



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:53 AM UTC

PDB ID : 2KZ1 / pdb_00002kz1
Title : Inter-molecular interactions in a 44 kDa interferon-receptor complex detected by asymmetric back-protonation and 2D NOESY
Authors : Nudelman, I.; Akabayov, S.R.; Schnur, E.; Biron, Z.; Levy, R.; Xu, Y.; Yang, D.; Anglister, J.
Deposited on : 2010-06-10

This is a Full wwPDB NMR 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/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

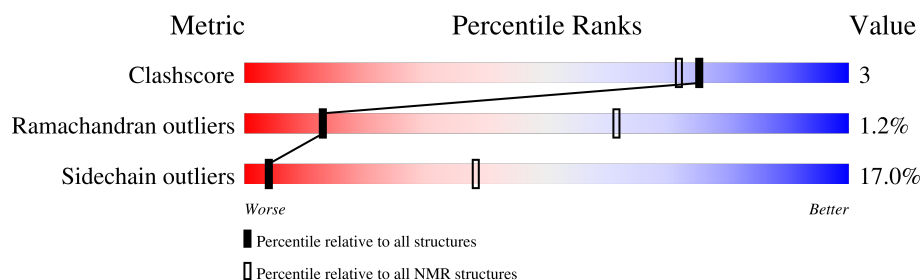
1 Overall quality at a glance

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	165	
2	B	212	

2 Ensemble composition and analysis

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:1-A:156, B:11-B:206 (352)	0.62	6

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 3 clusters and 3 single-model clusters were found.

Cluster number	Models
1	4, 9, 10
2	3, 6
3	2, 8
Single-model clusters	1; 5; 7

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5823 atoms, of which 2896 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Interferon alpha-2.

Mol	Chain	Residues	Atoms						Trace
1	A	165	Total	C	H	N	O	S	0
			2699	860	1348	227	255	9	

- Molecule 2 is a protein called Soluble IFN alpha/beta receptor.

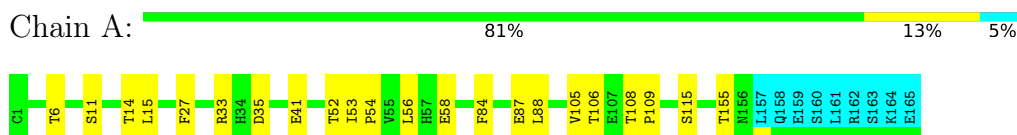
Mol	Chain	Residues	Atoms						Trace
2	B	196	Total	C	H	N	O	S	0
			3124	1014	1548	253	299	10	

4 Residue-property plots

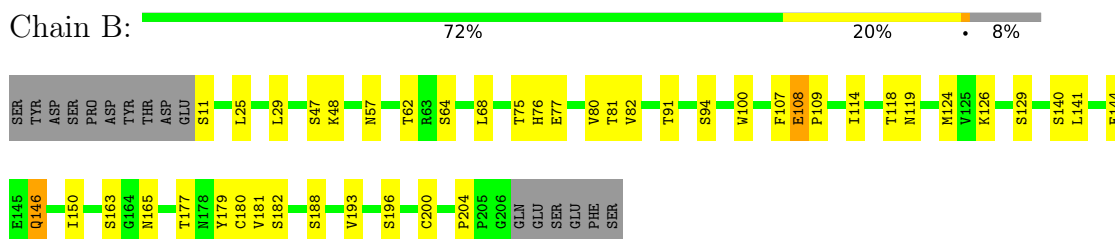
4.1 Average score per residue in the NMR ensemble

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: Interferon alpha-2



- Molecule 2: Soluble IFN alpha/beta receptor

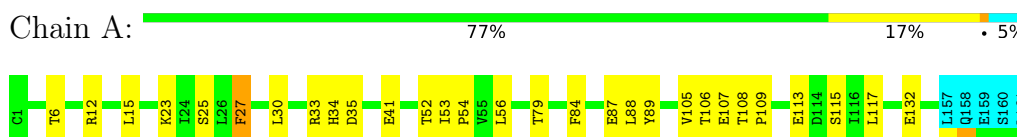


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

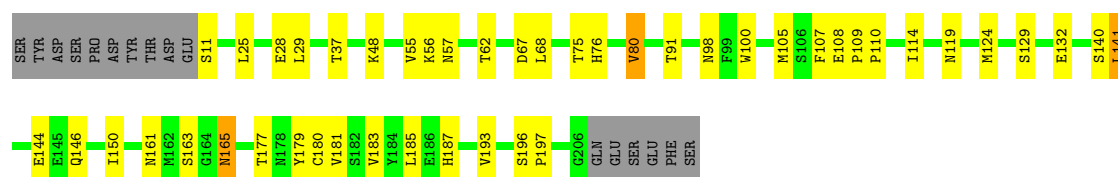
4.2.1 Score per residue for model 1

- Molecule 1: Interferon alpha-2



- Molecule 2: Soluble IFN alpha/beta receptor

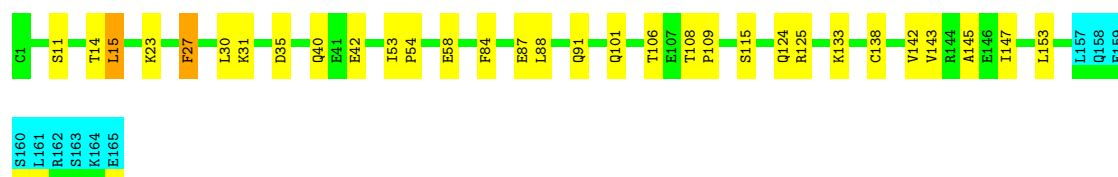




4.2.2 Score per residue for model 2

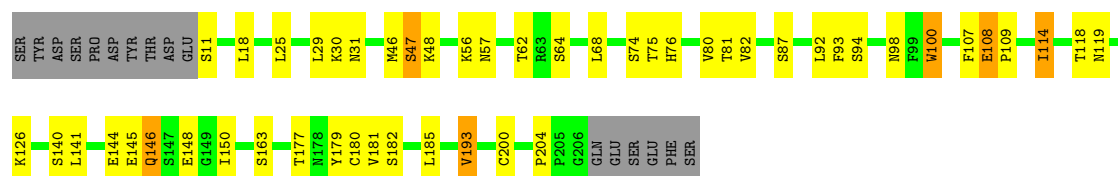
- Molecule 1: Interferon alpha-2

Chain A: 76% 18% 5%



- Molecule 2: Soluble IFN alpha/beta receptor

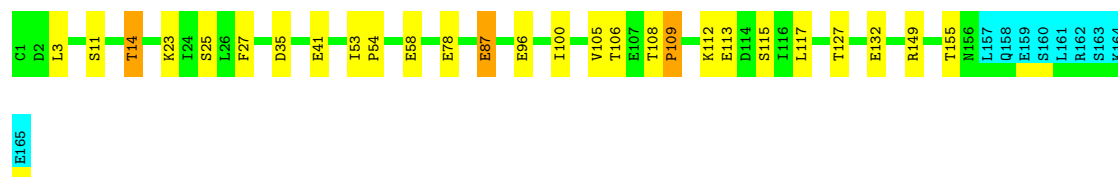
Chain B: 69% 21% 8%



4.2.3 Score per residue for model 3

- Molecule 1: Interferon alpha-2

Chain A: 78% 15% 5%



- Molecule 2: Soluble IFN alpha/beta receptor

Chain B: 70% 21% 8%

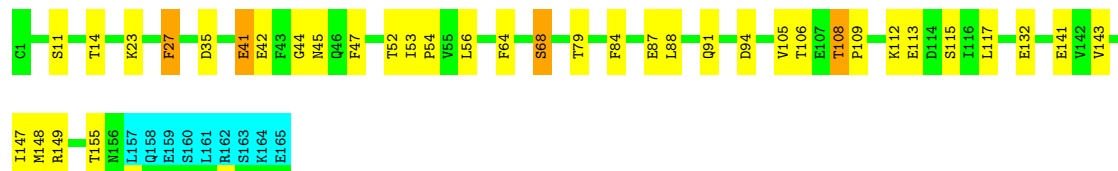




4.2.4 Score per residue for model 4

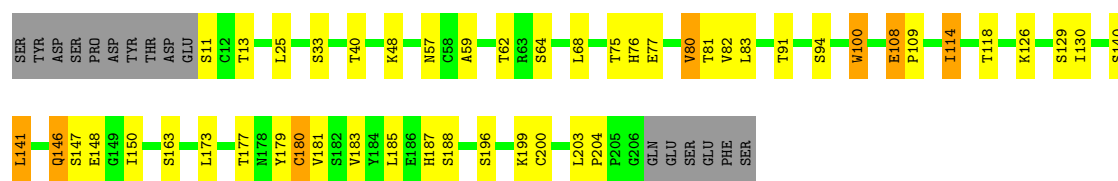
- Molecule 1: Interferon alpha-2

Chain A: 72% 20% 5%



- Molecule 2: Soluble IFN alpha/beta receptor

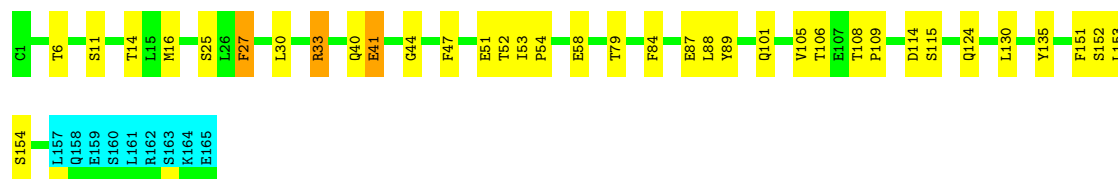
Chain B: 69% 20% 8%



4.2.5 Score per residue for model 5

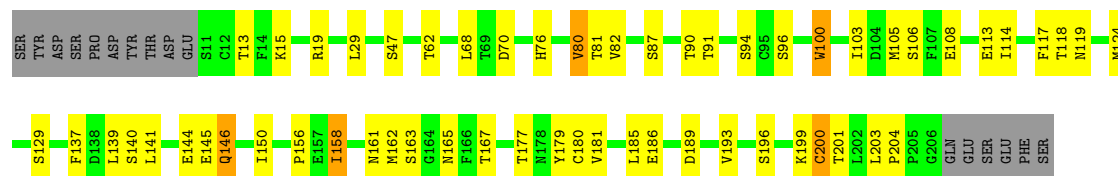
- Molecule 1: Interferon alpha-2

Chain A: 73% 20% 5%



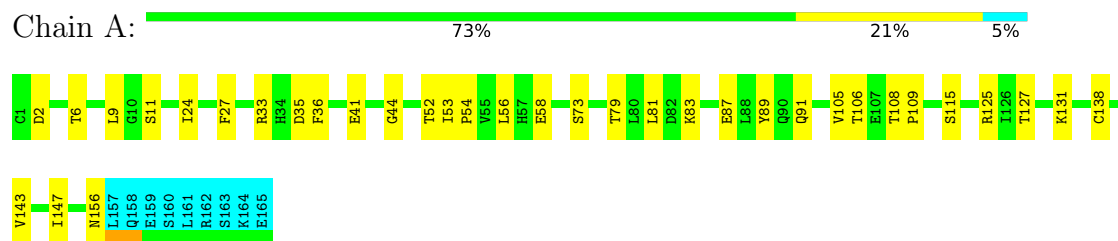
- Molecule 2: Soluble IFN alpha/beta receptor

Chain B: 65% 25% 8%

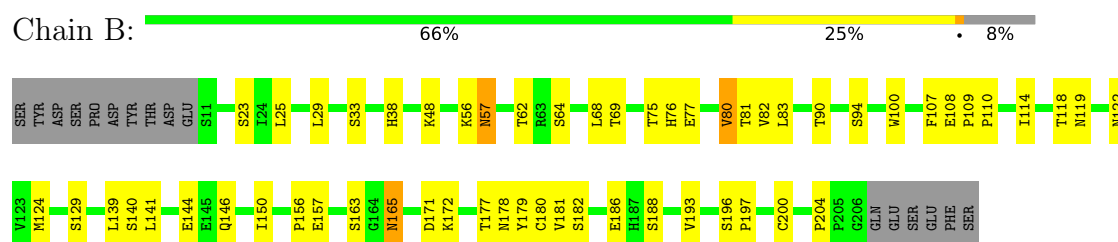


4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Interferon alpha-2

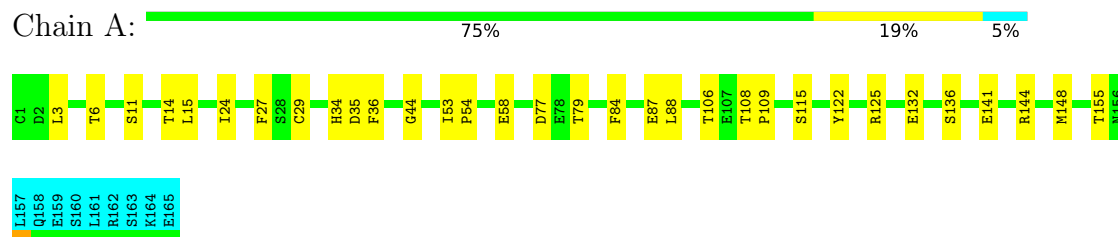


- Molecule 2: Soluble IFN alpha/beta receptor

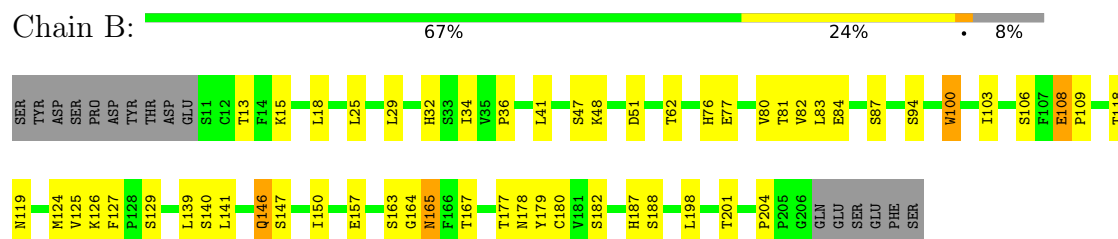


4.2.7 Score per residue for model 7

- Molecule 1: Interferon alpha-2



- Molecule 2: Soluble IFN alpha/beta receptor



4.2.8 Score per residue for model 8

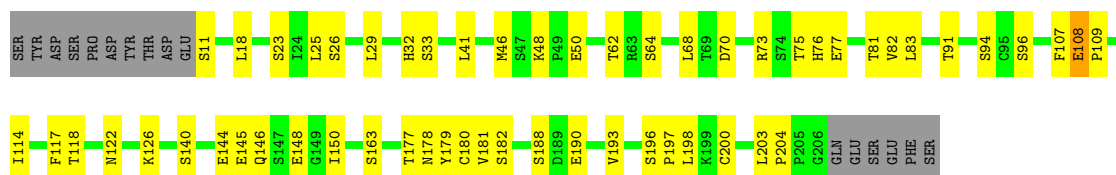
- Molecule 1: Interferon alpha-2

Chain A: 



- Molecule 2: Soluble IFN alpha/beta receptor

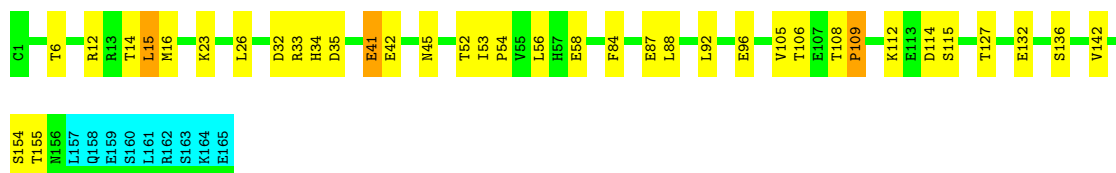
Chain B: 



4.2.9 Score per residue for model 9

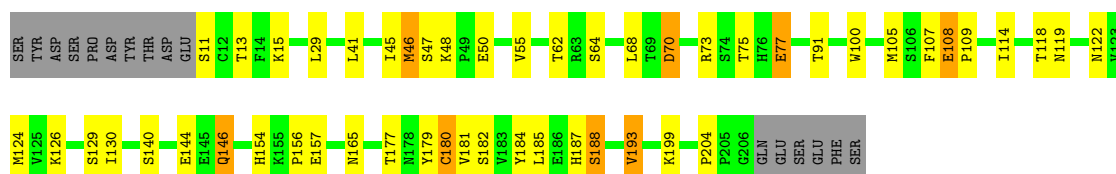
- Molecule 1: Interferon alpha-2

Chain A: 



- Molecule 2: Soluble IFN alpha/beta receptor

Chain B: 

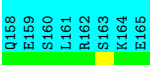


4.2.10 Score per residue for model 10

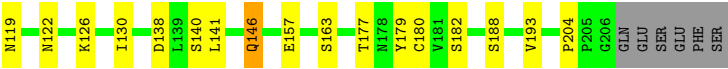
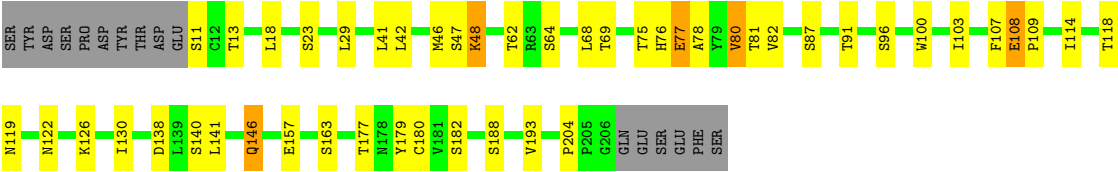
- Molecule 1: Interferon alpha-2

Chain A: 





● Molecule 2: Soluble IFN alpha/beta receptor



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, molecular dynamics*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
HADDOCK	refinement	2.0

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	1275	1270	1269	10±2
2	B	1576	1548	1547	10±2
All	All	28510	28180	28160	176

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:PHE:CE2	2:B:80:VAL:HB	0.65	2.27	4	6
2:B:146:GLN:O	2:B:179:TYR:HA	0.62	1.95	6	10
1:A:33:ARG:HD2	1:A:33:ARG:O	0.61	1.96	5	3
1:A:35:ASP:OD1	2:B:48:LYS:HE2	0.58	1.98	4	2
2:B:146:GLN:HA	2:B:150:ILE:O	0.57	2.00	6	8
2:B:141:LEU:HD11	2:B:183:VAL:HG13	0.56	1.77	4	3
1:A:64:PHE:O	1:A:68:SER:HB2	0.55	2.01	10	2
2:B:179:TYR:CE2	2:B:201:THR:HB	0.55	2.36	7	2
1:A:35:ASP:CB	2:B:48:LYS:HE2	0.53	2.33	7	2
1:A:36:PHE:HA	1:A:125:ARG:NH1	0.52	2.19	7	2
1:A:109:PRO:O	1:A:112:LYS:HG2	0.52	2.03	8	3
2:B:45:ILE:HB	2:B:77:GLU:OE2	0.52	2.05	9	1
1:A:53:ILE:N	1:A:54:PRO:HD2	0.51	2.21	6	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:109:PRO:N	2:B:110:PRO:HD2	0.51	2.21	3	3
1:A:52:THR:O	1:A:56:LEU:HG	0.51	2.06	10	5
1:A:84:PHE:O	1:A:88:LEU:HG	0.50	2.07	5	7
2:B:144:GLU:O	2:B:181:VAL:HA	0.49	2.06	5	7
2:B:83:LEU:O	2:B:94:SER:HA	0.49	2.07	4	4
2:B:124:MET:SD	2:B:165:ASN:HB2	0.49	2.48	1	6
2:B:40:THR:HG23	2:B:59:ALA:HA	0.48	1.83	4	1
1:A:15:LEU:HD11	2:B:100:TRP:CZ2	0.48	2.44	2	1
2:B:70:ASP:OD2	2:B:73:ARG:HD3	0.48	2.08	9	1
1:A:15:LEU:HD11	2:B:100:TRP:CH2	0.47	2.44	9	2
1:A:113:GLU:O	1:A:117:LEU:HG	0.47	2.09	3	3
1:A:47:PHE:O	1:A:52:THR:HB	0.47	2.09	4	2
1:A:143:VAL:O	1:A:147:ILE:HG12	0.47	2.09	2	3
1:A:144:ARG:NH1	1:A:145:ALA:HA	0.47	2.25	10	1
2:B:114:ILE:HD13	2:B:181:VAL:HB	0.46	1.87	2	2
2:B:108:GLU:H	2:B:109:PRO:CD	0.46	2.24	7	4
2:B:18:LEU:HD23	2:B:107:PHE:CZ	0.46	2.46	10	1
1:A:54:PRO:HD3	1:A:105:VAL:CG1	0.45	2.42	3	7
2:B:158:ILE:HG22	2:B:162:MET:HB2	0.45	1.88	5	1
2:B:56:LYS:O	2:B:57:ASN:HB3	0.45	2.11	2	3
1:A:56:LEU:HD22	1:A:154:SER:HB3	0.45	1.87	9	1
1:A:54:PRO:O	1:A:58:GLU:HG2	0.45	2.12	3	1
1:A:130:LEU:HB3	1:A:135:TYR:CE1	0.45	2.47	5	1
1:A:26:LEU:HG	2:B:46:MET:O	0.45	2.11	9	1
1:A:35:ASP:HA	2:B:48:LYS:HE2	0.45	1.89	3	4
1:A:138:CYS:O	1:A:142:VAL:HG23	0.44	2.12	8	3
1:A:16:MET:SD	2:B:189:ASP:HB2	0.44	2.52	5	1
2:B:46:MET:HB3	2:B:77:GLU:OE1	0.44	2.12	10	1
1:A:35:ASP:HB2	2:B:48:LYS:NZ	0.44	2.27	10	1
2:B:108:GLU:H	2:B:109:PRO:HD2	0.44	1.73	4	3
1:A:148:MET:HE2	2:B:100:TRP:HE1	0.44	1.73	4	1
2:B:117:PHE:O	2:B:203:LEU:HB2	0.44	2.13	8	2
2:B:180:CYS:HA	2:B:199:LYS:O	0.43	2.13	4	2
1:A:41:GLU:CD	1:A:41:GLU:H	0.43	2.21	5	2
1:A:36:PHE:HB2	1:A:122:TYR:CE1	0.43	2.48	7	1
1:A:12:ARG:HG2	2:B:187:HIS:CE1	0.43	2.49	1	1
1:A:144:ARG:O	1:A:148:MET:HB2	0.43	2.14	7	1
1:A:148:MET:SD	2:B:46:MET:HE1	0.43	2.54	8	1
2:B:77:GLU:HA	2:B:100:TRP:CH2	0.43	2.48	7	1
1:A:24:ILE:HD12	1:A:29:CYS:SG	0.43	2.54	7	1
2:B:34:ILE:O	2:B:36:PRO:HD3	0.42	2.14	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:147:SER:HA	2:B:178:ASN:O	0.42	2.14	7	1
2:B:92:LEU:HG	2:B:93:PHE:CD2	0.42	2.49	2	1
1:A:108:THR:O	1:A:112:LYS:HD3	0.42	2.14	4	1
2:B:100:TRP:HB3	2:B:103:ILE:HG22	0.42	1.90	5	1
2:B:125:VAL:O	2:B:165:ASN:HA	0.42	2.14	7	1
1:A:115:SER:O	1:A:119:VAL:HG23	0.42	2.14	10	2
1:A:41:GLU:O	1:A:45:ASN:HB2	0.42	2.15	9	2
2:B:70:ASP:OD1	2:B:73:ARG:HD3	0.42	2.14	8	1
2:B:154:HIS:O	2:B:156:PRO:HD3	0.42	2.14	9	1
2:B:113:GLU:OE1	2:B:199:LYS:HE2	0.42	2.15	5	1
1:A:73:SER:HA	1:A:81:LEU:HD13	0.42	1.91	6	2
2:B:46:MET:HB2	2:B:78:ALA:O	0.42	2.15	10	1
1:A:145:ALA:HB1	2:B:47:SER:HA	0.41	1.92	2	1
1:A:33:ARG:NH1	2:B:50:GLU:HB2	0.41	2.31	8	1
2:B:127:PHE:HB2	2:B:164:GLY:O	0.41	2.16	7	1
1:A:14:THR:HG23	1:A:87:GLU:HB3	0.41	1.92	3	1
1:A:35:ASP:HB2	2:B:48:LYS:HE2	0.41	1.92	7	1
1:A:16:MET:SD	2:B:188:SER:HB2	0.41	2.55	9	1
1:A:32:ASP:O	1:A:142:VAL:HG21	0.40	2.16	9	1
1:A:92:LEU:O	1:A:96:GLU:HG2	0.40	2.16	9	1
1:A:96:GLU:O	1:A:100:ILE:HG13	0.40	2.17	3	1
2:B:179:TYR:O	2:B:200:CYS:HA	0.40	2.17	5	1
2:B:171:ASP:O	2:B:172:LYS:HB2	0.40	2.17	6	1
1:A:57:HIS:CD2	1:A:96:GLU:HB3	0.40	2.52	8	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	155/165 (94%)	139±2 (90±2%)	14±2 (9±2%)	1±0 (1±0%)	18	68
2	B	194/212 (92%)	165±3 (85±1%)	26±2 (13±1%)	3±1 (1±1%)	11	57
All	All	3490/3770 (93%)	3046 (87%)	403 (12%)	41 (1%)	13	61

All 10 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	109	PRO	10
2	B	108	GLU	10
2	B	204	PRO	8
2	B	197	PRO	3
1	A	31	LYS	2
2	B	193	VAL	2
2	B	106	SER	2
2	B	156	PRO	2
2	B	119	ASN	1
2	B	188	SER	1

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	143/152 (94%)	124±2 (87±1%)	19±2 (13±1%)	6	46
2	B	185/201 (92%)	148±2 (80±1%)	37±2 (20±1%)	3	33
All	All	3280/3530 (93%)	2724 (83%)	556 (17%)	4	38

All 149 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	106	THR	10
1	A	108	THR	10
1	A	115	SER	10
2	B	62	THR	10
2	B	140	SER	10
2	B	177	THR	10
2	B	180	CYS	10
1	A	87	GLU	9
2	B	29	LEU	9
2	B	163	SER	9
2	B	118	THR	9
1	A	27	PHE	8
1	A	41	GLU	8

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Mol	Chain	Res	Type	Models (Total)
2	B	68	LEU	8
2	B	75	THR	8
2	B	76	HIS	8
2	B	114	ILE	8
2	B	141	LEU	8
2	B	193	VAL	8
1	A	11	SER	8
1	A	14	THR	8
2	B	81	THR	8
2	B	82	VAL	8
2	B	11	SER	7
2	B	100	TRP	7
2	B	119	ASN	7
2	B	64	SER	7
2	B	126	LYS	7
2	B	146	GLN	7
1	A	6	THR	6
2	B	25	LEU	6
2	B	80	VAL	6
2	B	91	THR	6
2	B	107	PHE	6
2	B	129	SER	6
2	B	196	SER	6
1	A	58	GLU	6
2	B	182	SER	6
2	B	200	CYS	6
1	A	155	THR	6
2	B	77	GLU	6
1	A	23	LYS	5
1	A	33	ARG	5
1	A	79	THR	5
1	A	132	GLU	5
2	B	185	LEU	5
2	B	47	SER	5
2	B	41	LEU	5
2	B	13	THR	5
2	B	188	SER	5
1	A	15	LEU	4
1	A	89	TYR	4
2	B	105	MET	4
1	A	42	GLU	4
2	B	18	LEU	4

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Mol	Chain	Res	Type	Models (Total)
2	B	87	SER	4
2	B	145	GLU	4
2	B	148	GLU	4
2	B	33	SER	4
2	B	122	ASN	4
2	B	157	GLU	4
1	A	25	SER	3
1	A	30	LEU	3
1	A	34	HIS	3
2	B	55	VAL	3
2	B	165	ASN	3
1	A	91	GLN	3
1	A	101	GLN	3
1	A	153	LEU	3
1	A	3	LEU	3
1	A	127	THR	3
1	A	149	ARG	3
2	B	32	HIS	3
2	B	57	ASN	3
2	B	130	ILE	3
2	B	187	HIS	3
1	A	114	ASP	3
2	B	15	LYS	3
2	B	96	SER	3
2	B	139	LEU	3
2	B	23	SER	3
2	B	28	GLU	2
2	B	98	ASN	2
2	B	161	ASN	2
1	A	40	GLN	2
1	A	124	GLN	2
2	B	31	ASN	2
2	B	46	MET	2
2	B	94	SER	2
2	B	26	SER	2
2	B	173	LEU	2
1	A	68	SER	2
1	A	141	GLU	2
2	B	70	ASP	2
2	B	90	THR	2
2	B	167	THR	2
2	B	186	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	2	ASP	2
1	A	83	LYS	2
2	B	69	THR	2
2	B	178	ASN	2
1	A	136	SER	2
2	B	103	ILE	2
2	B	198	LEU	2
1	A	107	GLU	1
2	B	37	THR	1
2	B	67	ASP	1
2	B	132	GLU	1
1	A	125	ARG	1
1	A	133	LYS	1
2	B	30	LYS	1
2	B	74	SER	1
1	A	78	GLU	1
2	B	56	LYS	1
2	B	108	GLU	1
2	B	202	LEU	1
1	A	56	LEU	1
1	A	94	ASP	1
2	B	147	SER	1
2	B	203	LEU	1
1	A	51	GLU	1
1	A	151	PHE	1
1	A	152	SER	1
1	A	154	SER	1
2	B	19	ARG	1
2	B	137	PHE	1
2	B	158	ILE	1
1	A	9	LEU	1
1	A	24	ILE	1
1	A	131	LYS	1
1	A	138	CYS	1
1	A	156	ASN	1
2	B	38	HIS	1
1	A	77	ASP	1
2	B	51	ASP	1
2	B	84	GLU	1
1	A	8	SER	1
1	A	146	GLU	1
2	B	190	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	12	ARG	1
2	B	50	GLU	1
2	B	184	TYR	1
1	A	5	GLN	1
1	A	31	LYS	1
1	A	71	ASP	1
1	A	72	SER	1
2	B	42	LEU	1
2	B	48	LYS	1
2	B	138	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided