDOXIN



- Molecule 2: TARGET SITE IN HUMAN NFkB

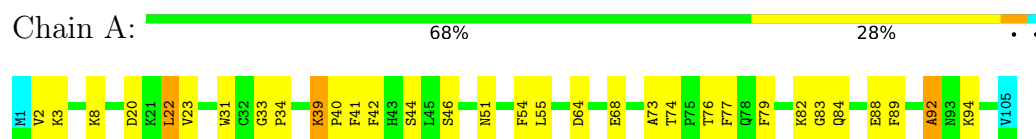


4.2 Scores per residue for each member of the ensemble

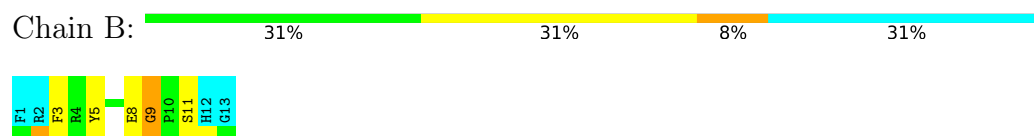
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: THIOREDOXIN

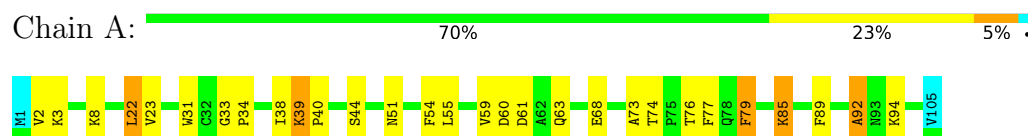


- Molecule 2: TARGET SITE IN HUMAN NFkB

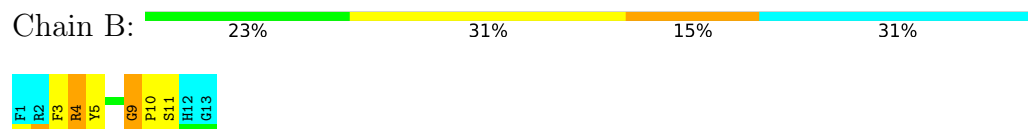


4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: THIOREDOXIN

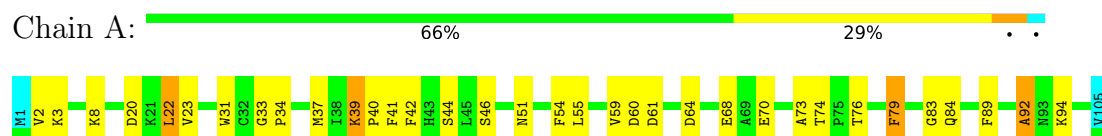


- Molecule 2: TARGET SITE IN HUMAN NFKB

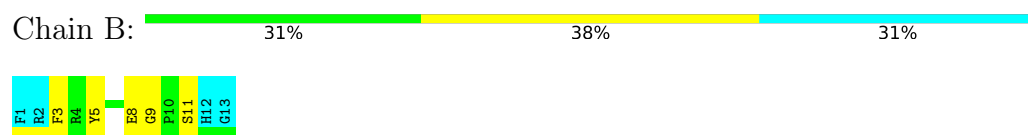


4.2.3 Score per residue for model 3

- Molecule 1: THIOREDOXIN

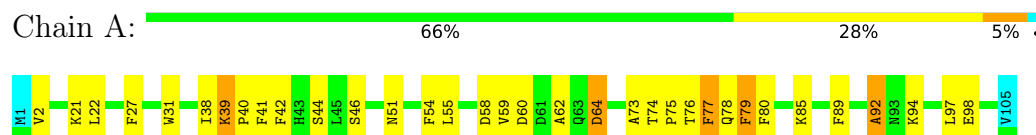


- Molecule 2: TARGET SITE IN HUMAN NFKB

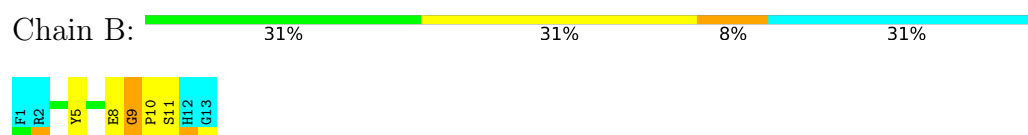


4.2.4 Score per residue for model 4

- Molecule 1: THIOREDOXIN

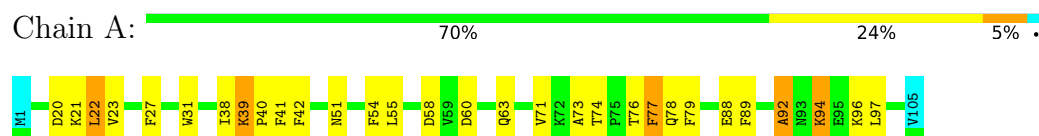


- Molecule 2: TARGET SITE IN HUMAN NFKB

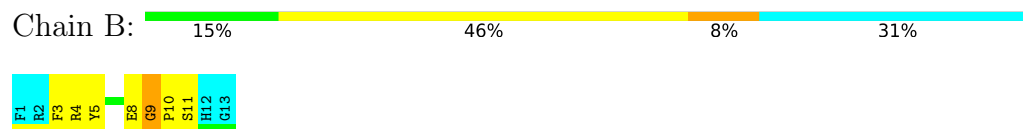


4.2.5 Score per residue for model 5

- Molecule 1: THIOREDOXIN

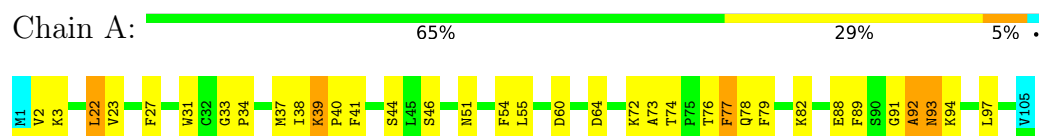


- Molecule 2: TARGET SITE IN HUMAN NFKB

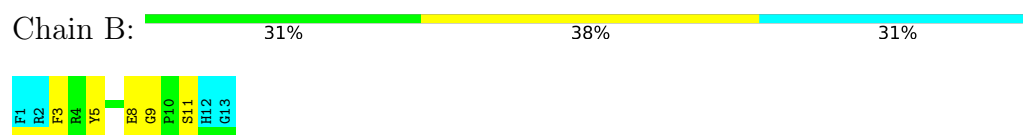


4.2.6 Score per residue for model 6

- Molecule 1: THIOREDOXIN

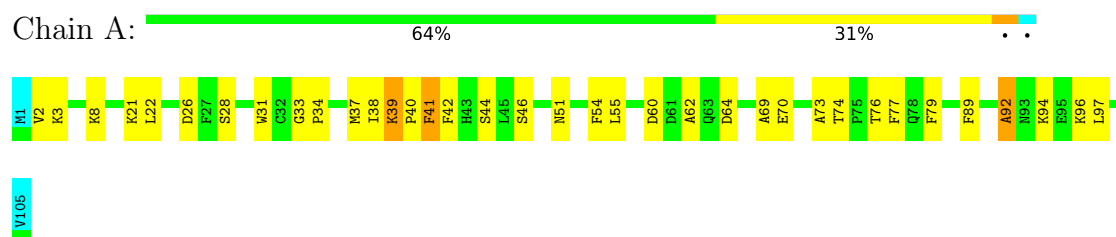


- Molecule 2: TARGET SITE IN HUMAN NFKB



4.2.7 Score per residue for model 7

- Molecule 1: THIOREDOXIN



- Molecule 2: TARGET SITE IN HUMAN NFKB

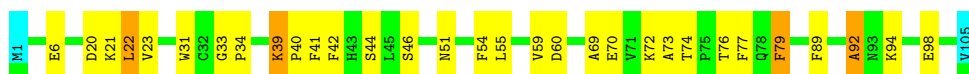




4.2.8 Score per residue for model 8

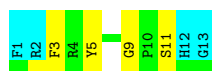
- Molecule 1: THIOREDOXIN

Chain A: 69% 26% . .



- Molecule 2: TARGET SITE IN HUMAN NFKB

Chain B: 38% 31% 31%



4.2.9 Score per residue for model 9

- Molecule 1: THIOREDOXIN

Chain A: 69% 27% . .



- Molecule 2: TARGET SITE IN HUMAN NFKB

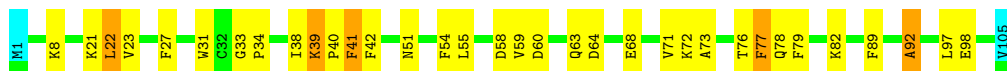
Chain B: 31% 31% 8% 31%



4.2.10 Score per residue for model 10

- Molecule 1: THIOREDOXIN

Chain A: 66% 28% 5% .



- Molecule 2: TARGET SITE IN HUMAN NFKB

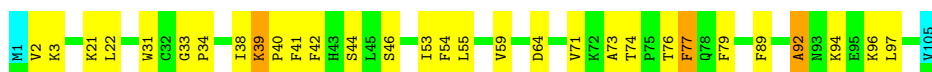
Chain B: 23% 38% 8% 31%



4.2.11 Score per residue for model 11

- Molecule 1: THIOREDOXIN

Chain A: 70% 26% . .



- Molecule 2: TARGET SITE IN HUMAN NFKB

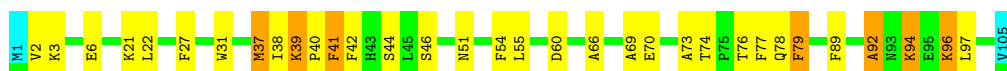
Chain B: 38% 31% 31%



4.2.12 Score per residue for model 12

- Molecule 1: THIOREDOXIN

Chain A: 67% 25% 7% .



- Molecule 2: TARGET SITE IN HUMAN NFKB

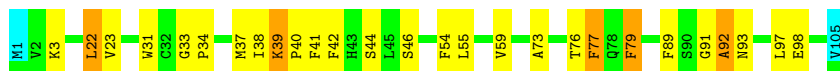
Chain B: 31% 31% 8% 31%



4.2.13 Score per residue for model 13

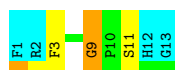
- Molecule 1: THIOREDOXIN

Chain A: 72% 21% 5% .



- Molecule 2: TARGET SITE IN HUMAN NFKB

Chain B: 46% 15% 8% 31%



4.2.14 Score per residue for model 14

- Molecule 1: THIOREDOXIN

Chain A: 70% 27%



- Molecule 2: TARGET SITE IN HUMAN NFKB

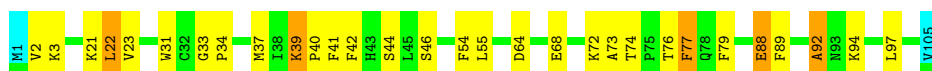
Chain B: 31% 31% 8% 31%



4.2.15 Score per residue for model 15

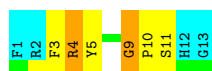
- Molecule 1: THIOREDOXIN

Chain A: 70% 24% 5%



- Molecule 2: TARGET SITE IN HUMAN NFKB

Chain B: 23% 31% 15% 31%



4.2.16 Score per residue for model 16

- Molecule 1: THIOREDOXIN

Chain A: 63% 30% 5%



- Molecule 2: TARGET SITE IN HUMAN NFKB

Chain B: 38% 31% 31%



4.2.17 Score per residue for model 17

- Molecule 1: THIOREDOXIN

Chain A: 67% 29%



- Molecule 2: TARGET SITE IN HUMAN NFKB

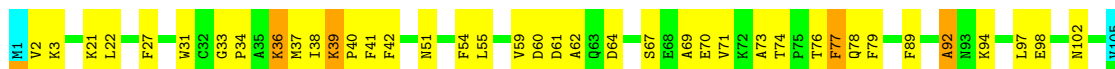
Chain B: 31% 23% 15% 31%



4.2.18 Score per residue for model 18

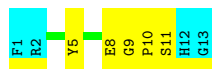
- Molecule 1: THIOREDOXIN

Chain A: 61% 33%



- Molecule 2: TARGET SITE IN HUMAN NFKB

Chain B: 31% 38% 31%



4.2.19 Score per residue for model 19

- Molecule 1: THIOREDOXIN

Chain A: 63% 30% 5%



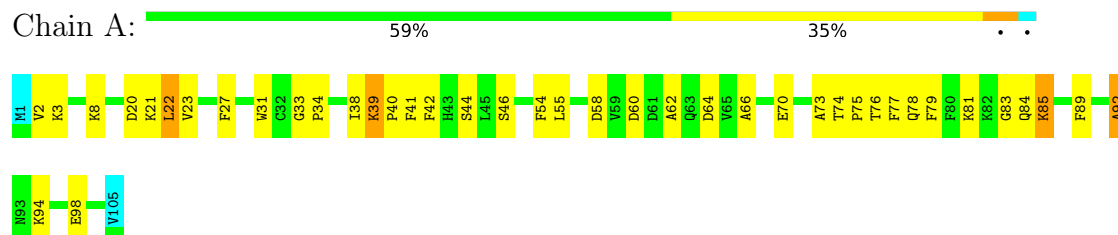
- Molecule 2: TARGET SITE IN HUMAN NFKB

Chain B: 31% 38% 31%

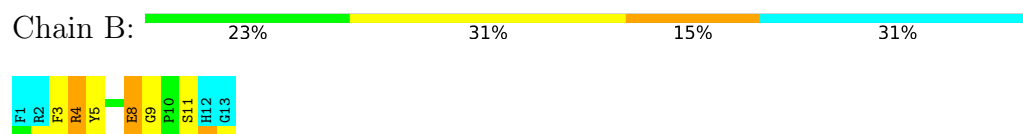


4.2.20 Score per residue for model 20

- Molecule 1: THIOREDOXIN

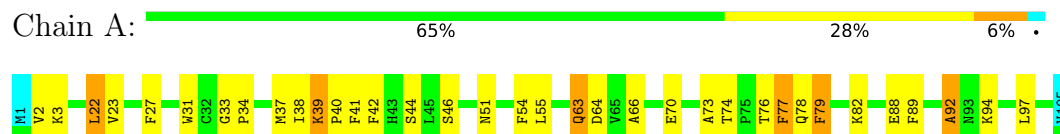


- Molecule 2: TARGET SITE IN HUMAN NFKB

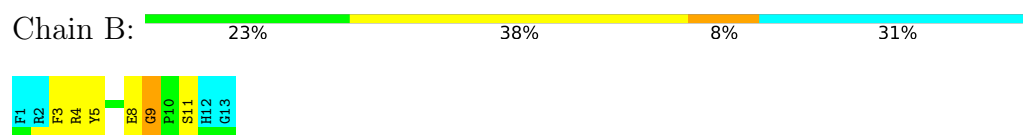


4.2.21 Score per residue for model 21

- Molecule 1: THIOREDOXIN

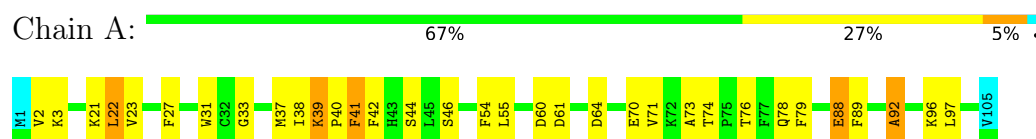


- Molecule 2: TARGET SITE IN HUMAN NFKB

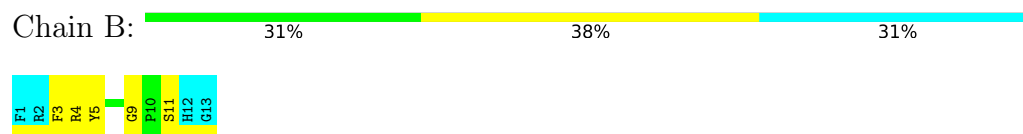


4.2.22 Score per residue for model 22

- Molecule 1: THIOREDOXIN

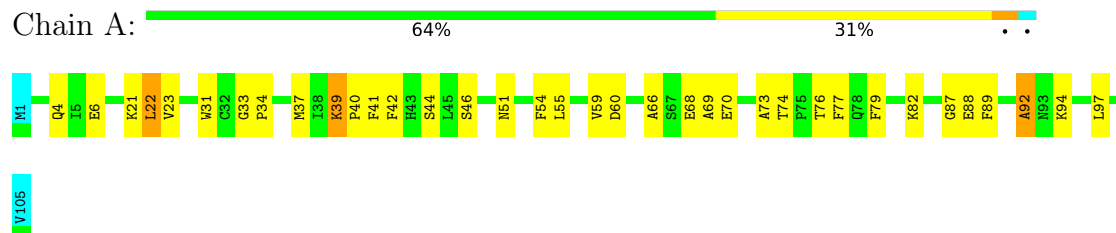


- Molecule 2: TARGET SITE IN HUMAN NFKB

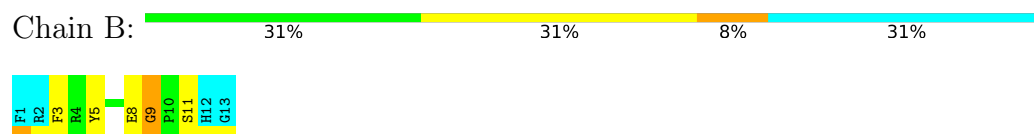


4.2.23 Score per residue for model 23

- Molecule 1: THIOREDOXIN

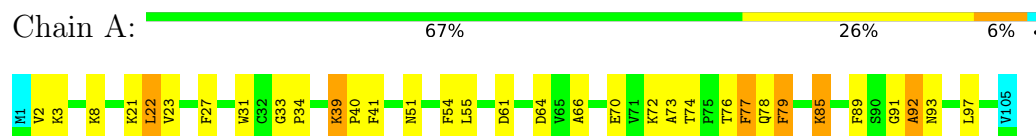


- Molecule 2: TARGET SITE IN HUMAN NFKB

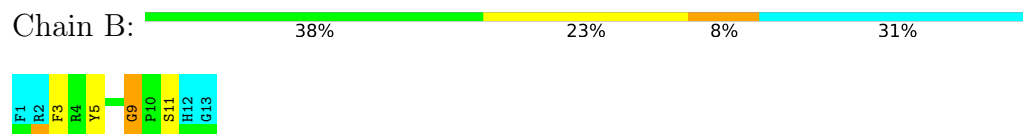


4.2.24 Score per residue for model 24

- Molecule 1: THIOREDOXIN

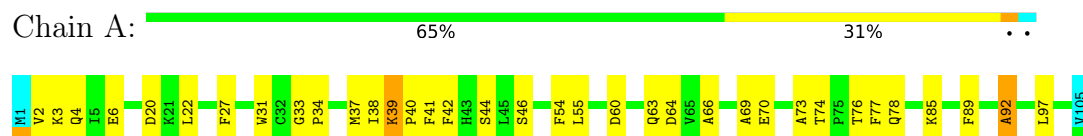


- Molecule 2: TARGET SITE IN HUMAN NFKB



4.2.25 Score per residue for model 25

- Molecule 1: THIOREDOXIN



- Molecule 2: TARGET SITE IN HUMAN NFKB

Chain B: 



4.2.26 Score per residue for model 26

- Molecule 1: THIOREDOXIN

Chain A: 



- Molecule 2: TARGET SITE IN HUMAN NFKB

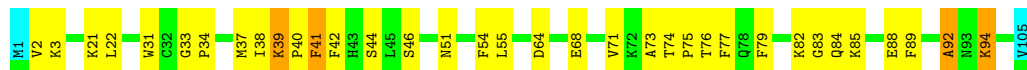
Chain B: 



4.2.27 Score per residue for model 27

- Molecule 1: THIOREDOXIN

Chain A: 



- Molecule 2: TARGET SITE IN HUMAN NFKB

Chain B: 

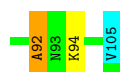


4.2.28 Score per residue for model 28

- Molecule 1: THIOREDOXIN

Chain A: 





- Molecule 2: TARGET SITE IN HUMAN NFKB



4.2.29 Score per residue for model 29

- Molecule 1: THIOREDOXIN



- Molecule 2: TARGET SITE IN HUMAN NFKB

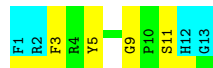


4.2.30 Score per residue for model 30

- Molecule 1: THIOREDOXIN



- Molecule 2: TARGET SITE IN HUMAN NFKB



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: ?.

Of the ? calculated structures, 30 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.

6 Model quality [i](#)

6.1 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 (average) 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	1.48±0.01	0±0/816 (0.0± 0.0%)	1.18±0.01	1±1/1101 (0.1± 0.1%)
2	B	1.46±0.03	0±0/76 (0.0± 0.0%)	1.14±0.03	0±0/103 (0.0± 0.0%)
All	All	1.48	1/26760 (0.0%)	1.17	41/36120 (0.1%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	87	GLY	N-CA	5.33	1.50	1.45	28	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	41	PHE	CA-CB-CG	-6.16	107.64	113.80	27	6
1	A	77	PHE	CA-CB-CG	-5.53	108.27	113.80	17	24
1	A	79	PHE	CA-CB-CG	-5.30	108.50	113.80	13	11

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	800	788	788	29±4
2	B	73	65	65	8±2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
3	A	6	12	0	1±1
All	All	26370	25950	25590	960

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 18.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:LYS:HB3	1:A:94:LYS:HZ3	0.68	1.48	12	1
1:A:77:PHE:CD1	1:A:97:LEU:HD21	0.68	2.23	29	16
1:A:74:THR:HG23	2:B:5:TYR:CE2	0.66	2.25	25	25
1:A:2:VAL:HG12	1:A:3:LYS:H	0.64	1.52	18	3
1:A:39:LYS:N	1:A:40:PRO:CD	0.64	2.61	27	30
1:A:38:ILE:HG22	1:A:38:ILE:O	0.63	1.92	12	18
1:A:21:LYS:NZ	1:A:51:ASN:ND2	0.62	2.48	28	2
1:A:73:ALA:HB1	2:B:8:GLU:CD	0.61	2.20	3	13
1:A:27:PHE:CE1	1:A:78:GLN:NE2	0.60	2.70	12	9
1:A:21:LYS:CE	1:A:53:ILE:HD11	0.60	2.26	11	1
1:A:54:PHE:C	1:A:55:LEU:HD12	0.59	2.22	2	30
1:A:94:LYS:HZ3	1:A:94:LYS:CB	0.59	2.10	12	1
1:A:2:VAL:HG12	1:A:3:LYS:N	0.58	2.13	18	22
2:B:9:GLY:C	2:B:11:SER:H	0.58	2.06	10	30
1:A:89:PHE:CD1	1:A:89:PHE:O	0.58	2.57	25	30
1:A:31:TRP:CZ3	2:B:3:PHE:CE2	0.57	2.92	1	25
1:A:74:THR:HG23	2:B:5:TYR:CE1	0.57	2.34	5	1
1:A:41:PHE:CD1	1:A:94:LYS:NZ	0.57	2.68	12	1
1:A:33:GLY:N	1:A:34:PRO:HD2	0.57	2.15	25	24
1:A:88:GLU:N	1:A:88:GLU:CD	0.56	2.64	19	6
1:A:80:PHE:CZ	1:A:85:LYS:NZ	0.56	2.73	4	1
1:A:73:ALA:O	1:A:76:THR:OG1	0.56	2.23	25	30
2:B:4:ARG:CG	2:B:4:ARG:HH11	0.56	2.14	25	6
1:A:22:LEU:HD23	1:A:23:VAL:H	0.55	1.62	14	21
1:A:89:PHE:C	1:A:89:PHE:CD1	0.55	2.85	5	9
1:A:92:ALA:HB2	2:B:9:GLY:C	0.55	2.26	29	30
1:A:63:GLN:NE2	2:B:4:ARG:NH1	0.54	2.55	5	1
1:A:6:GLU:N	1:A:6:GLU:OE2	0.54	2.40	23	1
1:A:51:ASN:O	1:A:51:ASN:ND2	0.54	2.41	14	14
1:A:21:LYS:HE2	1:A:53:ILE:HD11	0.54	1.79	11	1
1:A:63:GLN:NE2	2:B:4:ARG:CZ	0.54	2.71	21	1
1:A:64:ASP:N	1:A:64:ASP:OD1	0.53	2.39	11	8
1:A:89:PHE:CD1	1:A:89:PHE:C	0.53	2.86	18	21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:GLU:CD	1:A:6:GLU:N	0.53	2.67	30	3
1:A:63:GLN:NE2	2:B:4:ARG:HH11	0.53	2.02	5	1
1:A:33:GLY:N	1:A:34:PRO:CD	0.53	2.72	25	19
1:A:21:LYS:NZ	1:A:51:ASN:CG	0.53	2.67	18	1
1:A:41:PHE:CE1	1:A:94:LYS:NZ	0.52	2.67	7	1
1:A:27:PHE:CE1	1:A:78:GLN:OE1	0.52	2.63	19	6
2:B:4:ARG:NH1	2:B:4:ARG:CG	0.52	2.72	15	2
1:A:31:TRP:NE1	1:A:60:ASP:OD2	0.52	2.42	7	5
1:A:41:PHE:CG	1:A:94:LYS:NZ	0.52	2.70	12	1
2:B:4:ARG:CG	2:B:4:ARG:NH1	0.52	2.70	25	4
1:A:21:LYS:HZ1	1:A:51:ASN:CG	0.52	2.13	18	1
1:A:63:GLN:NE2	2:B:4:ARG:NE	0.52	2.57	21	1
1:A:20:ASP:OD1	1:A:82:LYS:NZ	0.52	2.41	28	1
1:A:38:ILE:O	1:A:38:ILE:CG2	0.51	2.59	5	6
1:A:37:MET:SD	1:A:37:MET:O	0.51	2.68	22	8
1:A:31:TRP:CH2	2:B:3:PHE:CD2	0.51	2.99	19	4
1:A:31:TRP:HE1	1:A:60:ASP:CG	0.51	2.13	23	6
1:A:58:ASP:C	1:A:60:ASP:H	0.50	2.15	4	4
1:A:58:ASP:O	1:A:60:ASP:N	0.50	2.44	4	2
1:A:44:SER:C	1:A:46:SER:N	0.49	2.69	3	24
1:A:38:ILE:C	1:A:40:PRO:HD2	0.49	2.32	2	9
1:A:83:GLY:C	1:A:84:GLN:HE21	0.49	2.15	20	4
1:A:83:GLY:C	1:A:84:GLN:NE2	0.49	2.71	3	4
1:A:26:ASP:CG	1:A:28:SER:HG	0.49	2.15	7	1
1:A:72:LYS:C	2:B:5:TYR:CD2	0.49	2.90	24	4
1:A:85:LYS:CB	1:A:85:LYS:NZ	0.49	2.76	26	4
1:A:66:ALA:O	1:A:70:GLU:N	0.49	2.45	20	10
1:A:91:GLY:O	1:A:93:ASN:N	0.49	2.46	24	3
1:A:37:MET:C	1:A:37:MET:SD	0.48	2.97	15	1
2:B:9:GLY:C	2:B:11:SER:N	0.48	2.71	25	29
1:A:63:GLN:HE22	2:B:4:ARG:CZ	0.48	2.21	21	1
1:A:44:SER:O	1:A:46:SER:N	0.48	2.46	19	14
1:A:22:LEU:CD2	1:A:23:VAL:H	0.48	2.22	6	16
1:A:39:LYS:N	1:A:40:PRO:HD2	0.48	2.24	2	3
1:A:33:GLY:O	1:A:37:MET:N	0.48	2.47	28	15
1:A:2:VAL:CG2	1:A:46:SER:OG	0.47	2.63	4	4
1:A:27:PHE:O	1:A:74:THR:HG22	0.47	2.08	17	2
1:A:31:TRP:CD1	1:A:60:ASP:OD2	0.47	2.68	7	4
1:A:51:ASN:O	1:A:51:ASN:OD1	0.47	2.33	19	7
1:A:39:LYS:C	1:A:41:PHE:H	0.47	2.16	27	1
1:A:93:ASN:ND2	1:A:96:LYS:NZ	0.47	2.63	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:LYS:N	1:A:64:ASP:OD2	0.47	2.48	17	9
1:A:70:GLU:CD	1:A:70:GLU:N	0.47	2.73	22	3
1:A:2:VAL:CG1	1:A:3:LYS:N	0.46	2.78	19	8
1:A:74:THR:O	2:B:8:GLU:N	0.46	2.48	1	4
1:A:40:PRO:O	1:A:44:SER:OG	0.46	2.30	25	6
1:A:71:VAL:O	2:B:5:TYR:CE2	0.46	2.69	10	1
1:A:79:PHE:CD1	1:A:79:PHE:N	0.45	2.83	2	29
1:A:59:VAL:HG11	2:B:5:TYR:OH	0.45	2.11	11	2
1:A:58:ASP:C	1:A:60:ASP:N	0.45	2.74	10	3
1:A:38:ILE:HD12	1:A:75:PRO:CG	0.45	2.41	20	1
1:A:41:PHE:O	1:A:42:PHE:C	0.45	2.60	4	25
1:A:38:ILE:HD12	1:A:75:PRO:HG3	0.45	1.88	20	3
1:A:21:LYS:HZ1	1:A:51:ASN:ND2	0.45	2.08	28	2
1:A:4:GLN:O	1:A:6:GLU:OE2	0.45	2.35	23	2
1:A:71:VAL:O	2:B:5:TYR:CE1	0.45	2.70	26	1
1:A:37:MET:SD	1:A:37:MET:C	0.45	3.00	22	4
1:A:31:TRP:CH2	2:B:3:PHE:CE2	0.44	3.04	2	2
1:A:71:VAL:CG1	2:B:5:TYR:OH	0.44	2.66	18	6
1:A:69:ALA:O	1:A:70:GLU:C	0.44	2.60	25	8
1:A:63:GLN:CD	2:B:4:ARG:NH1	0.44	2.75	5	2
2:B:8:GLU:O	2:B:9:GLY:O	0.44	2.36	25	4
1:A:63:GLN:CD	1:A:63:GLN:C	0.44	2.85	25	2
1:A:59:VAL:N	3:A:108:HOH:O	0.44	2.51	8	6
1:A:20:ASP:OD1	1:A:20:ASP:O	0.44	2.35	28	2
1:A:68:GLU:CD	1:A:68:GLU:C	0.44	2.86	23	7
2:B:9:GLY:O	2:B:11:SER:N	0.44	2.51	21	23
1:A:38:ILE:HG23	1:A:94:LYS:NZ	0.43	2.27	5	2
1:A:88:GLU:N	1:A:88:GLU:OE2	0.43	2.51	22	2
1:A:72:LYS:C	2:B:5:TYR:CD1	0.43	2.96	10	1
1:A:20:ASP:OD1	1:A:81:LYS:NZ	0.43	2.51	28	1
1:A:39:LYS:C	1:A:41:PHE:N	0.43	2.75	27	2
1:A:98:GLU:C	1:A:98:GLU:CD	0.43	2.87	8	7
1:A:87:GLY:C	1:A:88:GLU:CD	0.43	2.87	9	2
2:B:8:GLU:OE1	2:B:8:GLU:C	0.43	2.61	20	1
1:A:39:LYS:NZ	1:A:39:LYS:CB	0.43	2.81	26	2
1:A:88:GLU:CD	1:A:88:GLU:C	0.43	2.87	21	5
2:B:5:TYR:CD1	2:B:5:TYR:N	0.43	2.86	23	3
1:A:36:LYS:CB	1:A:36:LYS:NZ	0.43	2.82	18	1
1:A:67:SER:O	1:A:70:GLU:OE2	0.43	2.37	18	1
1:A:21:LYS:HZ2	1:A:51:ASN:ND2	0.43	2.11	28	1
1:A:21:LYS:N	3:A:109:HOH:O	0.42	2.52	22	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ALA:C	1:A:64:ASP:N	0.42	2.77	4	6
1:A:87:GLY:C	1:A:88:GLU:OE1	0.42	2.62	23	1
1:A:60:ASP:OD1	2:B:4:ARG:N	0.42	2.52	28	1
1:A:21:LYS:HZ1	1:A:51:ASN:HD21	0.42	1.57	28	1
1:A:44:SER:C	1:A:46:SER:H	0.42	2.23	19	4
1:A:8:LYS:HZ1	1:A:68:GLU:CD	0.42	2.22	2	1
1:A:6:GLU:OE1	1:A:6:GLU:N	0.42	2.52	12	1
1:A:55:LEU:N	1:A:55:LEU:CD1	0.42	2.83	11	11
1:A:60:ASP:OD1	2:B:3:PHE:C	0.42	2.62	26	7
1:A:6:GLU:N	1:A:6:GLU:CD	0.42	2.78	12	2
1:A:20:ASP:O	1:A:20:ASP:OD1	0.42	2.38	30	1
1:A:96:LYS:O	1:A:97:LEU:C	0.42	2.62	7	9
1:A:77:PHE:CE1	1:A:97:LEU:HD21	0.42	2.48	29	4
1:A:6:GLU:CD	1:A:6:GLU:H	0.41	2.23	30	1
1:A:39:LYS:CG	1:A:40:PRO:HD3	0.41	2.46	25	1
1:A:38:ILE:HG23	1:A:94:LYS:HZ2	0.41	1.76	5	1
1:A:68:GLU:O	1:A:70:GLU:OE1	0.41	2.38	3	1
1:A:20:ASP:O	1:A:20:ASP:CG	0.41	2.64	9	4
1:A:71:VAL:CG1	1:A:76:THR:OG1	0.41	2.69	5	2
1:A:60:ASP:OD2	2:B:3:PHE:C	0.41	2.64	12	1
2:B:8:GLU:OE1	2:B:8:GLU:O	0.41	2.37	20	1
1:A:49:TYR:C	1:A:51:ASN:N	0.41	2.78	26	1
1:A:59:VAL:CG1	2:B:5:TYR:OH	0.41	2.68	17	1
1:A:102:ASN:O	1:A:102:ASN:OD1	0.41	2.39	17	2
1:A:55:LEU:HD12	1:A:55:LEU:N	0.41	2.31	12	4
1:A:27:PHE:CE1	1:A:78:GLN:CD	0.40	2.98	25	1
1:A:21:LYS:NZ	1:A:51:ASN:HD21	0.40	2.12	28	1
1:A:41:PHE:CB	1:A:94:LYS:HZ2	0.40	2.28	12	1
1:A:98:GLU:C	1:A:98:GLU:OE2	0.40	2.64	20	1
1:A:74:THR:HG23	2:B:5:TYR:HE2	0.40	1.76	1	1
1:A:63:GLN:OE1	2:B:4:ARG:NH1	0.40	2.55	17	1
1:A:81:LYS:C	1:A:83:GLY:N	0.40	2.78	20	1
1:A:68:GLU:CD	1:A:68:GLU:O	0.40	2.65	27	1

6.3 Torsion angles ⓘ

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	103/105 (98%)	89±1 (87±1%)	13±1 (12±1%)	1±0 (1±0%)	15	65
2	B	9/13 (69%)	4±0 (50±6%)	4±1 (40±11%)	1±1 (10±8%)	1	9
All	All	3360/3540 (95%)	2812 (84%)	489 (15%)	59 (2%)	9	52

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	92	ALA	29
2	B	9	GLY	20
2	B	10	PRO	8
1	A	59	VAL	2

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	86/88 (98%)	82±1 (95±2%)	4±1 (5±2%)	23	73
2	B	8/11 (73%)	8±1 (97±6%)	0±1 (3±6%)	34	83
All	All	2820/2970 (95%)	2680 (95%)	140 (5%)	23	74

All 22 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	22	LEU	30
1	A	39	LYS	30
1	A	94	LYS	23
1	A	82	LYS	8
1	A	61	ASP	7
2	B	4	ARG	7
1	A	85	LYS	6
1	A	64	ASP	5
1	A	20	ASP	4
1	A	96	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	8	LYS	2
1	A	93	ASN	2
1	A	72	LYS	2
1	A	88	GLU	2
1	A	37	MET	1
1	A	3	LYS	1
1	A	36	LYS	1
2	B	8	GLU	1
1	A	63	GLN	1
1	A	21	LYS	1
1	A	48	LYS	1
1	A	84	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided