



Full wwPDB NMR Structure Validation Report ⓘ

Mar 24, 2026 – 12:28 AM UTC

PDB ID : 3CI2 / pdb_00003ci2
Title : REFINEMENT OF THE THREE-DIMENSIONAL SOLUTION STRUCTURE OF BARLEY SERINE PROTEINASE INHIBITOR 2 AND COMPARISON WITH THE STRUCTURES IN CRYSTALS
Authors : Poulsen, F.M.
Deposited on : 1991-09-10

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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

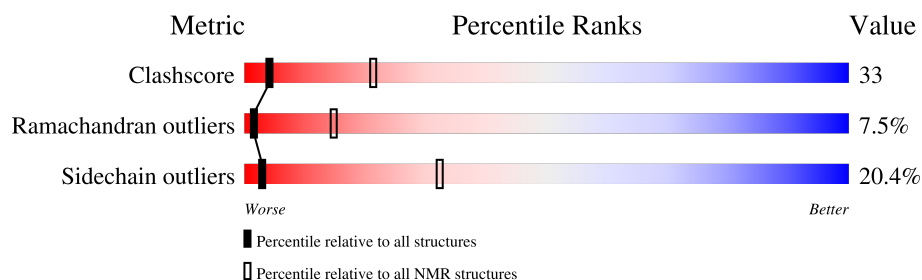
1 Overall quality at a glance

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	66	9% 62% 18% 6% • •

2 Ensemble composition and analysis

This entry contains 20 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:21-A:83 (63)	0.99	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 3 clusters and 6 single-model clusters were found.

Cluster number	Models
1	2, 5, 9, 10, 14, 19
2	1, 4, 6, 7, 15, 17
3	3, 18
Single-model clusters	8; 11; 12; 13; 16; 20

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1061 atoms, of which 549 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CHYMOTRYPSIN INHIBITOR 2.

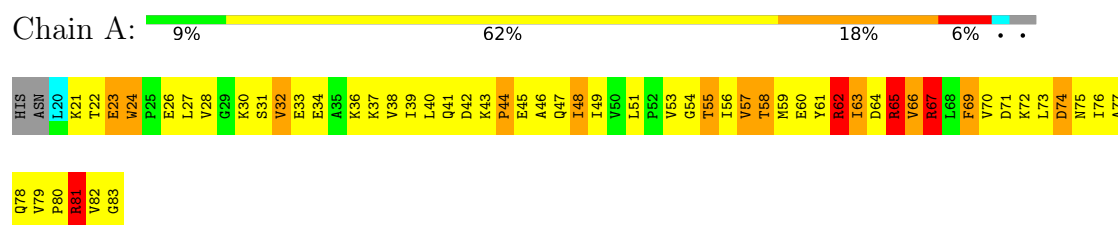
Mol	Chain	Residues	Atoms						Trace
1	A	64	Total	C	H	N	O	S	0
			1061	331	549	86	94	1	

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: CHYMOTRYPSIN INHIBITOR 2

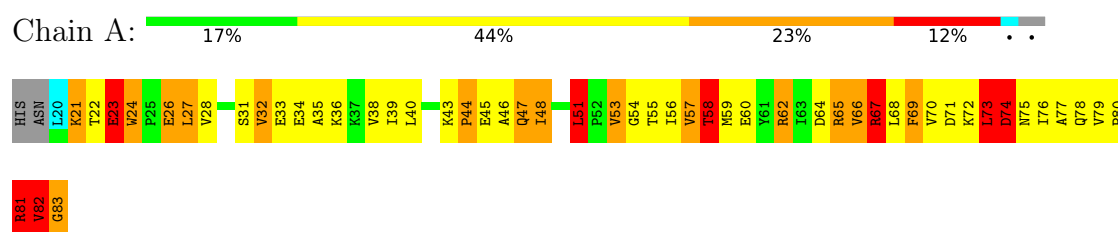


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

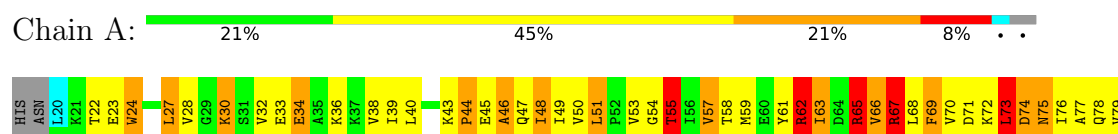
4.2.1 Score per residue for model 1

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



4.2.2 Score per residue for model 2

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



P80
R81
G83

4.2.3 Score per residue for model 3

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A: 30% 38% 20% 8% . .

HIS ASN L20 K21 E23 E24 E25 E26 L27 S31 V82 E33 E34 A35 K36 K37 V38 V39 L40 Q41 D42 K43 K44 P44 A45 E46 Q47 I48 I49 V50 V51 L51 T55 I56 V57 T58 M59 E60 Y61 R62 R65 V66 R67 L68 F69 V70 D71 K72 L73 D74 N75 I76 A77 Q78 V79 P80 R81 V82

G83

4.2.4 Score per residue for model 4

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A: 27% 36% 26% 6% . .

HIS ASN L20 K21 E23 E24 E25 E26 L27 S31 V82 E33 E34 A35 K36 K37 V38 V39 L40 Q41 D42 K43 K44 P44 A45 E46 Q47 I48 I49 V50 V51 L51 T55 I56 V57 T58 M59 E60 Y61 R62 R65 V66 R67 L68 F69 V70 D71 K72 L73 D74 N75 I76 A77 Q78 V79 P80 R81 V82

V82
G83

4.2.5 Score per residue for model 5

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A: 26% 41% 18% 11% . .

HIS ASN L20 K21 E23 E24 E25 E26 L27 S31 V82 E33 E34 A35 K36 K37 V38 V39 L40 Q41 D42 K43 K44 P44 A45 E46 Q47 I48 L51 P52 V53 G54 T55 I56 V57 T58 M59 E60 Y61 R62 R65 V66 R67 L68 F69 V70 D71 K72 L73 D74 N75 I76 A77 Q78 V79 P80 R81 V82

G83

4.2.6 Score per residue for model 6

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2

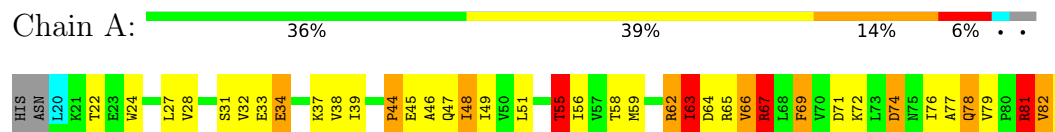
Chain A: 27% 36% 24% 8% . .

HIS ASN L20 K21 E23 E24 L27 V28 G29 S31 V82 E33 E34 A35 K36 K37 V38 V39 L40 Q41 D42 K43 K44 P44 A45 E46 Q47 I48 I49 V50 V51 G54 T55 I56 V57 T58 R62 I63 D64 R65 V66 R67 L68 F69 V70 D71 K72 L73 D74 N75 I76 A77 Q78 V79 P80 R81 V82

V82
G83

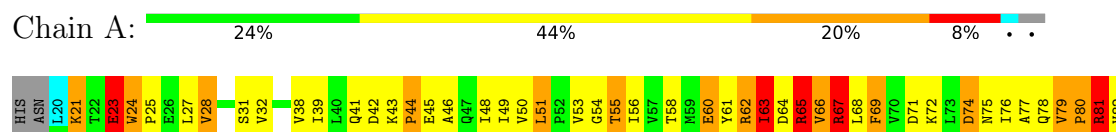
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



4.2.8 Score per residue for model 8

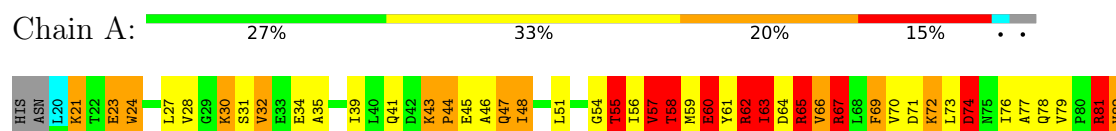
- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



G83

4.2.9 Score per residue for model 9

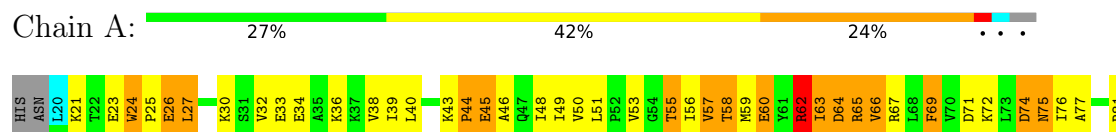
- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



G83

4.2.10 Score per residue for model 10

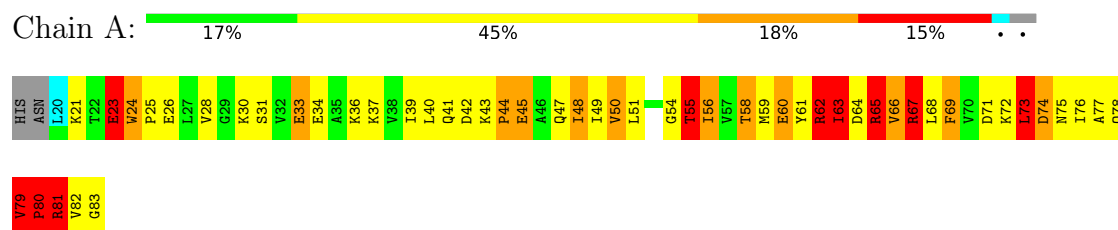
- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



V82
G83

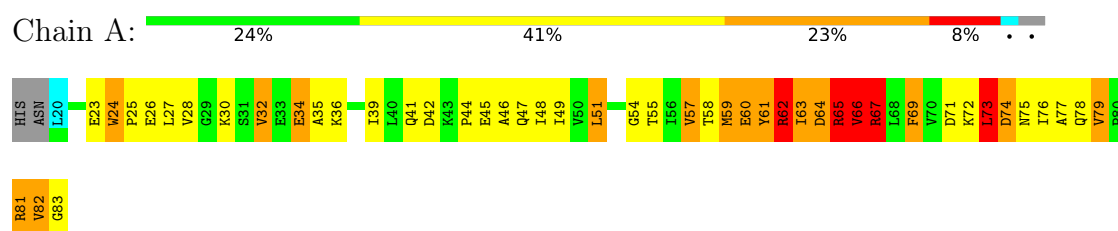
4.2.11 Score per residue for model 11

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



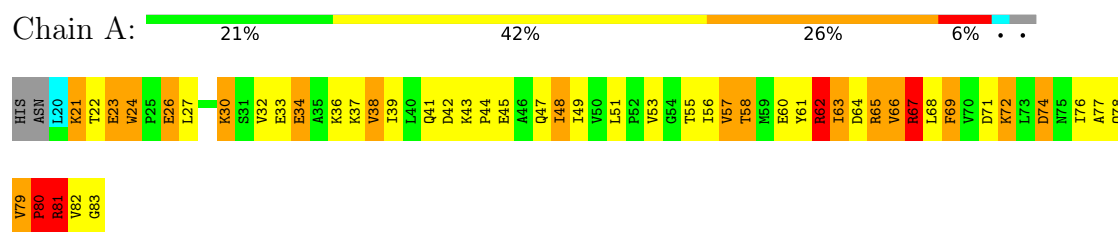
4.2.12 Score per residue for model 12

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



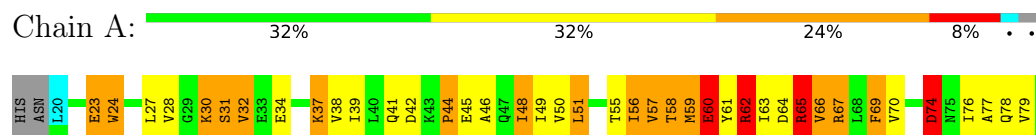
4.2.13 Score per residue for model 13

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



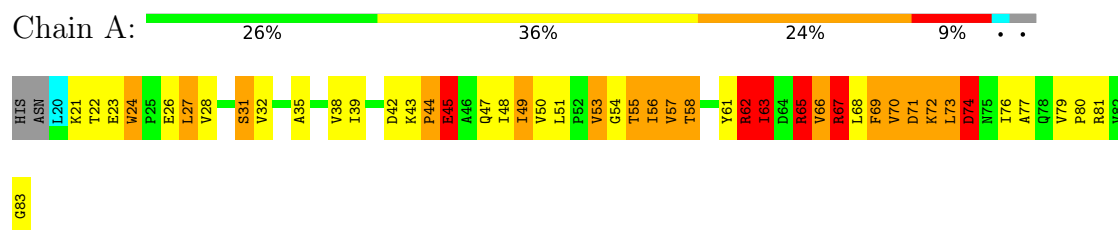
4.2.14 Score per residue for model 14

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



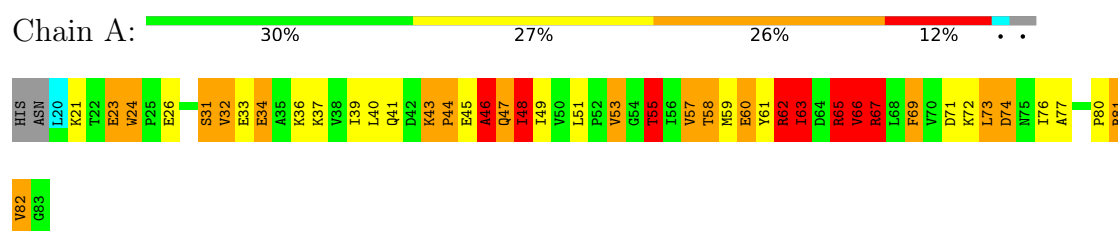
4.2.15 Score per residue for model 15

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



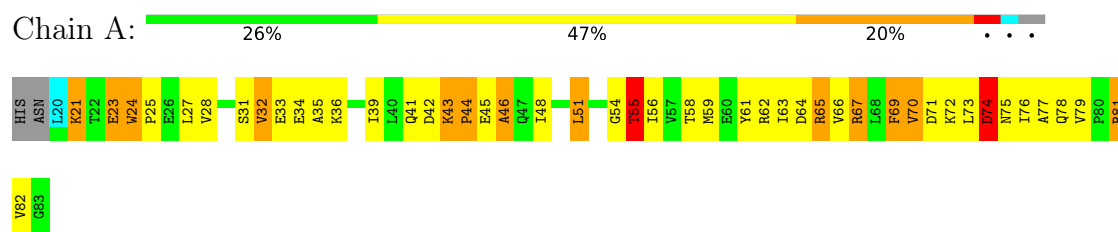
4.2.16 Score per residue for model 16

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



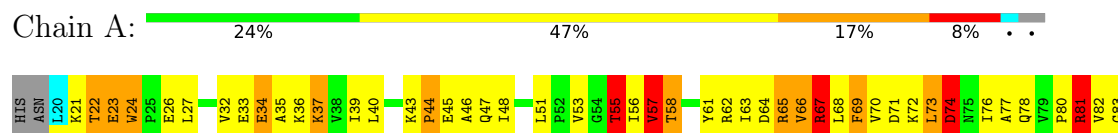
4.2.17 Score per residue for model 17

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



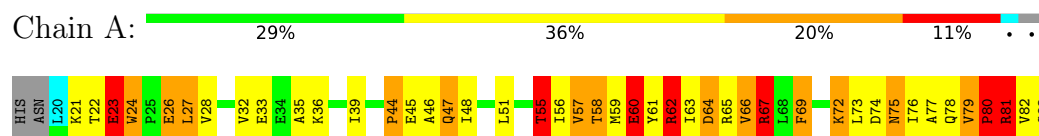
4.2.18 Score per residue for model 18

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



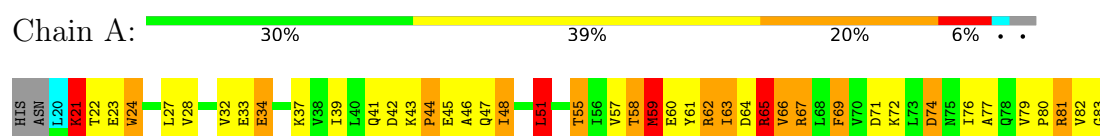
4.2.19 Score per residue for model 19

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



4.2.20 Score per residue for model 20

- Molecule 1: CHYMOTRYPSIN INHIBITOR 2



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 20 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

6.1 Standard geometry

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	2.02±0.04	6±2/512 (1.2± 0.5%)	2.40±0.09	29±5/692 (4.2± 0.8%)
All	All	2.02	126/10240 (1.2%)	2.40	588/13840 (4.2%)

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	0.0±0.0	3.7±0.5
All	All	0	74

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	69	PHE	CA-CB	9.07	1.64	1.52	8	13
1	A	46	ALA	CA-C	7.29	1.62	1.52	16	1
1	A	28	VAL	CA-CB	7.25	1.61	1.54	8	1
1	A	24	TRP	CG-CD2	-6.97	1.31	1.43	13	20
1	A	47	GLN	N-CA	6.61	1.54	1.46	16	1
1	A	62	ARG	CA-CB	6.56	1.61	1.52	11	1
1	A	46	ALA	N-CA	6.50	1.54	1.46	16	1
1	A	81	ARG	CZ-NH2	-6.39	1.25	1.33	6	5
1	A	43	LYS	CA-CB	6.33	1.62	1.53	16	1
1	A	70	VAL	N-CA	6.26	1.53	1.45	1	3
1	A	62	ARG	NE-CZ	-6.20	1.26	1.33	2	5
1	A	23	GLU	N-CA	6.08	1.53	1.46	19	3
1	A	54	GLY	N-CA	6.05	1.52	1.45	17	6
1	A	65	ARG	NE-CZ	-6.01	1.26	1.33	4	3
1	A	22	THR	N-CA	5.96	1.53	1.46	5	3
1	A	43	LYS	N-CA	5.96	1.53	1.45	16	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	51	LEU	N-CA	5.95	1.51	1.45	14	2
1	A	31	SER	CA-C	-5.94	1.44	1.53	6	2
1	A	57	VAL	CA-CB	5.85	1.62	1.54	20	1
1	A	56	ILE	N-CA	5.84	1.52	1.46	13	2
1	A	63	ILE	N-CA	5.83	1.53	1.46	4	1
1	A	59	MET	N-CA	5.75	1.49	1.46	5	3
1	A	42	ASP	CA-C	5.69	1.59	1.52	12	1
1	A	67	ARG	NE-CZ	-5.67	1.26	1.33	9	1
1	A	65	ARG	CZ-NH2	-5.63	1.26	1.33	9	6
1	A	67	ARG	CZ-NH2	-5.63	1.26	1.33	17	8
1	A	24	TRP	N-CA	5.57	1.52	1.46	12	1
1	A	78	GLN	N-CA	5.56	1.52	1.45	9	3
1	A	63	ILE	CA-CB	-5.51	1.47	1.54	4	1
1	A	55	THR	CA-CB	-5.46	1.44	1.53	6	1
1	A	62	ARG	CZ-NH2	-5.39	1.26	1.33	2	8
1	A	79	VAL	CA-C	5.39	1.58	1.52	11	1
1	A	48	ILE	CA-CB	-5.31	1.48	1.54	18	1
1	A	74	ASP	CA-CB	5.29	1.62	1.53	5	1
1	A	67	ARG	CZ-NH1	-5.29	1.25	1.32	15	1
1	A	56	ILE	CA-C	5.25	1.58	1.52	11	1
1	A	81	ARG	N-CA	5.23	1.52	1.46	9	1
1	A	44	PRO	CA-C	5.22	1.59	1.52	16	1
1	A	31	SER	N-CA	5.21	1.52	1.45	6	1
1	A	76	ILE	CA-C	-5.14	1.48	1.53	19	1
1	A	46	ALA	CA-CB	5.14	1.59	1.52	2	1
1	A	42	ASP	N-CA	5.12	1.52	1.46	6	1
1	A	65	ARG	CD-NE	5.11	1.53	1.46	7	1
1	A	23	GLU	CA-C	5.08	1.59	1.52	11	1
1	A	75	ASN	C-N	-5.05	1.28	1.33	19	1
1	A	62	ARG	CZ-NH1	-5.03	1.25	1.32	12	1
1	A	65	ARG	N-CA	5.01	1.52	1.46	19	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	69	PHE	CA-CB-CG	-19.45	94.35	113.80	14	20
1	A	66	VAL	N-CA-C	-12.11	88.03	107.28	20	6
1	A	77	ALA	N-CA-CB	-11.99	92.08	110.42	13	20
1	A	43	LYS	N-CA-C	10.89	128.30	108.69	16	1
1	A	55	THR	OG1-CB-CG2	-10.69	87.92	109.30	16	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	46	ALA	N-CA-C	10.35	132.85	110.80	16	2
1	A	80	PRO	N-CA-C	10.23	133.55	112.47	11	3
1	A	43	LYS	CB-CA-C	-10.21	100.07	110.17	16	1
1	A	32	VAL	N-CA-C	10.11	120.74	110.23	3	7
1	A	24	TRP	N-CA-C	10.01	126.55	108.94	13	7
1	A	77	ALA	CB-CA-C	9.85	125.82	109.56	13	19
1	A	62	ARG	N-CA-C	-9.77	94.97	109.62	12	3
1	A	48	ILE	N-CA-C	9.72	121.46	109.30	6	14
1	A	58	THR	N-CA-C	9.65	124.80	110.52	1	11
1	A	81	ARG	N-CA-C	9.55	131.14	110.80	11	3
1	A	61	TYR	CA-CB-CG	-9.28	97.20	113.90	4	1
1	A	67	ARG	NE-CZ-NH2	-9.20	110.92	119.20	1	2
1	A	65	ARG	N-CA-C	9.18	128.50	107.48	8	16
1	A	76	ILE	O-C-N	9.06	132.14	122.45	19	20
1	A	79	VAL	CA-C-N	9.02	131.11	119.84	13	3
1	A	79	VAL	C-N-CA	9.02	131.11	119.84	13	3
1	A	82	VAL	CB-CA-C	-9.00	99.82	111.25	4	4
1	A	22	THR	N-CA-C	-8.94	100.46	112.26	18	5
1	A	76	ILE	CA-CB-CG1	-8.93	95.21	110.40	11	20
1	A	77	ALA	N-CA-C	-8.91	101.98	113.12	13	2
1	A	59	MET	N-CA-C	-8.79	96.43	109.62	12	3
1	A	59	MET	CA-C-O	8.78	123.03	117.94	5	2
1	A	66	VAL	CG1-CB-CG2	-8.18	92.81	110.80	19	16
1	A	63	ILE	N-CA-C	7.84	125.65	109.34	11	4
1	A	32	VAL	N-CA-CB	-7.82	101.40	110.55	12	12
1	A	76	ILE	CA-C-N	7.80	131.05	120.44	15	4
1	A	76	ILE	C-N-CA	7.80	131.05	120.44	15	4
1	A	65	ARG	N-CA-CB	-7.78	97.05	111.52	18	15
1	A	47	GLN	OE1-CD-NE2	-7.75	114.85	122.60	5	9
1	A	24	TRP	NE1-CE2-CZ2	7.72	141.68	130.10	19	17
1	A	65	ARG	NE-CZ-NH2	-7.70	112.27	119.20	6	4
1	A	62	ARG	NE-CZ-NH2	-7.61	112.35	119.20	1	2
1	A	67	ARG	NH1-CZ-NH2	7.60	129.18	119.30	9	2
1	A	79	VAL	N-CA-C	7.53	125.15	108.88	13	3
1	A	57	VAL	N-CA-C	7.53	125.00	109.34	3	5
1	A	67	ARG	NE-CZ-NH1	-7.48	114.02	121.50	16	6
1	A	21	LYS	N-CA-C	-7.38	99.30	109.71	9	3
1	A	24	TRP	CB-CG-CD1	-7.32	115.92	126.90	3	15
1	A	82	VAL	N-CA-C	-7.24	97.05	107.98	20	3
1	A	81	ARG	NE-CZ-NH1	-7.16	114.34	121.50	16	2
1	A	34	GLU	N-CA-C	-7.16	103.41	111.07	13	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	GLY	N-CA-C	-7.16	96.22	113.18	11	1
1	A	56	ILE	N-CA-C	7.07	124.04	109.34	19	4
1	A	61	TYR	N-CA-C	7.06	120.07	108.99	4	1
1	A	64	ASP	N-CA-C	-7.04	104.56	113.01	13	5
1	A	60	GLU	N-CA-C	-7.02	98.84	109.79	10	2
1	A	78	GLN	OE1-CD-NE2	-6.97	115.63	122.60	2	12
1	A	41	GLN	OE1-CD-NE2	-6.93	115.67	122.60	11	5
1	A	35	ALA	N-CA-C	-6.93	102.57	111.02	9	1
1	A	55	THR	CA-CB-CG2	6.90	122.23	110.50	17	3
1	A	24	TRP	CG-CD2-CE3	-6.82	127.08	133.90	13	7
1	A	66	VAL	CA-C-N	-6.78	114.03	122.84	13	1
1	A	66	VAL	C-N-CA	-6.78	114.03	122.84	13	1
1	A	80	PRO	N-CA-CB	-6.75	96.17	103.25	13	2
1	A	42	ASP	CA-CB-CG	6.73	119.33	112.60	14	2
1	A	74	ASP	N-CA-CB	-6.72	99.14	110.49	7	5
1	A	62	ARG	NH1-CZ-NH2	6.64	127.94	119.30	19	4
1	A	65	ARG	NE-CZ-NH1	-6.55	114.95	121.50	13	4
1	A	60	GLU	N-CA-CB	-6.55	101.34	110.38	9	5
1	A	73	LEU	N-CA-CB	-6.52	98.94	111.53	1	6
1	A	81	ARG	NE-CZ-NH2	-6.52	113.33	119.20	6	2
1	A	45	GLU	N-CA-CB	-6.51	101.58	110.56	11	3
1	A	55	THR	N-CA-CB	-6.45	99.60	110.49	2	13
1	A	82	VAL	CA-C-N	6.44	133.30	121.70	1	1
1	A	82	VAL	C-N-CA	6.44	133.30	121.70	1	1
1	A	69	PHE	CA-C-O	6.36	127.85	120.98	7	7
1	A	24	TRP	CG-CD1-NE1	-6.34	101.95	110.20	16	19
1	A	27	LEU	N-CA-CB	-6.27	100.89	110.92	14	4
1	A	58	THR	N-CA-CB	-6.25	100.93	110.49	11	2
1	A	38	VAL	CB-CA-C	-6.21	104.02	111.97	1	9
1	A	82	VAL	N-CA-CB	6.20	118.94	111.31	4	1
1	A	76	ILE	N-CA-C	6.17	116.98	108.84	6	2
1	A	64	ASP	N-CA-CB	-6.14	101.67	110.57	19	3
1	A	63	ILE	N-CA-CB	-6.07	101.21	111.23	9	6
1	A	62	ARG	NE-CZ-NH1	-6.06	115.44	121.50	2	3
1	A	75	ASN	CA-CB-CG	-5.99	106.61	112.60	2	4
1	A	43	LYS	CA-C-N	5.96	127.29	119.84	17	2
1	A	43	LYS	C-N-CA	5.96	127.29	119.84	17	2
1	A	83	GLY	N-CA-C	-5.95	96.05	113.30	1	1
1	A	64	ASP	CA-CB-CG	-5.92	106.69	112.60	18	2
1	A	65	ARG	CD-NE-CZ	-5.84	116.22	124.40	10	1
1	A	24	TRP	CD2-CE2-CZ2	-5.83	116.57	122.40	19	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	78	GLN	N-CA-C	-5.82	100.66	109.85	7	3
1	A	55	THR	CB-CA-C	5.77	118.49	109.84	14	2
1	A	42	ASP	CB-CG-OD2	-5.75	105.18	118.40	20	1
1	A	53	VAL	O-C-N	5.75	129.75	122.57	1	2
1	A	50	VAL	N-CA-CB	-5.71	104.26	111.46	11	1
1	A	31	SER	CA-C-O	5.71	128.57	121.89	14	3
1	A	82	VAL	O-C-N	5.69	128.03	121.94	12	1
1	A	73	LEU	N-CA-C	-5.68	103.72	111.56	9	1
1	A	78	GLN	CA-C-O	-5.66	114.25	120.30	12	1
1	A	69	PHE	CB-CG-CD1	-5.63	111.12	120.70	6	7
1	A	59	MET	O-C-N	5.59	129.52	122.19	9	2
1	A	76	ILE	CA-C-O	5.58	127.76	120.78	14	4
1	A	70	VAL	CA-C-O	-5.57	117.28	121.68	4	1
1	A	23	GLU	N-CA-CB	-5.57	101.16	111.52	1	1
1	A	41	GLN	N-CA-C	-5.56	105.75	112.54	20	1
1	A	24	TRP	N-CA-CB	-5.55	102.04	110.75	11	1
1	A	55	THR	CA-CB-OG1	5.54	117.91	109.60	16	1
1	A	76	ILE	N-CA-CB	-5.49	105.98	111.90	19	2
1	A	23	GLU	N-CA-C	5.47	118.38	108.69	16	2
1	A	26	GLU	CA-C-O	5.47	126.34	120.55	13	1
1	A	59	MET	CA-C-N	5.46	132.15	121.66	9	3
1	A	59	MET	C-N-CA	5.46	132.15	121.66	9	3
1	A	47	GLN	N-CA-C	-5.46	101.30	109.15	5	1
1	A	45	GLU	N-CA-C	5.45	119.03	112.93	11	1
1	A	78	GLN	CA-C-N	-5.45	110.95	120.59	12	4
1	A	78	GLN	C-N-CA	-5.45	110.95	120.59	12	4
1	A	39	ILE	N-CA-CB	-5.45	104.17	110.55	4	1
1	A	80	PRO	N-CD-CG	-5.43	95.06	103.20	20	4
1	A	42	ASP	N-CA-CB	-5.34	101.35	110.33	8	1
1	A	46	ALA	N-CA-CB	-5.34	101.46	110.49	16	1
1	A	65	ARG	NH1-CZ-NH2	5.34	126.24	119.30	9	3
1	A	36	LYS	N-CA-CB	-5.32	101.11	109.78	12	1
1	A	48	ILE	N-CA-CB	-5.32	102.65	112.43	13	1
1	A	24	TRP	CE2-CD2-CE3	5.29	124.09	118.80	19	2
1	A	42	ASP	N-CA-C	5.29	119.66	112.04	17	1
1	A	31	SER	N-CA-C	5.27	118.31	110.52	16	1
1	A	56	ILE	CA-C-O	5.23	126.04	119.39	11	1
1	A	36	LYS	CB-CA-C	5.16	119.31	110.74	12	1
1	A	40	LEU	N-CA-CB	-5.16	101.55	110.32	18	1
1	A	62	ARG	CD-NE-CZ	-5.14	117.20	124.40	13	1
1	A	24	TRP	NE1-CE2-CD2	-5.10	100.77	107.40	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	58	THR	O-C-N	5.09	129.10	122.38	13	1
1	A	53	VAL	CA-C-N	-5.09	116.21	123.08	4	1
1	A	53	VAL	C-N-CA	-5.09	116.21	123.08	4	1
1	A	40	LEU	N-CA-C	-5.08	105.75	111.28	16	1
1	A	47	GLN	CG-CD-NE2	5.06	124.00	116.40	5	1
1	A	51	LEU	CB-CA-C	5.06	116.89	110.16	1	1
1	A	57	VAL	CA-C-N	5.06	129.57	122.09	15	1
1	A	57	VAL	C-N-CA	5.06	129.57	122.09	15	1
1	A	22	THR	OG1-CB-CG2	-5.05	99.20	109.30	2	1
1	A	43	LYS	N-CA-CB	-5.05	102.92	111.30	2	1
1	A	80	PRO	CB-CA-C	5.02	117.54	111.46	2	1
1	A	44	PRO	N-CA-C	5.00	122.77	112.47	17	1

There are no chirality outliers.

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	62	ARG	Sidechain	20
1	A	65	ARG	Sidechain	18
1	A	67	ARG	Sidechain	18
1	A	81	ARG	Sidechain	18

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	505	538	538	34±8
All	All	10100	10760	10760	685

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:TYR:CE2	1:A:63:ILE:HB	0.84	2.08	2	3
1:A:79:VAL:HB	1:A:80:PRO:HD3	0.77	1.56	11	1
1:A:79:VAL:HB	1:A:80:PRO:CD	0.77	2.10	11	3
1:A:79:VAL:CB	1:A:80:PRO:CD	0.73	2.67	11	2
1:A:28:VAL:CG2	1:A:79:VAL:HG22	0.72	2.15	11	10
1:A:51:LEU:HB3	1:A:69:PHE:CZ	0.70	2.21	11	7
1:A:28:VAL:HG23	1:A:79:VAL:CG2	0.68	2.19	8	2
1:A:39:ILE:HG21	1:A:66:VAL:HG21	0.67	1.65	4	20
1:A:51:LEU:HB3	1:A:69:PHE:CE1	0.66	2.26	17	10
1:A:66:VAL:HG22	1:A:82:VAL:HG22	0.64	1.67	19	3
1:A:71:ASP:CG	1:A:72:LYS:N	0.64	2.52	15	18
1:A:65:ARG:HB3	1:A:65:ARG:NH2	0.64	2.08	11	1
1:A:79:VAL:N	1:A:80:PRO:HD2	0.63	2.07	19	2
1:A:26:GLU:CD	1:A:26:GLU:H	0.63	2.02	11	9
1:A:39:ILE:CG2	1:A:66:VAL:HG21	0.62	2.25	12	19
1:A:32:VAL:CG2	1:A:70:VAL:HG11	0.62	2.24	6	3
1:A:24:TRP:CZ2	1:A:39:ILE:HG23	0.62	2.30	13	5
1:A:67:ARG:CZ	1:A:68:LEU:H	0.62	2.08	11	1
1:A:23:GLU:N	1:A:23:GLU:CD	0.62	2.58	11	8
1:A:65:ARG:HB3	1:A:65:ARG:CZ	0.62	2.25	11	1
1:A:57:VAL:HG22	1:A:69:PHE:CE2	0.62	2.30	19	4
1:A:21:LYS:NZ	1:A:23:GLU:O	0.62	2.32	19	2
1:A:79:VAL:CB	1:A:80:PRO:HD3	0.61	2.25	11	1
1:A:66:VAL:CG2	1:A:82:VAL:HG22	0.61	2.24	19	3
1:A:55:THR:HA	1:A:69:PHE:CZ	0.60	2.31	11	1
1:A:61:TYR:CD2	1:A:62:ARG:N	0.60	2.69	4	1
1:A:48:ILE:HD12	1:A:48:ILE:N	0.60	2.11	16	1
1:A:62:ARG:H	1:A:83:GLY:C	0.60	2.04	20	1
1:A:39:ILE:CG2	1:A:48:ILE:HD11	0.59	2.27	3	13
1:A:55:THR:HB	1:A:69:PHE:CE1	0.59	2.32	7	7
1:A:67:ARG:NH2	1:A:83:GLY:C	0.59	2.61	3	2
1:A:59:MET:SD	1:A:81:ARG:CD	0.58	2.91	12	1
1:A:40:LEU:HD21	1:A:46:ALA:O	0.58	1.99	2	2
1:A:62:ARG:HB2	1:A:65:ARG:CZ	0.58	2.28	5	1
1:A:23:GLU:C	1:A:24:TRP:CE3	0.58	2.82	11	6
1:A:28:VAL:CG2	1:A:79:VAL:CG2	0.58	2.82	8	3
1:A:57:VAL:HG21	1:A:69:PHE:CE2	0.57	2.33	12	4
1:A:56:ILE:H	1:A:56:ILE:HD12	0.57	1.60	14	1
1:A:61:TYR:CD2	1:A:83:GLY:HA2	0.57	2.35	4	1
1:A:27:LEU:CD1	1:A:27:LEU:N	0.57	2.67	15	1
1:A:32:VAL:HG23	1:A:70:VAL:HG11	0.57	1.75	17	1
1:A:67:ARG:HH21	1:A:83:GLY:C	0.57	2.07	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:GLU:CD	1:A:62:ARG:NH1	0.57	2.63	12	1
1:A:51:LEU:HD22	1:A:69:PHE:CZ	0.56	2.34	18	3
1:A:33:GLU:HG3	1:A:34:GLU:N	0.56	2.15	20	2
1:A:61:TYR:CE1	1:A:83:GLY:HA3	0.56	2.36	5	1
1:A:71:ASP:CG	1:A:72:LYS:H	0.56	2.08	15	13
1:A:61:TYR:CE1	1:A:63:ILE:HB	0.56	2.36	13	2
1:A:33:GLU:CD	1:A:34:GLU:N	0.56	2.63	17	1
1:A:63:ILE:HA	1:A:82:VAL:HG12	0.56	1.77	8	1
1:A:61:TYR:CD1	1:A:63:ILE:HB	0.56	2.36	18	6
1:A:62:ARG:H	1:A:62:ARG:CD	0.56	2.13	11	1
1:A:24:TRP:NE1	1:A:39:ILE:HA	0.55	2.17	15	1
1:A:63:ILE:HD12	1:A:82:VAL:HG11	0.55	1.76	5	6
1:A:39:ILE:HD12	1:A:48:ILE:CD1	0.55	2.31	13	1
1:A:60:GLU:CD	1:A:62:ARG:HE	0.55	2.09	16	1
1:A:62:ARG:CZ	1:A:62:ARG:HA	0.55	2.31	14	1
1:A:57:VAL:HA	1:A:67:ARG:NH1	0.55	2.16	10	2
1:A:53:VAL:HG23	1:A:70:VAL:O	0.55	2.02	15	1
1:A:55:THR:HG22	1:A:69:PHE:CE2	0.55	2.36	11	1
1:A:47:GLN:HB3	1:A:64:ASP:O	0.55	2.02	19	1
1:A:63:ILE:C	1:A:65:ARG:H	0.54	2.11	15	4
1:A:55:THR:HB	1:A:69:PHE:CZ	0.54	2.37	5	3
1:A:65:ARG:HH12	1:A:83:GLY:C	0.54	2.10	5	1
1:A:33:GLU:CG	1:A:34:GLU:N	0.54	2.70	20	2
1:A:43:LYS:HG3	1:A:46:ALA:N	0.54	2.18	16	1
1:A:37:LYS:NZ	1:A:41:GLN:OE1	0.54	2.39	13	2
1:A:27:LEU:N	1:A:27:LEU:HD12	0.54	2.18	15	1
1:A:51:LEU:CD2	1:A:55:THR:HG22	0.54	2.33	19	1
1:A:36:LYS:NZ	1:A:48:ILE:O	0.54	2.41	11	2
1:A:24:TRP:CG	1:A:39:ILE:HG12	0.54	2.38	3	1
1:A:24:TRP:CZ3	1:A:82:VAL:HG23	0.53	2.38	8	4
1:A:62:ARG:NH2	1:A:62:ARG:HB2	0.53	2.18	13	1
1:A:51:LEU:HB2	1:A:69:PHE:CE1	0.53	2.37	14	2
1:A:27:LEU:HD12	1:A:27:LEU:C	0.53	2.28	5	3
1:A:24:TRP:CE3	1:A:66:VAL:HG11	0.53	2.38	14	2
1:A:43:LYS:NZ	1:A:63:ILE:O	0.53	2.41	9	1
1:A:51:LEU:HD13	1:A:69:PHE:CE2	0.53	2.38	16	2
1:A:51:LEU:HG	1:A:69:PHE:CZ	0.53	2.39	17	2
1:A:51:LEU:HD12	1:A:67:ARG:HD2	0.53	1.80	11	1
1:A:63:ILE:HD12	1:A:82:VAL:CG1	0.52	2.34	8	2
1:A:61:TYR:CD2	1:A:63:ILE:N	0.52	2.77	4	1
1:A:51:LEU:CD1	1:A:55:THR:CG2	0.52	2.88	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ILE:HG21	1:A:48:ILE:HD11	0.52	1.80	6	8
1:A:51:LEU:CB	1:A:69:PHE:CZ	0.52	2.92	7	3
1:A:62:ARG:HB3	1:A:65:ARG:NH2	0.52	2.19	16	2
1:A:24:TRP:HB3	1:A:27:LEU:CG	0.52	2.35	3	5
1:A:43:LYS:HE3	1:A:45:GLU:C	0.52	2.30	16	1
1:A:24:TRP:HB3	1:A:27:LEU:HG	0.51	1.83	4	6
1:A:24:TRP:HB3	1:A:27:LEU:CD1	0.51	2.36	9	2
1:A:39:ILE:HD13	1:A:66:VAL:HG11	0.51	1.83	1	6
1:A:53:VAL:HG22	1:A:69:PHE:HB3	0.51	1.83	13	3
1:A:51:LEU:HD23	1:A:55:THR:CG2	0.51	2.35	19	3
1:A:62:ARG:O	1:A:64:ASP:N	0.51	2.44	6	4
1:A:27:LEU:HD13	1:A:35:ALA:HB1	0.51	1.81	18	2
1:A:59:MET:SD	1:A:60:GLU:N	0.51	2.83	14	1
1:A:45:GLU:C	1:A:82:VAL:HG11	0.51	2.30	16	1
1:A:66:VAL:HG22	1:A:82:VAL:CG2	0.51	2.36	12	3
1:A:81:ARG:HH22	1:A:83:GLY:C	0.51	2.13	18	1
1:A:37:LYS:HD3	1:A:37:LYS:C	0.51	2.31	20	1
1:A:21:LYS:HE3	1:A:24:TRP:NE1	0.51	2.21	8	1
1:A:23:GLU:CD	1:A:23:GLU:H	0.51	2.13	9	3
1:A:62:ARG:C	1:A:64:ASP:H	0.50	2.13	8	3
1:A:59:MET:O	1:A:62:ARG:HD2	0.50	2.05	20	1
1:A:65:ARG:CZ	1:A:65:ARG:CB	0.50	2.89	11	1
1:A:72:LYS:NZ	1:A:72:LYS:HA	0.50	2.20	19	1
1:A:22:THR:O	1:A:81:ARG:CB	0.50	2.60	19	2
1:A:57:VAL:HG21	1:A:67:ARG:CD	0.50	2.37	18	1
1:A:67:ARG:NH2	1:A:69:PHE:CE2	0.50	2.78	18	1
1:A:34:GLU:N	1:A:34:GLU:CD	0.50	2.70	12	1
1:A:56:ILE:HD12	1:A:56:ILE:N	0.50	2.20	14	1
1:A:48:ILE:N	1:A:48:ILE:CD1	0.50	2.75	16	1
1:A:48:ILE:HA	1:A:65:ARG:HG3	0.50	1.83	4	1
1:A:61:TYR:CE2	1:A:63:ILE:CB	0.49	2.92	2	1
1:A:49:ILE:H	1:A:65:ARG:NH2	0.49	2.05	2	1
1:A:56:ILE:H	1:A:56:ILE:CD1	0.49	2.19	14	1
1:A:27:LEU:HA	1:A:30:LYS:CE	0.49	2.37	5	1
1:A:61:TYR:CE1	1:A:83:GLY:C	0.49	2.90	18	1
1:A:25:PRO:HA	1:A:79:VAL:HG21	0.49	1.85	12	2
1:A:27:LEU:HD21	1:A:39:ILE:CG1	0.49	2.38	15	1
1:A:47:GLN:O	1:A:65:ARG:NH1	0.49	2.45	20	1
1:A:28:VAL:HG21	1:A:79:VAL:HG22	0.49	1.82	4	2
1:A:67:ARG:NE	1:A:67:ARG:HA	0.49	2.22	11	3
1:A:57:VAL:HG13	1:A:69:PHE:CE2	0.49	2.42	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:VAL:HA	1:A:67:ARG:CZ	0.49	2.37	5	1
1:A:51:LEU:HD23	1:A:55:THR:HG21	0.49	1.84	9	4
1:A:79:VAL:O	1:A:81:ARG:NH1	0.49	2.45	9	1
1:A:58:THR:OG1	1:A:62:ARG:NH1	0.49	2.46	11	1
1:A:21:LYS:CE	1:A:23:GLU:O	0.49	2.61	16	1
1:A:66:VAL:HG22	1:A:82:VAL:HA	0.49	1.84	11	1
1:A:33:GLU:CD	1:A:36:LYS:HZ3	0.49	2.15	19	1
1:A:24:TRP:CE2	1:A:39:ILE:HG23	0.49	2.43	16	2
1:A:48:ILE:HG12	1:A:66:VAL:H	0.49	1.68	14	2
1:A:61:TYR:CE2	1:A:83:GLY:N	0.49	2.81	4	1
1:A:51:LEU:CB	1:A:69:PHE:CE1	0.48	2.97	6	4
1:A:60:GLU:HG2	1:A:61:TYR:N	0.48	2.24	16	1
1:A:49:ILE:H	1:A:65:ARG:CZ	0.48	2.21	2	1
1:A:76:ILE:HG21	1:A:80:PRO:HG3	0.48	1.84	3	1
1:A:33:GLU:CG	1:A:34:GLU:H	0.48	2.21	13	2
1:A:60:GLU:CG	1:A:61:TYR:N	0.48	2.76	16	1
1:A:80:PRO:O	1:A:81:ARG:CB	0.48	2.61	11	1
1:A:55:THR:OG1	1:A:69:PHE:CE1	0.48	2.66	16	1
1:A:26:GLU:CD	1:A:26:GLU:N	0.48	2.72	1	4
1:A:24:TRP:CH2	1:A:82:VAL:HG23	0.48	2.43	4	2
1:A:61:TYR:O	1:A:62:ARG:NH1	0.48	2.46	4	1
1:A:79:VAL:HG22	1:A:80:PRO:HD2	0.48	1.85	8	1
1:A:72:LYS:N	1:A:72:LYS:HD2	0.48	2.22	1	1
1:A:48:ILE:CG2	1:A:68:LEU:HD12	0.48	2.39	2	1
1:A:53:VAL:HA	1:A:69:PHE:CG	0.48	2.43	2	1
1:A:24:TRP:CH2	1:A:39:ILE:HG23	0.48	2.43	13	1
1:A:59:MET:HG2	1:A:60:GLU:H	0.48	1.68	19	1
1:A:49:ILE:CG2	1:A:50:VAL:N	0.48	2.77	4	6
1:A:62:ARG:NE	1:A:62:ARG:HA	0.48	2.24	19	1
1:A:32:VAL:CG1	1:A:33:GLU:N	0.48	2.76	5	3
1:A:33:GLU:OE2	1:A:36:LYS:NZ	0.47	2.47	10	4
1:A:24:TRP:HB3	1:A:27:LEU:CD2	0.47	2.39	10	4
1:A:30:LYS:NZ	1:A:34:GLU:CD	0.47	2.72	6	2
1:A:27:LEU:HA	1:A:30:LYS:NZ	0.47	2.24	13	1
1:A:57:VAL:O	1:A:62:ARG:NH2	0.47	2.47	16	1
1:A:21:LYS:HZ3	1:A:24:TRP:CD1	0.47	2.27	17	1
1:A:43:LYS:HE3	1:A:46:ALA:C	0.47	2.34	16	1
1:A:31:SER:HA	1:A:74:ASP:O	0.47	2.10	11	5
1:A:62:ARG:CD	1:A:62:ARG:N	0.47	2.78	11	1
1:A:73:LEU:CD1	1:A:75:ASN:HD22	0.47	2.23	2	1
1:A:53:VAL:HA	1:A:69:PHE:CD1	0.47	2.45	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ARG:HH11	1:A:83:GLY:C	0.47	2.18	8	1
1:A:60:GLU:CD	1:A:62:ARG:HH21	0.47	2.17	9	1
1:A:34:GLU:OE1	1:A:37:LYS:NZ	0.47	2.48	18	1
1:A:49:ILE:HG22	1:A:50:VAL:N	0.47	2.24	11	3
1:A:23:GLU:HB2	1:A:81:ARG:NH2	0.47	2.25	6	1
1:A:36:LYS:HG2	1:A:48:ILE:HB	0.47	1.87	13	1
1:A:23:GLU:H	1:A:23:GLU:CD	0.47	2.18	19	1
1:A:27:LEU:CD1	1:A:39:ILE:HG13	0.47	2.40	8	3
1:A:61:TYR:CE2	1:A:63:ILE:HD13	0.47	2.45	19	2
1:A:59:MET:N	1:A:59:MET:SD	0.47	2.88	1	2
1:A:63:ILE:HD12	1:A:82:VAL:HG12	0.47	1.87	4	1
1:A:60:GLU:CD	1:A:62:ARG:NH2	0.47	2.73	9	1
1:A:67:ARG:HD2	1:A:69:PHE:CE2	0.46	2.45	11	1
1:A:60:GLU:CD	1:A:62:ARG:HH11	0.46	2.18	5	1
1:A:57:VAL:HG12	1:A:67:ARG:HD3	0.46	1.86	14	1
1:A:51:LEU:HD12	1:A:67:ARG:CD	0.46	2.41	11	1
1:A:30:LYS:O	1:A:75:ASN:HA	0.46	2.10	2	3
1:A:34:GLU:HA	1:A:37:LYS:HE3	0.46	1.87	7	1
1:A:24:TRP:HB3	1:A:27:LEU:HD12	0.46	1.88	18	2
1:A:64:ASP:CG	1:A:65:ARG:HH22	0.46	2.18	11	1
1:A:45:GLU:O	1:A:82:VAL:HG11	0.46	2.11	16	1
1:A:54:GLY:O	1:A:56:ILE:N	0.46	2.49	8	3
1:A:63:ILE:C	1:A:65:ARG:N	0.46	2.71	2	5
1:A:79:VAL:HG12	1:A:80:PRO:N	0.46	2.23	11	1
1:A:27:LEU:CD1	1:A:27:LEU:H	0.46	2.24	15	1
1:A:23:GLU:CD	1:A:23:GLU:N	0.46	2.73	19	1
1:A:63:ILE:CD1	1:A:82:VAL:HG11	0.46	2.41	14	1
1:A:59:MET:O	1:A:62:ARG:CD	0.46	2.64	20	1
1:A:51:LEU:HD11	1:A:67:ARG:CZ	0.46	2.41	9	1
1:A:65:ARG:HD2	1:A:67:ARG:CZ	0.46	2.40	9	1
1:A:24:TRP:O	1:A:80:PRO:HD2	0.46	2.10	16	2
1:A:53:VAL:O	1:A:72:LYS:NZ	0.46	2.48	8	1
1:A:67:ARG:NH2	1:A:83:GLY:OXT	0.46	2.49	2	2
1:A:43:LYS:NZ	1:A:45:GLU:OE1	0.45	2.49	1	5
1:A:25:PRO:N	1:A:79:VAL:HG13	0.45	2.26	11	1
1:A:53:VAL:HG23	1:A:69:PHE:C	0.45	2.36	8	2
1:A:39:ILE:CD1	1:A:68:LEU:HD11	0.45	2.42	13	2
1:A:45:GLU:O	1:A:47:GLN:N	0.45	2.49	20	2
1:A:43:LYS:NZ	1:A:45:GLU:OE2	0.45	2.49	20	3
1:A:66:VAL:HG13	1:A:81:ARG:C	0.45	2.37	12	2
1:A:30:LYS:NZ	1:A:34:GLU:OE2	0.45	2.50	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:GLU:CD	1:A:81:ARG:HH22	0.45	2.19	1	1
1:A:27:LEU:O	1:A:28:VAL:C	0.45	2.60	7	2
1:A:51:LEU:CD1	1:A:67:ARG:HE	0.45	2.25	9	1
1:A:66:VAL:HA	1:A:81:ARG:O	0.45	2.12	12	1
1:A:21:LYS:NZ	1:A:42:ASP:CG	0.45	2.75	11	2
1:A:59:MET:HA	1:A:59:MET:HE3	0.45	1.87	10	1
1:A:21:LYS:HB3	1:A:42:ASP:HB3	0.45	1.89	13	1
1:A:34:GLU:CD	1:A:37:LYS:HZ1	0.45	2.19	7	1
1:A:65:ARG:HD2	1:A:67:ARG:NH1	0.45	2.28	9	1
1:A:28:VAL:HG23	1:A:79:VAL:HG21	0.44	1.88	8	1
1:A:27:LEU:HD23	1:A:35:ALA:HB1	0.44	1.89	15	1
1:A:57:VAL:HG13	1:A:69:PHE:HE2	0.44	1.71	14	1
1:A:57:VAL:HG13	1:A:69:PHE:CD2	0.44	2.48	19	1
1:A:24:TRP:CD1	1:A:39:ILE:HG12	0.44	2.47	3	1
1:A:36:LYS:O	1:A:40:LEU:HG	0.44	2.12	1	3
1:A:51:LEU:HG	1:A:69:PHE:CE2	0.44	2.48	17	1
1:A:35:ALA:O	1:A:36:LYS:C	0.44	2.60	19	4
1:A:43:LYS:HD2	1:A:46:ALA:C	0.44	2.37	16	1
1:A:23:GLU:OE1	1:A:24:TRP:N	0.44	2.51	1	1
1:A:58:THR:C	1:A:59:MET:HE3	0.44	2.37	1	1
1:A:71:ASP:CG	1:A:73:LEU:H	0.44	2.20	1	3
1:A:24:TRP:HE1	1:A:42:ASP:CG	0.44	2.20	3	1
1:A:51:LEU:HB2	1:A:69:PHE:CZ	0.44	2.47	19	2
1:A:27:LEU:HD11	1:A:39:ILE:HG13	0.44	1.88	17	2
1:A:43:LYS:CE	1:A:45:GLU:C	0.44	2.91	16	1
1:A:34:GLU:O	1:A:37:LYS:HB3	0.44	2.13	6	1
1:A:57:VAL:HG21	1:A:69:PHE:HE2	0.44	1.72	15	4
1:A:66:VAL:O	1:A:67:ARG:NH1	0.44	2.48	9	1
1:A:50:VAL:C	1:A:51:LEU:HD12	0.44	2.38	10	1
1:A:58:THR:O	1:A:67:ARG:NH1	0.44	2.50	15	1
1:A:48:ILE:CG2	1:A:49:ILE:N	0.44	2.80	16	1
1:A:57:VAL:CG2	1:A:67:ARG:HD2	0.44	2.43	16	1
1:A:21:LYS:HE3	1:A:24:TRP:CD1	0.44	2.48	20	1
1:A:47:GLN:O	1:A:65:ARG:NH2	0.44	2.51	6	1
1:A:34:GLU:OE2	1:A:37:LYS:NZ	0.44	2.51	16	1
1:A:60:GLU:CD	1:A:62:ARG:NE	0.44	2.75	16	1
1:A:72:LYS:HA	1:A:72:LYS:CE	0.44	2.43	19	1
1:A:67:ARG:C	1:A:68:LEU:HD12	0.43	2.38	15	2
1:A:27:LEU:HA	1:A:30:LYS:HE2	0.43	1.90	4	1
1:A:36:LYS:O	1:A:40:LEU:HD12	0.43	2.13	4	1
1:A:34:GLU:CD	1:A:37:LYS:NZ	0.43	2.76	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LYS:HZ3	1:A:42:ASP:CG	0.43	2.22	15	1
1:A:61:TYR:O	1:A:61:TYR:CD1	0.43	2.71	8	1
1:A:51:LEU:CD1	1:A:55:THR:HG21	0.43	2.43	20	1
1:A:38:VAL:O	1:A:41:GLN:HB3	0.43	2.13	4	4
1:A:74:ASP:O	1:A:74:ASP:CG	0.43	2.61	11	2
1:A:73:LEU:O	1:A:75:ASN:N	0.43	2.51	19	2
1:A:33:GLU:OE1	1:A:36:LYS:NZ	0.43	2.52	16	1
1:A:43:LYS:HZ3	1:A:45:GLU:CD	0.43	2.22	5	2
1:A:59:MET:SD	1:A:81:ARG:HD3	0.43	2.54	12	1
1:A:61:TYR:CE1	1:A:63:ILE:HD13	0.43	2.48	16	2
1:A:51:LEU:HD12	1:A:69:PHE:CE1	0.43	2.49	20	1
1:A:43:LYS:O	1:A:45:GLU:N	0.43	2.51	1	1
1:A:43:LYS:HE3	1:A:46:ALA:CA	0.43	2.44	16	1
1:A:82:VAL:HG12	1:A:83:GLY:N	0.43	2.28	1	1
1:A:24:TRP:HZ3	1:A:82:VAL:HG23	0.43	1.74	8	1
1:A:68:LEU:O	1:A:70:VAL:HG13	0.43	2.13	18	1
1:A:62:ARG:O	1:A:65:ARG:HB3	0.43	2.14	4	1
1:A:28:VAL:CG2	1:A:79:VAL:HB	0.43	2.43	8	1
1:A:62:ARG:HB2	1:A:65:ARG:NH2	0.43	2.28	9	1
1:A:26:GLU:O	1:A:30:LYS:CE	0.43	2.66	11	1
1:A:64:ASP:OD2	1:A:65:ARG:NH2	0.43	2.52	12	1
1:A:21:LYS:NZ	1:A:26:GLU:OE2	0.42	2.52	16	2
1:A:51:LEU:HD13	1:A:69:PHE:CZ	0.42	2.48	12	2
1:A:51:LEU:CD1	1:A:69:PHE:CZ	0.42	3.02	20	1
1:A:35:ALA:O	1:A:39:ILE:HG13	0.42	2.14	4	2
1:A:50:VAL:HG22	1:A:51:LEU:N	0.42	2.29	6	1
1:A:48:ILE:HG12	1:A:66:VAL:HB	0.42	1.92	17	2
1:A:67:ARG:O	1:A:80:PRO:HA	0.42	2.14	18	1
1:A:51:LEU:HD13	1:A:67:ARG:CD	0.42	2.44	2	1
1:A:57:VAL:HG21	1:A:67:ARG:NE	0.42	2.29	1	1
1:A:60:GLU:CD	1:A:62:ARG:HB2	0.42	2.39	8	1
1:A:68:LEU:HD23	1:A:80:PRO:HG3	0.42	1.91	8	1
1:A:24:TRP:CH2	1:A:46:ALA:HB2	0.42	2.50	16	1
1:A:34:GLU:O	1:A:35:ALA:C	0.42	2.61	6	2
1:A:57:VAL:HG21	1:A:67:ARG:HD3	0.42	1.91	15	1
1:A:46:ALA:HB1	1:A:66:VAL:CG2	0.42	2.44	16	1
1:A:81:ARG:NH2	1:A:82:VAL:O	0.42	2.53	17	1
1:A:67:ARG:NE	1:A:69:PHE:CD2	0.42	2.88	18	1
1:A:70:VAL:HB	1:A:74:ASP:C	0.42	2.40	18	1
1:A:78:GLN:O	1:A:79:VAL:C	0.42	2.63	8	1
1:A:67:ARG:HA	1:A:67:ARG:NH2	0.42	2.30	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:VAL:CG2	1:A:69:PHE:CE2	0.42	3.03	18	1
1:A:25:PRO:CA	1:A:79:VAL:HG13	0.42	2.45	11	1
1:A:28:VAL:CG2	1:A:79:VAL:CB	0.42	2.97	8	1
1:A:24:TRP:HB3	1:A:27:LEU:HD22	0.42	1.91	15	1
1:A:57:VAL:HG21	1:A:67:ARG:HD2	0.42	1.91	16	1
1:A:39:ILE:CG2	1:A:48:ILE:CD1	0.42	2.98	5	2
1:A:28:VAL:CG2	1:A:79:VAL:HG23	0.42	2.45	8	1
1:A:73:LEU:HD12	1:A:73:LEU:O	0.42	2.14	11	2
1:A:61:TYR:CZ	1:A:83:GLY:C	0.42	2.98	12	1
1:A:65:ARG:NH2	1:A:65:ARG:HB3	0.42	2.29	16	1
1:A:24:TRP:CZ3	1:A:82:VAL:CG2	0.41	3.03	1	1
1:A:48:ILE:C	1:A:49:ILE:HD12	0.41	2.40	10	1
1:A:60:GLU:O	1:A:81:ARG:NH2	0.41	2.53	11	1
1:A:43:LYS:NZ	1:A:45:GLU:CD	0.41	2.78	20	1
1:A:30:LYS:NZ	1:A:34:GLU:OE1	0.41	2.48	9	3
1:A:37:LYS:N	1:A:37:LYS:HD3	0.41	2.30	14	1
1:A:70:VAL:CG2	1:A:74:ASP:HA	0.41	2.45	17	1
1:A:81:ARG:NH2	1:A:82:VAL:C	0.41	2.78	17	1
1:A:63:ILE:CD1	1:A:82:VAL:CG1	0.41	2.98	8	1
1:A:36:LYS:HG2	1:A:48:ILE:CG2	0.41	2.45	16	1
1:A:26:GLU:HG2	1:A:27:LEU:N	0.41	2.31	3	1
1:A:57:VAL:HG21	1:A:81:ARG:HH12	0.41	1.75	14	1
1:A:62:ARG:C	1:A:64:ASP:N	0.41	2.78	19	1
1:A:47:GLN:N	1:A:64:ASP:O	0.41	2.53	1	2
1:A:24:TRP:NE1	1:A:42:ASP:OD2	0.41	2.53	6	1
1:A:32:VAL:CG2	1:A:68:LEU:HD13	0.41	2.46	2	1
1:A:59:MET:SD	1:A:62:ARG:HG3	0.41	2.56	2	1
1:A:28:VAL:HG21	1:A:79:VAL:CG2	0.41	2.44	11	1
1:A:43:LYS:N	1:A:44:PRO:CD	0.41	2.84	11	1
1:A:21:LYS:NZ	1:A:24:TRP:CD1	0.41	2.89	1	1
1:A:21:LYS:HE2	1:A:23:GLU:O	0.41	2.15	16	1
1:A:51:LEU:HD11	1:A:67:ARG:NH2	0.41	2.30	9	1
1:A:81:ARG:HH21	1:A:83:GLY:C	0.41	2.24	11	1
1:A:53:VAL:HA	1:A:69:PHE:HD1	0.41	1.76	16	1
1:A:51:LEU:HD23	1:A:55:THR:HG22	0.41	1.91	19	1
1:A:62:ARG:H	1:A:83:GLY:CA	0.41	2.28	20	1
1:A:49:ILE:CG2	1:A:50:VAL:H	0.41	2.29	4	1
1:A:63:ILE:CD1	1:A:82:VAL:HG12	0.41	2.45	4	1
1:A:50:VAL:CG2	1:A:51:LEU:N	0.41	2.84	6	1
1:A:69:PHE:HB3	1:A:78:GLN:CD	0.41	2.41	6	1
1:A:32:VAL:HB	1:A:70:VAL:HG11	0.41	1.91	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:GLU:OE2	1:A:65:ARG:NH2	0.41	2.54	9	1
1:A:40:LEU:O	1:A:44:PRO:HA	0.41	2.16	11	1
1:A:60:GLU:CD	1:A:67:ARG:HH11	0.41	2.24	12	1
1:A:49:ILE:O	1:A:67:ARG:NH2	0.41	2.53	13	1
1:A:31:SER:HA	1:A:75:ASN:HA	0.41	1.93	8	1
1:A:33:GLU:OE1	1:A:37:LYS:NZ	0.41	2.51	11	1
1:A:32:VAL:HG21	1:A:50:VAL:CG2	0.40	2.46	14	1
1:A:25:PRO:C	1:A:27:LEU:H	0.40	2.24	17	1
1:A:54:GLY:N	1:A:69:PHE:CE2	0.40	2.89	2	1
1:A:61:TYR:CD2	1:A:63:ILE:HB	0.40	2.51	11	2
1:A:76:ILE:CG2	1:A:80:PRO:HG3	0.40	2.47	3	1
1:A:61:TYR:O	1:A:61:TYR:CG	0.40	2.74	8	1
1:A:36:LYS:HG2	1:A:48:ILE:HG21	0.40	1.92	16	1
1:A:51:LEU:HD12	1:A:69:PHE:CZ	0.40	2.51	20	1
1:A:39:ILE:HG21	1:A:48:ILE:CD1	0.40	2.46	2	1
1:A:47:GLN:O	1:A:65:ARG:HA	0.40	2.15	16	1
1:A:51:LEU:HB3	1:A:69:PHE:CD1	0.40	2.51	17	1
1:A:23:GLU:OE1	1:A:81:ARG:NH2	0.40	2.55	1	1
1:A:47:GLN:O	1:A:47:GLN:NE2	0.40	2.55	1	1
1:A:22:THR:O	1:A:81:ARG:HB2	0.40	2.17	3	1
1:A:28:VAL:CG2	1:A:79:VAL:HA	0.40	2.47	19	1
1:A:60:GLU:HG3	1:A:61:TYR:N	0.40	2.32	11	1
1:A:53:VAL:CG2	1:A:69:PHE:HB3	0.40	2.45	13	1
1:A:62:ARG:NH1	1:A:83:GLY:O	0.40	2.53	13	1
1:A:39:ILE:CB	1:A:48:ILE:HD11	0.40	2.47	16	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	62/66 (94%)	48±2 (77±3%)	9±2 (15±3%)	5±1 (8±2%)	1	15
All	All	1240/1320 (94%)	958 (77%)	189 (15%)	93 (8%)	1	15

All 15 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	44	PRO	20
1	A	74	ASP	19
1	A	46	ALA	16
1	A	55	THR	10
1	A	63	ILE	8
1	A	56	ILE	4
1	A	60	GLU	4
1	A	57	VAL	2
1	A	82	VAL	2
1	A	80	PRO	2
1	A	21	LYS	2
1	A	67	ARG	1
1	A	58	THR	1
1	A	79	VAL	1
1	A	59	MET	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	57/60 (95%)	45±2 (80±4%)	12±2 (20±4%)	3	32
All	All	1140/1200 (95%)	907 (80%)	233 (20%)	3	32

All 45 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	THR	19
1	A	74	ASP	17
1	A	44	PRO	15
1	A	23	GLU	13
1	A	45	GLU	12
1	A	62	ARG	10
1	A	81	ARG	10
1	A	32	VAL	9
1	A	57	VAL	9
1	A	60	GLU	8
1	A	51	LEU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	73	LEU	7
1	A	27	LEU	6
1	A	30	LYS	6
1	A	67	ARG	6
1	A	72	LYS	6
1	A	34	GLU	5
1	A	21	LYS	5
1	A	31	SER	5
1	A	55	THR	5
1	A	26	GLU	4
1	A	49	ILE	4
1	A	80	PRO	4
1	A	63	ILE	3
1	A	41	GLN	3
1	A	43	LYS	3
1	A	53	VAL	3
1	A	66	VAL	3
1	A	56	ILE	3
1	A	65	ARG	2
1	A	40	LEU	2
1	A	70	VAL	2
1	A	33	GLU	2
1	A	79	VAL	2
1	A	47	GLN	2
1	A	37	LYS	2
1	A	68	LEU	1
1	A	78	GLN	1
1	A	25	PRO	1
1	A	75	ASN	1
1	A	61	TYR	1
1	A	59	MET	1
1	A	71	ASP	1
1	A	48	ILE	1
1	A	22	THR	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 [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