



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:37 PM BST

PDB ID : 1RGD
Title : STRUCTURE REFINEMENT OF THE GLUCOCORTICOID RECEPTOR-DNA BINDING DOMAIN FROM NMR DATA BY RELAXATION MATRIX CALCULATIONS
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Deposited on : 1995-01-06

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We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

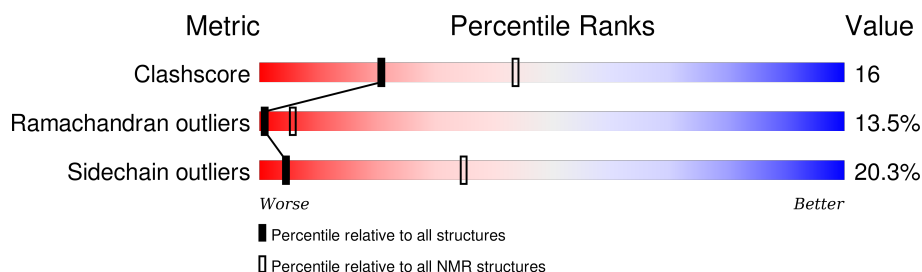
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	71	

2 Ensemble composition and analysis ⓘ

This entry contains 11 models. Model 7 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:1-A:37, A:43-A:70 (65)	0.84	7

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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 3, 4, 7, 9, 10
2	5, 6, 8, 11
Single-model clusters	1

3 Entry composition [i](#)

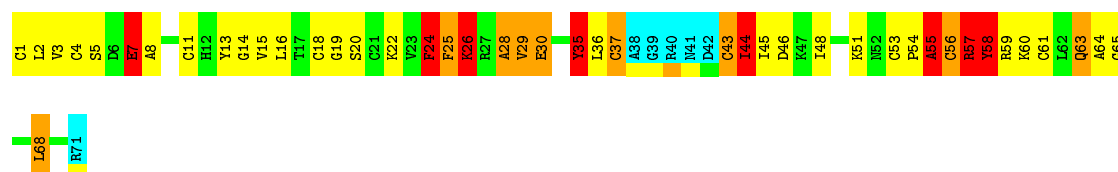
There are 2 unique types of molecules in this entry. The entry contains 550 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GLUCOCORTICOID RECEPTOR.

Mol	Chain	Residues	Atoms					Trace
1	A	71	Total	C	N	O	S	0
			548	333	107	97	11	

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

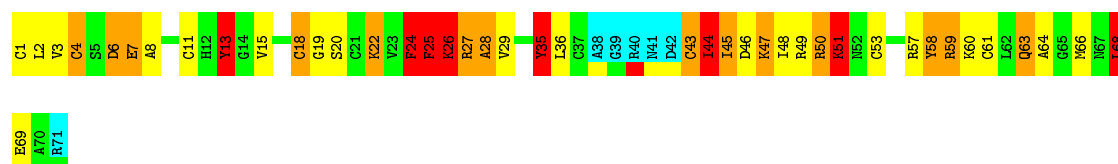
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2



4.2.3 Score per residue for model 3

- Molecule 1: GLUCOCORTICOID RECEPTOR

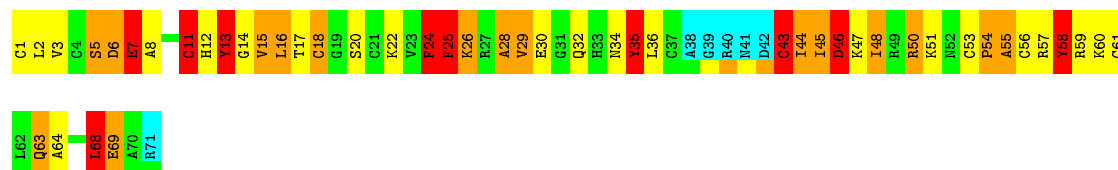
Chain A: 32% 28% 20% 11% 8%



4.2.4 Score per residue for model 4

- Molecule 1: GLUCOCORTICOID RECEPTOR

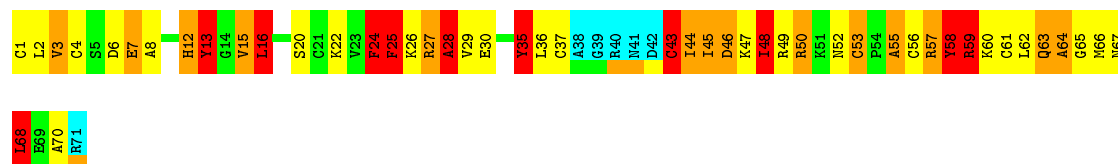
Chain A: 24% 31% 23% 14% 8%



4.2.5 Score per residue for model 5

- Molecule 1: GLUCOCORTICOID RECEPTOR

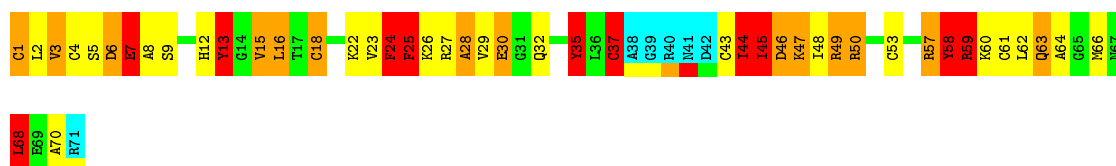
Chain A: 24% 32% 20% 15% 8%



4.2.6 Score per residue for model 6

- Molecule 1: GLUCOCORTICOID RECEPTOR

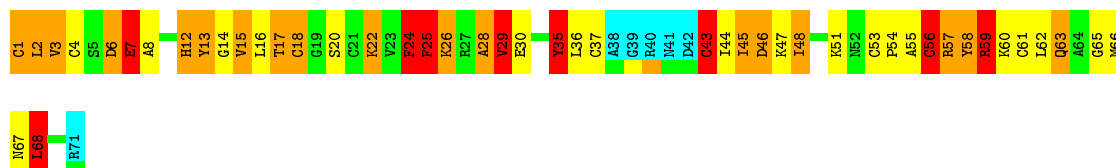
Chain A: 27% 30% 20% 15% 8%



4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: GLUCOCORTICOID RECEPTOR

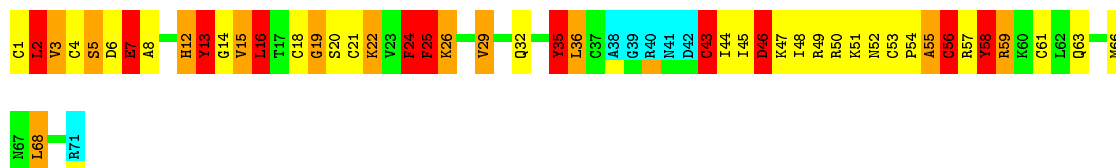
Chain A: 25% 28% 25% 13% 8%



4.2.8 Score per residue for model 8

- Molecule 1: GLUCOCORTICOID RECEPTOR

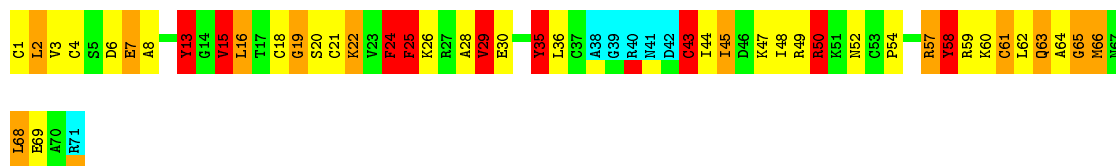
Chain A: 27% 32% 17% 15% 8%



4.2.9 Score per residue for model 9

- Molecule 1: GLUCOCORTICOID RECEPTOR

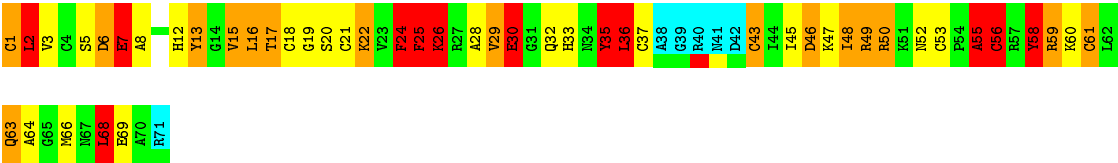
Chain A: 30% 32% 17% 13% 8%



4.2.10 Score per residue for model 10

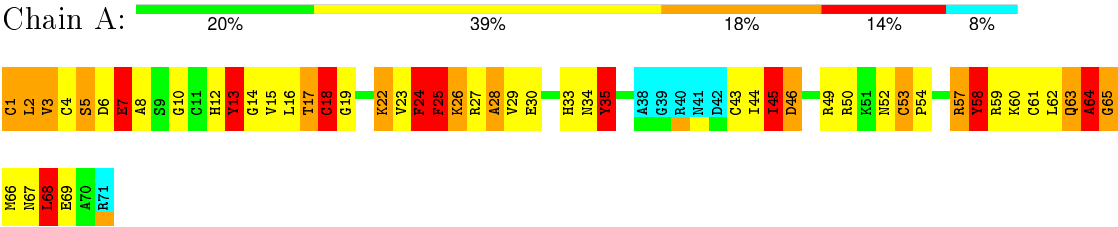
- Molecule 1: GLUCOCORTICOID RECEPTOR

Chain A: 24% 28% 23% 17% 8%



4.2.11 Score per residue for model 11

- Molecule 1: GLUCOCORTICOID RECEPTOR



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 11 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
IRMA	refinement	
DINOSAUR	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.04±0.10	1±1/508 (0.2±0.1%)	3.07±0.16	37±5/680 (5.4±0.7%)
All	All	1.04	13/5588 (0.2%)	3.07	405/7480 (5.4%)

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	Planarity
1	A	0.7±0.7	17.6±2.1
All	All	8	194

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	26	LYS	CA-CB	-8.30	1.35	1.53	7	9
1	A	3	VAL	CA-CB	-5.63	1.43	1.54	7	2
1	A	1	CYS	CA-CB	-5.43	1.42	1.53	5	1
1	A	29	VAL	CA-CB	-5.31	1.43	1.54	4	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	35	TYR	CB-CG-CD2	-38.38	97.97	121.00	11	11
1	A	13	TYR	CB-CG-CD1	-34.92	100.05	121.00	3	10
1	A	24	PHE	CB-CG-CD2	-29.83	99.92	120.80	3	11
1	A	13	TYR	CB-CG-CD2	21.29	133.78	121.00	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	24	PHE	CB-CG-CD1	-20.69	106.31	120.80	10	8
1	A	25	PHE	CB-CG-CD1	-16.88	108.98	120.80	6	4
1	A	58	TYR	CB-CG-CD2	-16.81	110.92	121.00	3	11
1	A	35	TYR	CB-CG-CD1	16.01	130.61	121.00	3	11
1	A	3	VAL	CA-CB-CG1	14.48	132.63	110.90	3	11
1	A	8	ALA	N-CA-CB	-13.49	91.22	110.10	9	11
1	A	2	LEU	CA-CB-CG	-13.01	85.37	115.30	8	11
1	A	68	LEU	CB-CG-CD1	-12.43	89.87	111.00	11	9
1	A	15	VAL	CB-CA-C	11.13	132.55	111.40	10	10
1	A	7	GLU	CA-C-N	-10.29	94.57	117.20	10	11
1	A	25	PHE	CB-CG-CD2	9.48	127.44	120.80	6	8
1	A	55	ALA	N-CA-CB	9.40	123.27	110.10	5	1
1	A	29	VAL	CB-CA-C	8.90	128.31	111.40	6	8
1	A	13	TYR	N-CA-CB	8.82	126.47	110.60	3	7
1	A	58	TYR	CB-CG-CD1	8.76	126.26	121.00	3	6
1	A	68	LEU	N-CA-CB	8.44	127.27	110.40	10	2
1	A	29	VAL	CA-CB-CG1	8.41	123.51	110.90	3	4
1	A	4	CYS	N-CA-CB	8.39	125.71	110.60	11	4
1	A	56	CYS	CA-CB-SG	8.35	129.03	114.00	2	5
1	A	46	ASP	N-CA-CB	8.34	125.61	110.60	10	7
1	A	28	ALA	CB-CA-C	8.12	122.28	110.10	11	4
1	A	63	GLN	CB-CA-C	7.65	125.71	110.40	3	11
1	A	30	GLU	CB-CA-C	7.64	125.67	110.40	6	1
1	A	2	LEU	N-CA-CB	7.61	125.62	110.40	4	2
1	A	45	ILE	CA-CB-CG1	7.51	125.26	111.00	6	3
1	A	43	CYS	CA-CB-SG	7.46	127.43	114.00	10	4
1	A	29	VAL	CA-C-N	-7.35	101.03	117.20	9	6
1	A	66	MET	N-CA-CB	7.31	123.76	110.60	10	1
1	A	15	VAL	CA-CB-CG2	7.28	121.82	110.90	10	2
1	A	44	ILE	CB-CA-C	7.26	126.12	111.60	5	4
1	A	18	CYS	N-CA-CB	7.16	123.49	110.60	8	5
1	A	26	LYS	N-CA-CB	7.09	123.36	110.60	10	1
1	A	1	CYS	N-CA-CB	7.08	123.34	110.60	10	4
1	A	68	LEU	CB-CG-CD2	-7.05	99.01	111.00	7	1
1	A	23	VAL	CG1-CB-CG2	7.02	122.14	110.90	11	1
1	A	1	CYS	CB-CA-C	7.00	124.39	110.40	2	4
1	A	26	LYS	CB-CA-C	6.99	124.38	110.40	2	7
1	A	35	TYR	N-CA-CB	6.95	123.11	110.60	1	1
1	A	29	VAL	CA-CB-CG2	-6.93	100.51	110.90	8	1
1	A	13	TYR	CD1-CG-CD2	6.92	125.51	117.90	11	9
1	A	35	TYR	CD1-CG-CD2	6.88	125.46	117.90	5	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	26	LYS	CA-CB-CG	6.87	128.52	113.40	2	7
1	A	28	ALA	C-N-CA	6.85	138.81	121.70	5	9
1	A	68	LEU	CB-CA-C	6.80	123.11	110.20	7	4
1	A	1	CYS	CA-CB-SG	6.77	126.19	114.00	9	5
1	A	17	THR	CA-CB-CG2	6.74	121.83	112.40	10	3
1	A	57	ARG	N-CA-CB	-6.68	98.57	110.60	7	2
1	A	16	LEU	CA-C-N	-6.61	102.65	117.20	8	3
1	A	48	ILE	CG1-CB-CG2	-6.60	96.88	111.40	10	3
1	A	35	TYR	CG-CD1-CE1	-6.54	116.07	121.30	5	8
1	A	50	ARG	NE-CZ-NH1	6.45	123.53	120.30	4	2
1	A	43	CYS	CA-C-N	-6.44	103.04	117.20	4	2
1	A	5	SER	CA-C-N	-6.37	103.18	117.20	11	2
1	A	58	TYR	CA-CB-CG	6.35	125.47	113.40	3	1
1	A	29	VAL	N-CA-CB	6.34	125.45	111.50	9	1
1	A	43	CYS	CB-CA-C	6.33	123.06	110.40	3	4
1	A	55	ALA	C-N-CA	6.32	137.50	121.70	2	4
1	A	13	TYR	CD1-CE1-CZ	-6.29	114.14	119.80	2	4
1	A	7	GLU	N-CA-C	6.26	127.91	111.00	10	1
1	A	53	CYS	CB-CA-C	6.25	122.91	110.40	8	1
1	A	2	LEU	CB-CG-CD2	6.21	121.55	111.00	8	1
1	A	44	ILE	N-CA-CB	6.20	125.06	110.80	2	2
1	A	13	TYR	CG-CD2-CE2	-6.18	116.36	121.30	2	5
1	A	35	TYR	CZ-CE2-CD2	-6.18	114.24	119.80	3	1
1	A	23	VAL	CB-CA-C	6.15	123.08	111.40	11	1
1	A	15	VAL	CA-C-N	-6.14	103.69	117.20	9	4
1	A	48	ILE	CA-CB-CG2	6.11	123.13	110.90	8	6
1	A	45	ILE	CG1-CB-CG2	5.97	124.53	111.40	1	1
1	A	13	TYR	CB-CA-C	5.96	122.31	110.40	10	2
1	A	65	GLY	CA-C-N	-5.93	104.15	117.20	9	5
1	A	7	GLU	N-CA-CB	-5.79	100.17	110.60	6	1
1	A	59	ARG	NE-CZ-NH1	5.77	123.18	120.30	8	2
1	A	48	ILE	CA-CB-CG1	5.76	121.95	111.00	9	2
1	A	46	ASP	C-N-CA	5.75	136.08	121.70	1	1
1	A	37	CYS	CB-CA-C	5.75	121.89	110.40	6	1
1	A	25	PHE	C-N-CA	5.66	135.85	121.70	10	1
1	A	67	ASN	C-N-CA	5.53	135.52	121.70	1	1
1	A	3	VAL	N-CA-CB	5.49	123.58	111.50	8	2
1	A	18	CYS	CB-CA-C	-5.47	99.47	110.40	8	1
1	A	6	ASP	CB-CA-C	5.42	121.23	110.40	10	1
1	A	51	LYS	CB-CA-C	5.41	121.23	110.40	1	1
1	A	2	LEU	CB-CG-CD1	5.39	120.17	111.00	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	68	LEU	CA-CB-CG	5.39	127.69	115.30	11	1
1	A	49	ARG	NE-CZ-NH1	5.38	122.99	120.30	6	1
1	A	66	MET	CG-SD-CE	5.36	108.78	100.20	3	1
1	A	64	ALA	C-N-CA	5.36	133.55	122.30	5	2
1	A	27	ARG	NE-CZ-NH1	5.34	122.97	120.30	3	1
1	A	29	VAL	CG1-CB-CG2	-5.32	102.38	110.90	8	2
1	A	22	LYS	N-CA-CB	-5.32	101.02	110.60	1	1
1	A	58	TYR	CD1-CG-CD2	5.24	123.67	117.90	2	3
1	A	36	LEU	N-CA-C	5.22	125.11	111.00	10	1
1	A	27	ARG	N-CA-C	5.20	125.03	111.00	5	1
1	A	5	SER	N-CA-C	5.19	125.02	111.00	10	1
1	A	26	LYS	CB-CG-CD	5.19	125.09	111.60	11	1
1	A	25	PHE	CD1-CG-CD2	5.17	125.02	118.30	3	2
1	A	6	ASP	N-CA-CB	-5.15	101.33	110.60	10	1
1	A	8	ALA	N-CA-C	5.08	124.73	111.00	2	1
1	A	45	ILE	CB-CA-C	5.08	121.77	111.60	11	1
1	A	16	LEU	N-CA-C	5.06	124.66	111.00	1	1
1	A	27	ARG	C-N-CA	5.05	134.33	121.70	11	1
1	A	55	ALA	CA-C-N	-5.05	106.09	117.20	8	1
1	A	47	LYS	N-CA-CB	-5.04	101.52	110.60	1	1
1	A	62	LEU	C-N-CA	5.04	134.30	121.70	6	1
1	A	1	CYS	CA-C-N	-5.04	106.12	117.20	10	1
1	A	46	ASP	CB-CA-C	5.02	120.44	110.40	8	1
1	A	34	ASN	N-CA-CB	5.01	119.62	110.60	11	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	15	VAL	CA	6
1	A	44	ILE	CA	1
1	A	13	TYR	CA	1

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	25	PHE	Mainchain,Sidechain	11
1	A	35	TYR	Sidechain	11
1	A	61	CYS	Mainchain	11
1	A	24	PHE	Sidechain,Mainchain	11
1	A	59	ARG	Mainchain	11

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	64	ALA	Mainchain	9
1	A	20	SER	Mainchain	9
1	A	6	ASP	Mainchain	8
1	A	13	TYR	Mainchain,Sidechain	8
1	A	57	ARG	Mainchain	8
1	A	15	VAL	Mainchain	7
1	A	7	GLU	Mainchain	7
1	A	43	CYS	Mainchain	6
1	A	58	TYR	Sidechain,Mainchain	6
1	A	55	ALA	Mainchain	6
1	A	22	LYS	Mainchain	5
1	A	4	CYS	Mainchain	5
1	A	16	LEU	Mainchain	5
1	A	44	ILE	Mainchain	4
1	A	5	SER	Mainchain	4
1	A	56	CYS	Mainchain	4
1	A	46	ASP	Mainchain	4
1	A	28	ALA	Mainchain	4
1	A	29	VAL	Mainchain	3
1	A	49	ARG	Mainchain	3
1	A	3	VAL	Mainchain	3
1	A	65	GLY	Mainchain	2
1	A	69	GLU	Mainchain	2
1	A	50	ARG	Sidechain,Mainchain	2
1	A	37	CYS	Mainchain	2
1	A	21	CYS	Mainchain	1
1	A	68	LEU	Mainchain	1
1	A	11	CYS	Mainchain	1
1	A	54	PRO	Mainchain	1
1	A	45	ILE	Mainchain	1
1	A	1	CYS	Mainchain	1
1	A	34	ASN	Mainchain	1

6.2 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 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	500	0	497	16±3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	5522	0	5473	173

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:HIS:H	1:A:22:LYS:HZ2	0.84	1.10	8	1
1:A:25:PHE:HE2	1:A:68:LEU:H	0.82	1.17	5	5
1:A:17:THR:H	1:A:22:LYS:NZ	0.73	1.82	7	3
1:A:12:HIS:H	1:A:22:LYS:NZ	0.70	1.84	8	1
1:A:25:PHE:O	1:A:29:VAL:HG23	0.70	1.86	1	6
1:A:1:CYS:HA	1:A:17:THR:HA	0.69	1.63	7	3
1:A:17:THR:H	1:A:22:LYS:HZ3	0.66	1.34	7	1
1:A:43:CYS:SG	1:A:53:CYS:HB3	0.65	2.31	5	5
1:A:35:TYR:O	1:A:55:ALA:HB2	0.63	1.94	10	1
1:A:51:LYS:H	1:A:51:LYS:NZ	0.60	1.93	3	1
1:A:49:ARG:CZ	1:A:52:ASN:HD22	0.60	2.08	5	1
1:A:60:LYS:HA	1:A:63:GLN:HB2	0.59	1.72	7	10
1:A:45:ILE:HB	1:A:56:CYS:SG	0.58	2.38	8	2
1:A:37:CYS:HB3	1:A:55:ALA:HB3	0.57	1.73	2	1
1:A:24:PHE:CD1	1:A:24:PHE:C	0.57	2.77	11	6
1:A:59:ARG:HE	1:A:60:LYS:HE3	0.57	1.58	6	1
1:A:29:VAL:HG11	1:A:68:LEU:HD22	0.57	1.76	9	1
1:A:13:TYR:HB2	1:A:22:LYS:HE2	0.57	1.75	1	1
1:A:4:CYS:HB2	1:A:46:ASP:O	0.57	1.99	8	1
1:A:25:PHE:O	1:A:28:ALA:HB3	0.56	2.00	1	5
1:A:13:TYR:CD1	1:A:68:LEU:HA	0.56	2.36	7	4
1:A:44:ILE:HB	1:A:52:ASN:HD21	0.56	1.60	5	1
1:A:49:ARG:HG3	1:A:50:ARG:H	0.56	1.61	10	1
1:A:49:ARG:HE	1:A:51:LYS:NZ	0.56	1.98	8	1
1:A:50:ARG:NE	1:A:52:ASN:HD21	0.55	1.99	1	1
1:A:19:GLY:O	1:A:22:LYS:HB2	0.55	2.01	10	4
1:A:60:LYS:NZ	1:A:63:GLN:HE22	0.55	1.99	4	1
1:A:17:THR:H	1:A:22:LYS:HZ1	0.55	1.43	11	1
1:A:24:PHE:HD1	1:A:24:PHE:C	0.54	2.05	11	1
1:A:45:ILE:H	1:A:60:LYS:NZ	0.54	2.01	9	2
1:A:15:VAL:HB	1:A:66:MET:HA	0.53	1.80	9	1
1:A:53:CYS:O	1:A:56:CYS:HB3	0.52	2.04	7	1
1:A:36:LEU:H	1:A:36:LEU:HD23	0.52	1.64	10	1
1:A:6:ASP:O	1:A:18:CYS:HB3	0.52	2.05	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:ARG:CZ	1:A:52:ASN:HD21	0.52	2.17	1	2
1:A:47:LYS:HZ3	1:A:47:LYS:H	0.52	1.47	6	1
1:A:59:ARG:CZ	1:A:63:GLN:HE22	0.52	2.18	1	3
1:A:12:HIS:N	1:A:22:LYS:HZ2	0.51	1.92	8	1
1:A:1:CYS:HB2	1:A:18:CYS:H	0.50	1.65	1	1
1:A:53:CYS:HB3	1:A:56:CYS:SG	0.50	2.46	2	1
1:A:50:ARG:HB3	1:A:52:ASN:OD1	0.50	2.06	8	1
1:A:26:LYS:O	1:A:30:GLU:HB2	0.50	2.07	2	2
1:A:13:TYR:CD2	1:A:68:LEU:HD23	0.50	2.41	1	1
1:A:47:LYS:HZ3	1:A:47:LYS:N	0.50	2.05	6	1
1:A:45:ILE:HD13	1:A:57:ARG:HB2	0.49	1.84	4	1
1:A:44:ILE:HA	1:A:60:LYS:HZ3	0.49	1.68	1	1
1:A:13:TYR:CD2	1:A:22:LYS:HG3	0.48	2.42	1	1
1:A:29:VAL:HG11	1:A:68:LEU:CD2	0.48	2.37	9	1
1:A:29:VAL:HG11	1:A:68:LEU:HD21	0.48	1.84	2	2
1:A:25:PHE:C	1:A:29:VAL:HG23	0.48	2.28	9	2
1:A:11:CYS:O	1:A:22:LYS:HD3	0.48	2.08	4	1
1:A:25:PHE:CE1	1:A:62:LEU:HD21	0.48	2.43	9	4
1:A:16:LEU:HA	1:A:22:LYS:HZ1	0.47	1.69	4	1
1:A:34:ASN:HD21	1:A:36:LEU:HD12	0.47	1.69	1	1
1:A:19:GLY:O	1:A:22:LYS:HB3	0.47	2.08	8	1
1:A:24:PHE:HD1	1:A:25:PHE:N	0.47	2.06	11	1
1:A:53:CYS:SG	1:A:56:CYS:HB2	0.47	2.49	10	1
1:A:46:ASP:OD1	1:A:48:ILE:HG22	0.47	2.10	5	1
1:A:13:TYR:CD2	1:A:68:LEU:HD12	0.47	2.44	11	1
1:A:24:PHE:C	1:A:24:PHE:CD1	0.47	2.88	3	2
1:A:32:GLN:O	1:A:35:TYR:HE1	0.46	1.93	1	1
1:A:45:ILE:HG12	1:A:60:LYS:HE3	0.46	1.86	9	1
1:A:24:PHE:HE2	1:A:57:ARG:HE	0.46	1.53	4	1
1:A:25:PHE:CD2	1:A:29:VAL:HG21	0.45	2.46	10	1
1:A:13:TYR:HB3	1:A:67:ASN:O	0.45	2.11	5	1
1:A:37:CYS:CB	1:A:55:ALA:HB3	0.45	2.42	5	1
1:A:22:LYS:HG2	1:A:23:VAL:N	0.45	2.26	6	1
1:A:45:ILE:HD11	1:A:57:ARG:HB2	0.45	1.87	6	1
1:A:19:GLY:O	1:A:22:LYS:HG2	0.45	2.12	9	1
1:A:2:LEU:HD12	1:A:16:LEU:O	0.44	2.12	10	2
1:A:24:PHE:CZ	1:A:35:TYR:HE2	0.44	2.30	10	1
1:A:13:TYR:HB2	1:A:22:LYS:HE3	0.44	1.88	3	1
1:A:3:VAL:HG11	1:A:57:ARG:HA	0.44	1.90	8	1
1:A:12:HIS:HB3	1:A:22:LYS:HD2	0.44	1.89	6	1
1:A:11:CYS:HB2	1:A:22:LYS:NZ	0.44	2.28	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ASN:HD22	1:A:57:ARG:CZ	0.44	2.25	9	1
1:A:24:PHE:CD1	1:A:25:PHE:N	0.43	2.86	10	1
1:A:9:SER:H	1:A:12:HIS:CE1	0.43	2.31	6	1
1:A:53:CYS:HA	1:A:54:PRO:HD3	0.43	1.65	4	1
1:A:21:CYS:O	1:A:24:PHE:HB3	0.43	2.13	8	1
1:A:51:LYS:H	1:A:51:LYS:HZ3	0.43	1.57	3	1
1:A:60:LYS:HZ1	1:A:63:GLN:HE22	0.43	1.56	4	1
1:A:47:LYS:NZ	1:A:51:LYS:NZ	0.43	2.66	7	1
1:A:24:PHE:CE1	1:A:35:TYR:CE2	0.42	3.07	5	2
1:A:13:TYR:C	1:A:15:VAL:H	0.42	2.18	10	1
1:A:19:GLY:HA2	1:A:22:LYS:HE3	0.42	1.91	9	1
1:A:21:CYS:HB3	1:A:61:CYS:SG	0.42	2.53	9	1
1:A:26:LYS:CG	1:A:68:LEU:HD21	0.42	2.44	1	1
1:A:1:CYS:HB2	1:A:18:CYS:N	0.42	2.30	1	1
1:A:29:VAL:HG22	1:A:58:TYR:OH	0.42	2.14	4	1
1:A:46:ASP:H	1:A:50:ARG:HB2	0.42	1.75	6	1
1:A:58:TYR:O	1:A:62:LEU:HG	0.41	2.15	9	1
1:A:44:ILE:O	1:A:45:ILE:HG22	0.41	2.15	3	1
1:A:13:TYR:CG	1:A:66:MET:HE3	0.41	2.50	9	1
1:A:37:CYS:HA	1:A:53:CYS:SG	0.41	2.55	6	1
1:A:12:HIS:HB3	1:A:22:LYS:HB2	0.41	1.92	5	1
1:A:50:ARG:HH21	1:A:57:ARG:CZ	0.41	2.29	5	1
1:A:59:ARG:NH2	1:A:63:GLN:HE22	0.41	2.13	1	1
1:A:13:TYR:CZ	1:A:26:LYS:HG3	0.41	2.51	4	2
1:A:25:PHE:CE1	1:A:58:TYR:CZ	0.41	3.09	11	1
1:A:17:THR:O	1:A:22:LYS:HE2	0.41	2.15	10	1
1:A:58:TYR:O	1:A:61:CYS:HB2	0.41	2.15	10	1
1:A:12:HIS:HB2	1:A:22:LYS:HE3	0.41	1.93	7	1
1:A:19:GLY:HA2	1:A:22:LYS:HD2	0.41	1.92	2	1
1:A:49:ARG:NH2	1:A:52:ASN:HD22	0.41	2.13	5	1
1:A:1:CYS:O	1:A:5:SER:HA	0.41	2.15	6	1
1:A:13:TYR:HE2	1:A:26:LYS:HB2	0.40	1.75	3	1
1:A:26:LYS:NZ	1:A:27:ARG:HE	0.40	2.14	3	1
1:A:3:VAL:CG2	1:A:64:ALA:HB2	0.40	2.46	11	1
1:A:49:ARG:HH21	1:A:50:ARG:CZ	0.40	2.29	10	1
1:A:25:PHE:HE1	1:A:58:TYR:CE1	0.40	2.35	11	1
1:A:13:TYR:HB3	1:A:67:ASN:C	0.40	2.37	7	1
1:A:24:PHE:HE2	1:A:57:ARG:HD3	0.40	1.76	2	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	64/71 (90%)	40±2 (63±4%)	15±3 (24±4%)	9±2 (13±3%)	1	6
All	All	704/781 (90%)	441 (63%)	168 (24%)	95 (13%)	1	6

All 30 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	7	GLU	10
1	A	36	LEU	8
1	A	45	ILE	6
1	A	14	GLY	6
1	A	12	HIS	5
1	A	37	CYS	5
1	A	54	PRO	5
1	A	44	ILE	5
1	A	11	CYS	4
1	A	46	ASP	4
1	A	68	LEU	4
1	A	47	LYS	3
1	A	18	CYS	3
1	A	70	ALA	3
1	A	33	HIS	2
1	A	19	GLY	2
1	A	50	ARG	2
1	A	26	LYS	2
1	A	32	GLN	2
1	A	53	CYS	2
1	A	43	CYS	2
1	A	49	ARG	2
1	A	13	TYR	1
1	A	35	TYR	1
1	A	6	ASP	1
1	A	51	LYS	1
1	A	69	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	5	SER	1
1	A	30	GLU	1
1	A	10	GLY	1

6.3.2 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 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	55/59 (93%)	44±2 (80±4%)	11±2 (20±4%)	4	35
All	All	605/649 (93%)	482 (80%)	123 (20%)	4	35

All 30 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	58	TYR	10
1	A	30	GLU	9
1	A	16	LEU	9
1	A	35	TYR	8
1	A	68	LEU	7
1	A	66	MET	7
1	A	47	LYS	6
1	A	59	ARG	6
1	A	2	LEU	6
1	A	45	ILE	5
1	A	50	ARG	5
1	A	26	LYS	5
1	A	7	GLU	5
1	A	43	CYS	5
1	A	69	GLU	4
1	A	48	ILE	4
1	A	51	LYS	3
1	A	18	CYS	3
1	A	46	ASP	2
1	A	32	GLN	2
1	A	27	ARG	2
1	A	44	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	36	LEU	1
1	A	13	TYR	1
1	A	12	HIS	1
1	A	52	ASN	1
1	A	24	PHE	1
1	A	22	LYS	1
1	A	57	ARG	1
1	A	15	VAL	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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