



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 06:17 pm GMT

PDB ID : 1HRA
Title : THE SOLUTION STRUCTURE OF THE HUMAN RETINOIC ACID
RECEPTOR-BETA DNA-BINDING DOMAIN
Authors : Knegt, R.M.A.; Katahira, M.; Schilthuis, J.G.; Bonvin, A.M.J.J.; Boelens,
R.; Eib, D.; Van Der Saag, P.T.; Kaptein, R.
Deposited on : 1993-07-25

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

<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
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

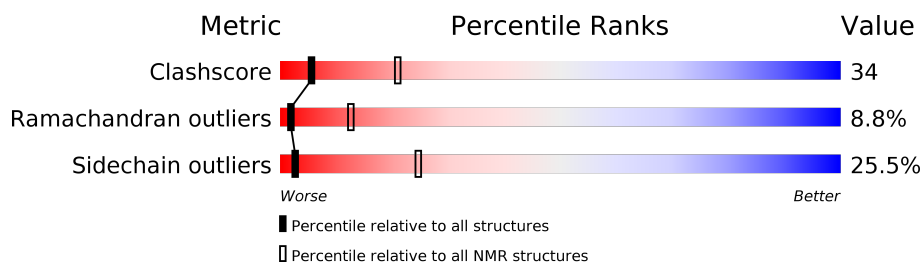
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	80	

2 Ensemble composition and analysis

This entry contains 15 models. Model 13 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:6-A:12, A:16-A:80 (72)	0.50	13

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 4 single-model clusters were found.

Cluster number	Models
1	1, 2, 6, 12, 13, 14
2	3, 7, 9
3	10, 15
Single-model clusters	4; 5; 8; 11

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 654 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RETINOIC ACID RECEPTOR.

Mol	Chain	Residues	Atoms					Trace
1	A	80	Total	C	N	O	S	0
			652	402	125	113	12	

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

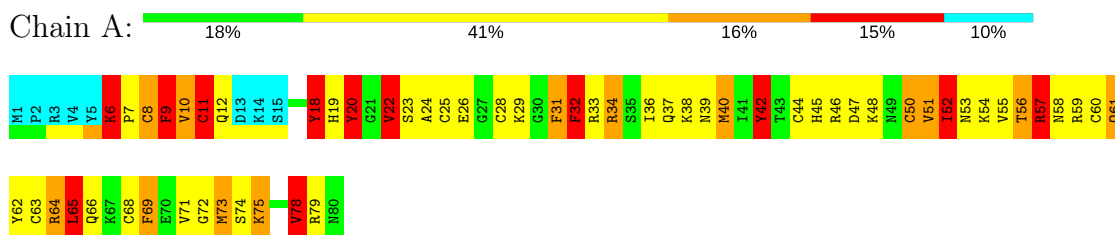
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: RETINOIC ACID RECEPTOR

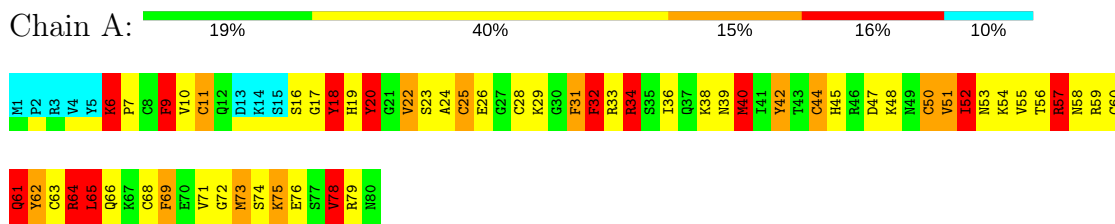


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

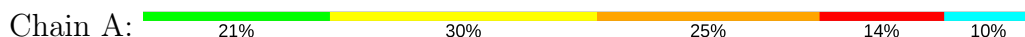
4.2.1 Score per residue for model 1

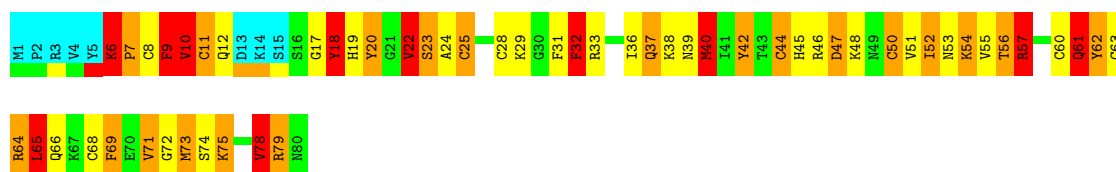
- Molecule 1: RETINOIC ACID RECEPTOR



4.2.2 Score per residue for model 2

- Molecule 1: RETINOIC ACID RECEPTOR

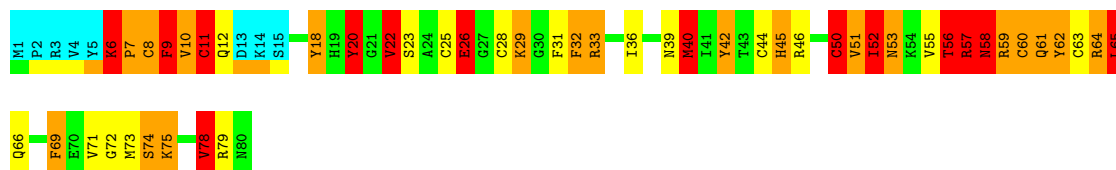




4.2.3 Score per residue for model 3

- Molecule 1: RETINOIC ACID RECEPTOR

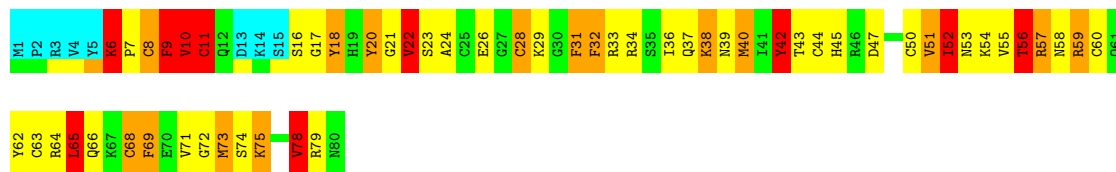
Chain A: 29% 20% 24% 18% 10%



4.2.4 Score per residue for model 4

- Molecule 1: RETINOIC ACID RECEPTOR

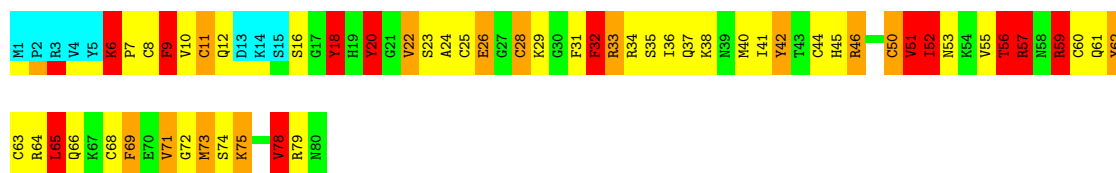
Chain A: 20% 39% 19% 13% 10%



4.2.5 Score per residue for model 5

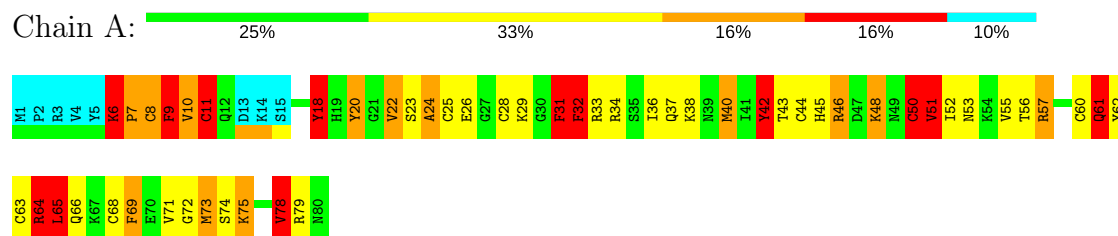
- Molecule 1: RETINOIC ACID RECEPTOR

Chain A: 21% 38% 16% 15% 10%



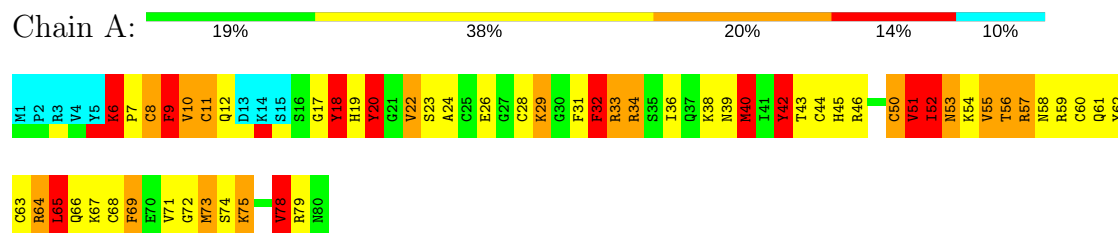
4.2.6 Score per residue for model 6

- Molecule 1: RETINOIC ACID RECEPTOR



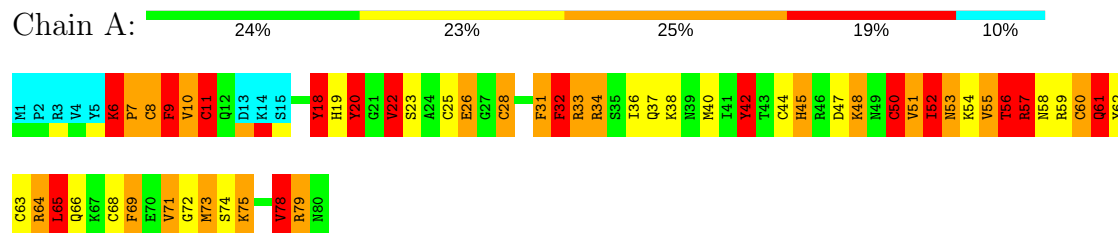
4.2.7 Score per residue for model 7

- Molecule 1: RETINOIC ACID RECEPTOR



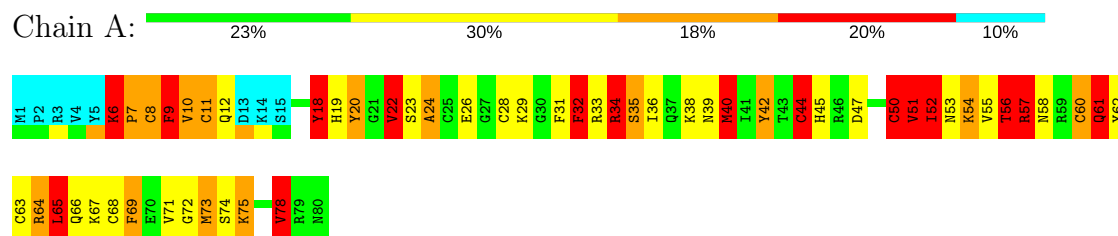
4.2.8 Score per residue for model 8

- Molecule 1: RETINOIC ACID RECEPTOR



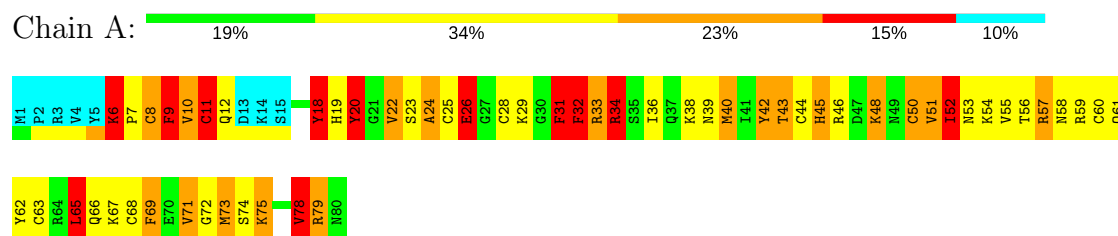
4.2.9 Score per residue for model 9

- Molecule 1: RETINOIC ACID RECEPTOR



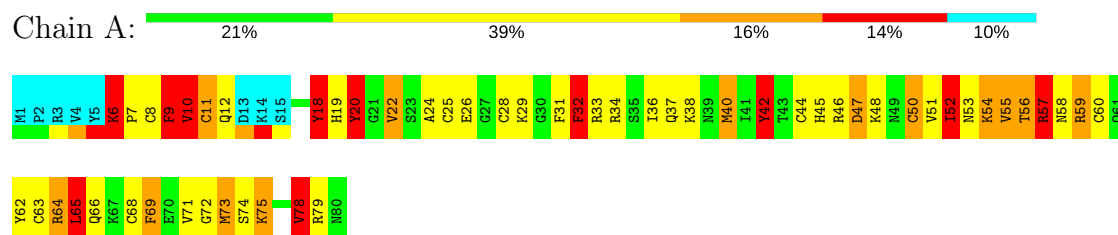
4.2.10 Score per residue for model 10

• Molecule 1: RETINOIC ACID RECEPTOR



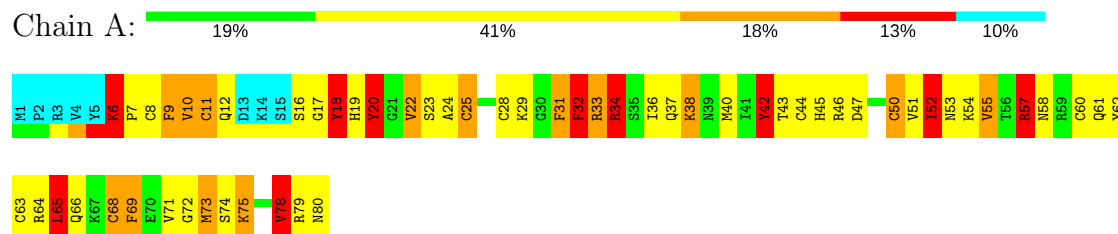
4.2.11 Score per residue for model 11

• Molecule 1: RETINOIC ACID RECEPTOR



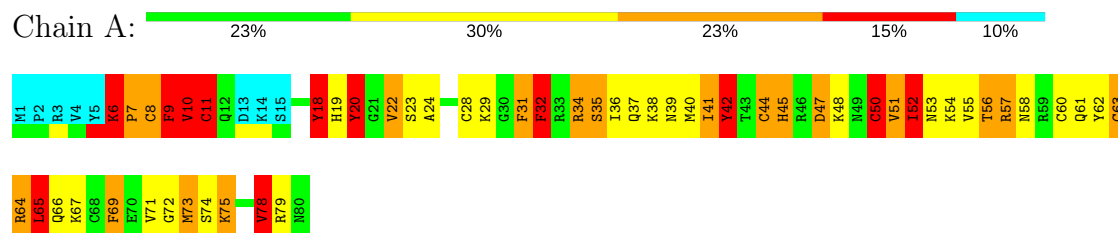
4.2.12 Score per residue for model 12

• Molecule 1: RETINOIC ACID RECEPTOR



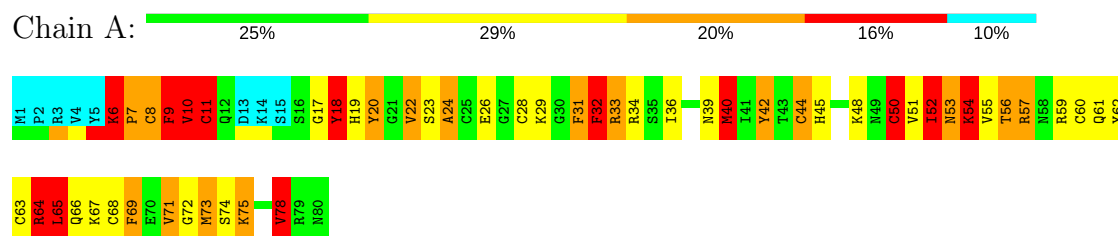
4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: RETINOIC ACID RECEPTOR



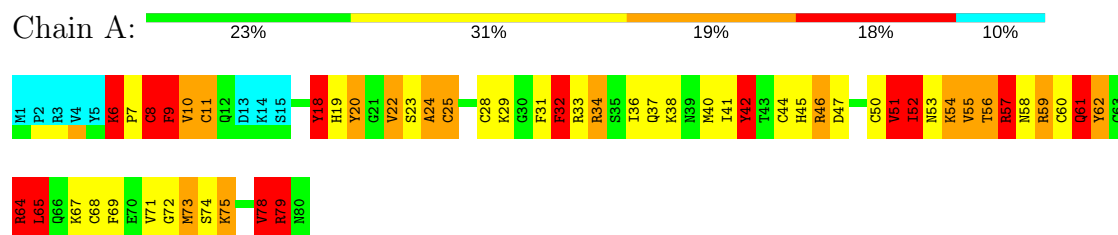
4.2.14 Score per residue for model 14

• Molecule 1: RETINOIC ACID RECEPTOR



4.2.15 Score per residue for model 15

• Molecule 1: RETINOIC ACID RECEPTOR



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 15 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. 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	0.87±0.01	0±0/594 (0.0±0.0%)	2.01±0.04	21±3/788 (2.7±0.4%)
All	All	0.87	0/8910 (0.0%)	2.01	318/11820 (2.7%)

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	0.1±0.2	21.6±3.7
All	All	1	324

There are no bond-length outliers.

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	42	TYR	CB-CG-CD2	-17.33	110.60	121.00	13	15
1	A	18	TYR	CB-CG-CD2	-15.17	111.90	121.00	5	13
1	A	20	TYR	CB-CG-CD2	-10.41	114.75	121.00	10	15
1	A	9	PHE	CB-CG-CD1	-10.05	113.76	120.80	11	11
1	A	42	TYR	CB-CG-CD1	9.77	126.86	121.00	12	7
1	A	18	TYR	CB-CG-CD1	-9.76	115.14	121.00	7	10
1	A	22	VAL	CG1-CB-CG2	-9.38	95.89	110.90	7	15
1	A	10	VAL	CA-CB-CG1	9.30	124.86	110.90	11	15
1	A	9	PHE	CB-CG-CD2	-9.27	114.31	120.80	12	4
1	A	22	VAL	CA-CB-CG2	8.35	123.42	110.90	3	15
1	A	62	TYR	CB-CG-CD2	-8.02	116.19	121.00	15	6
1	A	69	PHE	CB-CG-CD1	-7.81	115.33	120.80	9	15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	64	ARG	NE-CZ-NH1	7.39	123.99	120.30	11	8
1	A	11	CYS	C-N-CA	7.34	140.06	121.70	15	4
1	A	34	ARG	NE-CZ-NH1	7.03	123.82	120.30	10	7
1	A	57	ARG	CB-CA-C	6.89	124.19	110.40	12	8
1	A	50	CYS	CA-CB-SG	6.68	126.03	114.00	9	7
1	A	51	VAL	CB-CA-C	-6.64	98.78	111.40	15	6
1	A	34	ARG	NE-CZ-NH2	-6.56	117.02	120.30	10	2
1	A	10	VAL	CA-CB-CG2	6.53	120.70	110.90	2	1
1	A	51	VAL	CG1-CB-CG2	-6.50	100.49	110.90	6	5
1	A	6	LYS	N-CA-CB	-6.47	98.94	110.60	11	1
1	A	57	ARG	NE-CZ-NH1	6.43	123.51	120.30	12	5
1	A	41	ILE	C-N-CA	6.39	137.69	121.70	5	2
1	A	25	CYS	CA-CB-SG	6.37	125.46	114.00	5	10
1	A	51	VAL	C-N-CA	6.34	137.56	121.70	6	1
1	A	79	ARG	NE-CZ-NH1	6.33	123.47	120.30	2	3
1	A	78	VAL	CA-CB-CG2	6.33	120.39	110.90	9	2
1	A	33	ARG	NE-CZ-NH1	6.21	123.41	120.30	12	7
1	A	78	VAL	CA-CB-CG1	6.16	120.15	110.90	12	14
1	A	46	ARG	NE-CZ-NH1	6.15	123.38	120.30	2	6
1	A	18	TYR	N-CA-CB	6.12	121.61	110.60	1	1
1	A	59	ARG	NE-CZ-NH1	6.10	123.35	120.30	14	5
1	A	52	ILE	CA-CB-CG1	5.96	122.33	111.00	15	4
1	A	57	ARG	N-CA-CB	-5.96	99.87	110.60	11	1
1	A	50	CYS	CB-CA-C	5.95	122.30	110.40	14	3
1	A	11	CYS	O-C-N	-5.87	113.31	122.70	12	5
1	A	56	THR	CA-C-N	-5.78	104.48	117.20	8	2
1	A	10	VAL	N-CA-CB	-5.75	98.85	111.50	6	12
1	A	31	PHE	CB-CG-CD1	-5.67	116.83	120.80	1	4
1	A	8	CYS	N-CA-C	5.66	126.27	111.00	13	9
1	A	58	ASN	C-N-CA	5.64	135.79	121.70	8	2
1	A	33	ARG	NE-CZ-NH2	-5.61	117.50	120.30	7	3
1	A	38	LYS	O-C-N	-5.56	113.81	122.70	2	1
1	A	11	CYS	CA-C-N	-5.56	104.97	117.20	4	1
1	A	8	CYS	N-CA-CB	-5.52	100.66	110.60	15	1
1	A	56	THR	N-CA-CB	-5.47	99.91	110.30	7	4
1	A	43	THR	N-CA-C	5.46	125.74	111.00	6	1
1	A	28	CYS	N-CA-CB	5.46	120.42	110.60	4	3
1	A	31	PHE	CB-CG-CD2	-5.45	116.98	120.80	10	2
1	A	55	VAL	CA-C-N	-5.45	105.21	117.20	8	2
1	A	52	ILE	N-CA-CB	5.42	123.27	110.80	11	1
1	A	57	ARG	CA-C-N	-5.41	105.30	117.20	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	CYS	CA-CB-SG	5.40	123.72	114.00	2	1
1	A	51	VAL	CA-C-N	5.34	128.94	117.20	6	1
1	A	76	GLU	N-CA-CB	-5.23	101.18	110.60	1	1
1	A	24	ALA	N-CA-CB	5.18	117.36	110.10	9	1
1	A	18	TYR	N-CA-C	5.17	124.95	111.00	6	1
1	A	59	ARG	CA-C-N	-5.14	105.88	117.20	11	1
1	A	25	CYS	N-CA-CB	-5.11	101.41	110.60	11	1
1	A	55	VAL	N-CA-CB	-5.08	100.32	111.50	12	1
1	A	56	THR	C-N-CA	5.00	134.21	121.70	5	1
1	A	40	MET	CA-C-N	-5.00	106.20	117.20	4	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	18	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	6	LYS	Mainchain,Peptide	15
1	A	55	VAL	Peptide,Mainchain	15
1	A	74	SER	Peptide	15
1	A	9	PHE	Sidechain,Mainchain	15
1	A	65	LEU	Mainchain	15
1	A	45	HIS	Peptide	15
1	A	18	TYR	Sidechain,Peptide,Mainchain	15
1	A	75	LYS	Peptide	15
1	A	32	PHE	Sidechain,Mainchain	13
1	A	62	TYR	Sidechain,Mainchain	13
1	A	50	CYS	Peptide,Mainchain	10
1	A	40	MET	Peptide,Mainchain	8
1	A	26	GLU	Mainchain	8
1	A	52	ILE	Peptide,Mainchain	8
1	A	42	TYR	Sidechain,Peptide	8
1	A	7	PRO	Peptide,Mainchain	8
1	A	11	CYS	Peptide,Mainchain	8
1	A	20	TYR	Sidechain,Mainchain	7
1	A	64	ARG	Peptide	7
1	A	71	VAL	Mainchain	7
1	A	56	THR	Mainchain,Peptide	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	24	ALA	Mainchain	6
1	A	34	ARG	Mainchain	5
1	A	51	VAL	Peptide,Mainchain	4
1	A	47	ASP	Mainchain	4
1	A	22	VAL	Peptide,Mainchain	4
1	A	35	SER	Peptide,Mainchain	3
1	A	57	ARG	Mainchain,Peptide	3
1	A	54	LYS	Mainchain	3
1	A	10	VAL	Mainchain	3
1	A	53	ASN	Peptide	2
1	A	19	HIS	Sidechain	2
1	A	31	PHE	Sidechain	2
1	A	37	GLN	Mainchain,Peptide	1
1	A	63	CYS	Mainchain	1
1	A	46	ARG	Sidechain	1
1	A	44	CYS	Peptide	1
1	A	23	SER	Mainchain	1
1	A	58	ASN	Peptide	1
1	A	41	ILE	Mainchain	1
1	A	79	ARG	Sidechain	1
1	A	59	ARG	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	584	0	573	39±5
All	All	8790	0	8585	592

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LYS:NZ	1:A:39:ASN:HD22	0.80	1.74	1	2
1:A:53:ASN:HD22	1:A:54:LYS:NZ	0.77	1.77	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ILE:HA	1:A:40:MET:HG2	0.77	1.54	8	15
1:A:60:CYS:HB2	1:A:63:CYS:SG	0.77	2.19	5	1
1:A:37:GLN:HE21	1:A:38:LYS:NZ	0.76	1.77	12	7
1:A:33:ARG:HH21	1:A:75:LYS:HZ3	0.76	1.22	12	2
1:A:38:LYS:HZ3	1:A:39:ASN:HD21	0.74	1.25	10	2
1:A:52:ILE:HG12	1:A:64:ARG:HG3	0.73	1.59	15	4
1:A:33:ARG:HB3	1:A:75:LYS:HE2	0.72	1.59	11	11
1:A:8:CYS:SG	1:A:11:CYS:HB3	0.72	2.24	14	7
1:A:52:ILE:HG23	1:A:57:ARG:HB3	0.71	1.62	12	14
1:A:18:TYR:CZ	1:A:24:ALA:HB3	0.71	2.20	15	10
1:A:60:CYS:HB3	1:A:63:CYS:SG	0.71	2.26	13	9
1:A:38:LYS:HZ2	1:A:39:ASN:HD22	0.70	1.27	7	2
1:A:33:ARG:HE	1:A:75:LYS:HZ3	0.70	1.29	10	3
1:A:31:PHE:CZ	1:A:65:LEU:HD22	0.69	2.22	9	15
1:A:52:ILE:H	1:A:67:LYS:NZ	0.69	1.85	10	1
1:A:78:VAL:HG22	1:A:79:ARG:HG3	0.69	1.65	3	5
1:A:22:VAL:HG21	1:A:73:MET:SD	0.68	2.28	8	14
1:A:6:LYS:HB2	1:A:7:PRO:HA	0.68	1.66	5	6
1:A:37:GLN:HE21	1:A:38:LYS:HZ2	0.67	1.32	15	2
1:A:32:PHE:CE2	1:A:73:MET:HB2	0.66	2.25	13	15
1:A:75:LYS:HB3	1:A:78:VAL:HG11	0.66	1.68	11	15
1:A:53:ASN:HD22	1:A:54:LYS:HZ3	0.66	1.34	11	1
1:A:56:THR:HG23	1:A:57:ARG:HG2	0.66	1.65	9	6
1:A:52:ILE:H	1:A:64:ARG:CZ	0.65	2.04	4	6
1:A:44:CYS:SG	1:A:63:CYS:HB3	0.65	2.30	14	6
1:A:51:VAL:H	1:A:52:ILE:HD13	0.65	1.51	7	3
1:A:8:CYS:HB3	1:A:10:VAL:H	0.65	1.52	6	8
1:A:22:VAL:HG11	1:A:73:MET:SD	0.64	2.33	10	12
1:A:52:ILE:HD12	1:A:57:ARG:O	0.63	1.93	11	1
1:A:68:CYS:HB3	1:A:73:MET:SD	0.63	2.33	11	10
1:A:54:LYS:HA	1:A:56:THR:HG22	0.63	1.71	2	1
1:A:52:ILE:HA	1:A:56:THR:OG1	0.63	1.94	14	7
1:A:38:LYS:NZ	1:A:39:ASN:HD21	0.62	1.91	10	2
1:A:44:CYS:HA	1:A:62:TYR:HB3	0.62	1.71	13	1
1:A:47:ASP:O	1:A:50:CYS:HB2	0.61	1.95	9	8
1:A:8:CYS:SG	1:A:25:CYS:HB2	0.61	2.36	2	2
1:A:33:ARG:NH1	1:A:37:GLN:HE22	0.60	1.94	6	1
1:A:8:CYS:HB3	1:A:11:CYS:H	0.60	1.55	9	7
1:A:6:LYS:NZ	1:A:6:LYS:H	0.60	1.93	5	1
1:A:11:CYS:HB2	1:A:52:ILE:HB	0.60	1.71	8	2
1:A:22:VAL:HG22	1:A:23:SER:H	0.60	1.55	9	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ILE:HD13	1:A:75:LYS:O	0.60	1.96	13	5
1:A:66:GLN:HA	1:A:69:PHE:HB2	0.59	1.74	13	14
1:A:51:VAL:N	1:A:52:ILE:HD13	0.59	2.12	7	3
1:A:57:ARG:HB2	1:A:59:ARG:HB3	0.58	1.74	5	3
1:A:33:ARG:HE	1:A:75:LYS:NZ	0.58	1.96	7	3
1:A:75:LYS:HZ2	1:A:79:ARG:NH2	0.58	1.97	8	2
1:A:34:ARG:HH22	1:A:61:GLN:NE2	0.58	1.95	10	2
1:A:51:VAL:C	1:A:52:ILE:HD13	0.58	2.18	12	9
1:A:6:LYS:HB2	1:A:8:CYS:H	0.57	1.59	7	9
1:A:53:ASN:H	1:A:56:THR:HG21	0.57	1.58	15	4
1:A:75:LYS:HZ2	1:A:79:ARG:CZ	0.57	2.13	8	1
1:A:33:ARG:HH21	1:A:75:LYS:HZ2	0.57	1.42	7	1
1:A:52:ILE:HG23	1:A:57:ARG:H	0.56	1.59	11	1
1:A:44:CYS:H	1:A:48:LYS:NZ	0.56	1.99	6	1
1:A:9:PHE:CD2	1:A:71:VAL:HG21	0.56	2.36	4	11
1:A:18:TYR:CZ	1:A:23:SER:HA	0.55	2.36	3	4
1:A:22:VAL:HG22	1:A:23:SER:O	0.55	2.02	14	10
1:A:28:CYS:O	1:A:32:PHE:HB2	0.55	2.01	8	15
1:A:52:ILE:H	1:A:67:LYS:HZ2	0.55	1.44	10	1
1:A:75:LYS:HA	1:A:78:VAL:HG21	0.54	1.80	7	15
1:A:50:CYS:SG	1:A:60:CYS:HB3	0.54	2.43	8	3
1:A:18:TYR:OH	1:A:24:ALA:HB3	0.54	2.03	11	7
1:A:54:LYS:NZ	1:A:57:ARG:HH12	0.53	1.99	9	1
1:A:33:ARG:HH21	1:A:75:LYS:NZ	0.53	2.01	8	1
1:A:54:LYS:NZ	1:A:54:LYS:H	0.53	2.02	14	1
1:A:64:ARG:HD3	1:A:67:LYS:HB2	0.53	1.81	15	3
1:A:9:PHE:CD1	1:A:71:VAL:HG21	0.53	2.39	7	2
1:A:54:LYS:HZ2	1:A:54:LYS:H	0.53	1.44	14	1
1:A:50:CYS:SG	1:A:58:ASN:HB3	0.52	2.44	3	1
1:A:33:ARG:NH2	1:A:75:LYS:HZ3	0.52	1.98	12	2
1:A:20:TYR:OH	1:A:29:LYS:HG2	0.52	2.05	12	4
1:A:46:ARG:HG3	1:A:60:CYS:HB2	0.52	1.82	15	3
1:A:6:LYS:O	1:A:8:CYS:HB2	0.52	2.05	2	1
1:A:32:PHE:CZ	1:A:73:MET:HG3	0.51	2.41	4	13
1:A:51:VAL:H	1:A:58:ASN:ND2	0.51	2.03	11	1
1:A:38:LYS:HZ3	1:A:39:ASN:HD22	0.51	1.43	1	1
1:A:35:SER:O	1:A:40:MET:HB3	0.51	2.05	13	1
1:A:37:GLN:HB3	1:A:38:LYS:HZ2	0.50	1.64	8	1
1:A:36:ILE:CG2	1:A:78:VAL:HG12	0.50	2.37	2	5
1:A:78:VAL:HG22	1:A:79:ARG:HG2	0.50	1.82	11	3
1:A:37:GLN:NE2	1:A:79:ARG:HE	0.50	2.04	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LYS:HE3	1:A:78:VAL:HG11	0.50	1.83	11	4
1:A:9:PHE:HB2	1:A:23:SER:H	0.50	1.66	9	1
1:A:63:CYS:SG	1:A:64:ARG:N	0.50	2.85	5	7
1:A:8:CYS:H	1:A:9:PHE:HA	0.50	1.67	8	6
1:A:22:VAL:HG22	1:A:23:SER:N	0.50	2.22	9	4
1:A:75:LYS:HE3	1:A:78:VAL:CG1	0.49	2.37	6	3
1:A:8:CYS:N	1:A:9:PHE:HA	0.49	2.22	5	5
1:A:8:CYS:HB3	1:A:10:VAL:N	0.49	2.23	15	6
1:A:53:ASN:HD22	1:A:54:LYS:N	0.49	2.04	8	2
1:A:33:ARG:CZ	1:A:37:GLN:HE22	0.49	2.20	6	1
1:A:8:CYS:CB	1:A:11:CYS:H	0.49	2.21	7	3
1:A:38:LYS:NZ	1:A:39:ASN:ND2	0.49	2.60	10	2
1:A:12:GLN:HG2	1:A:53:ASN:O	0.48	2.08	3	1
1:A:41:ILE:H	1:A:42:TYR:HB3	0.48	1.69	13	1
1:A:55:VAL:HB	1:A:56:THR:HG23	0.48	1.84	11	2
1:A:37:GLN:HE21	1:A:38:LYS:HZ1	0.48	1.46	12	1
1:A:57:ARG:HA	1:A:58:ASN:C	0.48	2.29	7	7
1:A:60:CYS:SG	1:A:61:GLN:N	0.47	2.87	15	7
1:A:34:ARG:NE	1:A:39:ASN:HD21	0.47	2.06	13	1
1:A:6:LYS:HB3	1:A:9:PHE:O	0.47	2.09	1	2
1:A:32:PHE:CD2	1:A:75:LYS:HB2	0.47	2.45	4	11
1:A:51:VAL:O	1:A:57:ARG:HA	0.47	2.09	8	1
1:A:64:ARG:HG3	1:A:67:LYS:HB3	0.47	1.87	14	1
1:A:65:LEU:HB3	1:A:66:GLN:NE2	0.47	2.25	11	4
1:A:37:GLN:HE21	1:A:75:LYS:NZ	0.47	2.07	6	1
1:A:18:TYR:CE2	1:A:23:SER:HA	0.47	2.45	8	1
1:A:36:ILE:HD11	1:A:65:LEU:HD12	0.46	1.87	9	10
1:A:50:CYS:HB3	1:A:63:CYS:HB3	0.46	1.87	10	1
1:A:51:VAL:HG12	1:A:53:ASN:ND2	0.46	2.26	5	2
1:A:6:LYS:HB2	1:A:7:PRO:CA	0.46	2.38	5	1
1:A:53:ASN:ND2	1:A:54:LYS:H	0.46	2.09	11	1
1:A:20:TYR:OH	1:A:75:LYS:HG2	0.46	2.10	13	2
1:A:37:GLN:NE2	1:A:38:LYS:NZ	0.45	2.64	13	2
1:A:36:ILE:HG22	1:A:78:VAL:HG12	0.45	1.86	2	3
1:A:48:LYS:H	1:A:48:LYS:NZ	0.45	2.08	10	1
1:A:34:ARG:HG2	1:A:39:ASN:HD21	0.45	1.70	7	2
1:A:52:ILE:HD12	1:A:57:ARG:HB3	0.45	1.88	5	2
1:A:42:TYR:HD2	1:A:61:GLN:HB2	0.45	1.72	6	1
1:A:60:CYS:HB3	1:A:63:CYS:HG	0.45	1.70	13	1
1:A:20:TYR:HB2	1:A:74:SER:H	0.44	1.71	3	1
1:A:51:VAL:O	1:A:56:THR:HB	0.44	2.12	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LYS:HZ1	1:A:57:ARG:HH12	0.44	1.54	9	1
1:A:18:TYR:HD2	1:A:20:TYR:O	0.44	1.94	8	1
1:A:12:GLN:HB2	1:A:52:ILE:O	0.44	2.13	2	2
1:A:64:ARG:O	1:A:68:CYS:HB2	0.44	2.13	4	2
1:A:52:ILE:HD13	1:A:52:ILE:N	0.44	2.28	14	1
1:A:37:GLN:HE21	1:A:38:LYS:HZ3	0.43	1.56	4	1
1:A:59:ARG:H	1:A:59:ARG:CZ	0.43	2.26	4	2
1:A:46:ARG:HG3	1:A:60:CYS:SG	0.43	2.54	5	1
1:A:52:ILE:HG22	1:A:53:ASN:O	0.43	2.14	1	2
1:A:36:ILE:HG22	1:A:78:VAL:O	0.43	2.13	1	1
1:A:78:VAL:HA	1:A:79:ARG:HA	0.43	1.48	13	4
1:A:57:ARG:HG3	1:A:59:ARG:HH21	0.43	1.74	3	1
1:A:46:ARG:HG2	1:A:60:CYS:HB2	0.42	1.91	11	1
1:A:44:CYS:N	1:A:48:LYS:NZ	0.42	2.68	6	1
1:A:35:SER:HB3	1:A:40:MET:HB3	0.42	1.92	9	1
1:A:40:MET:HB2	1:A:42:TYR:CZ	0.42	2.50	4	1
1:A:17:GLY:HA3	1:A:18:TYR:HA	0.42	1.70	12	4
1:A:8:CYS:HA	1:A:24:ALA:HA	0.42	1.92	7	1
1:A:34:ARG:HG2	1:A:38:LYS:HZ1	0.42	1.75	9	1
1:A:51:VAL:H	1:A:58:ASN:HB3	0.41	1.75	4	3
1:A:52:ILE:N	1:A:52:ILE:HD13	0.41	2.30	11	1
1:A:10:VAL:HG11	1:A:67:LYS:HB3	0.41	1.93	10	1
1:A:25:CYS:HB3	1:A:28:CYS:H	0.41	1.74	1	1
1:A:10:VAL:HG13	1:A:64:ARG:HE	0.41	1.75	4	1
1:A:6:LYS:C	1:A:8:CYS:H	0.41	2.19	12	2
1:A:56:THR:HB	1:A:57:ARG:H	0.41	1.60	15	1
1:A:59:ARG:H	1:A:59:ARG:NE	0.41	2.13	4	1
1:A:50:CYS:O	1:A:64:ARG:HD3	0.41	2.16	12	1
1:A:10:VAL:HG12	1:A:68:CYS:SG	0.41	2.55	2	1
1:A:46:ARG:HB2	1:A:50:CYS:SG	0.41	2.56	11	1
1:A:48:LYS:NZ	1:A:48:LYS:H	0.41	2.14	8	1
1:A:50:CYS:HB3	1:A:63:CYS:CB	0.40	2.46	10	1
1:A:20:TYR:HD1	1:A:73:MET:HB3	0.40	1.76	3	1
1:A:43:THR:HA	1:A:44:CYS:HA	0.40	1.75	10	1
1:A:26:GLU:O	1:A:29:LYS:HG3	0.40	2.16	3	1
1:A:9:PHE:HD2	1:A:71:VAL:HG21	0.40	1.74	9	1
1:A:8:CYS:SG	1:A:28:CYS:SG	0.40	3.19	4	1
1:A:73:MET:H	1:A:73:MET:HG2	0.40	1.48	4	1
1:A:35:SER:O	1:A:36:ILE:HG13	0.40	2.15	13	1
1:A:31:PHE:HZ	1:A:65:LEU:HD22	0.40	1.72	10	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	71/80 (89%)	44±2 (62±3%)	20±2 (29±3%)	6±2 (9±2%)	2	12
All	All	1065/1200 (89%)	665 (62%)	306 (29%)	94 (9%)	2	12

All 18 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	72	GLY	15
1	A	6	LYS	11
1	A	57	ARG	10
1	A	61	GLN	9
1	A	19	HIS	9
1	A	44	CYS	6
1	A	26	GLU	6
1	A	52	ILE	5
1	A	22	VAL	5
1	A	16	SER	4
1	A	50	CYS	3
1	A	43	THR	3
1	A	20	TYR	2
1	A	17	GLY	2
1	A	51	VAL	1
1	A	58	ASN	1
1	A	42	TYR	1
1	A	21	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	66/74 (89%)	49±2 (75±3%)	17±2 (25±3%)	3	24
All	All	990/1110 (89%)	738 (75%)	252 (25%)	3	24

All 40 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	11	CYS	15
1	A	65	LEU	15
1	A	6	LYS	15
1	A	78	VAL	15
1	A	32	PHE	15
1	A	42	TYR	15
1	A	73	MET	14
1	A	52	ILE	14
1	A	20	TYR	12
1	A	29	LYS	11
1	A	18	TYR	10
1	A	61	GLN	9
1	A	48	LYS	8
1	A	40	MET	7
1	A	34	ARG	7
1	A	53	ASN	6
1	A	56	THR	5
1	A	54	LYS	5
1	A	44	CYS	5
1	A	59	ARG	4
1	A	45	HIS	4
1	A	10	VAL	4
1	A	57	ARG	4
1	A	39	ASN	4
1	A	12	GLN	3
1	A	68	CYS	3
1	A	50	CYS	3
1	A	38	LYS	3
1	A	60	CYS	3
1	A	26	GLU	2
1	A	79	ARG	2
1	A	31	PHE	2
1	A	51	VAL	1
1	A	64	ARG	1
1	A	43	THR	1
1	A	80	ASN	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	37	GLN	1
1	A	58	ASN	1
1	A	8	CYS	1
1	A	33	ARG	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