



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 10:51 PM UTC

PDB ID : 1TIZ / pdb_00001tiz
Title : Solution Structure of a Calmodulin-Like Calcium-Binding Domain from *Arabidopsis thaliana*
Authors : Song, J.; Zhao, Q.; Thao, S.; Frederick, R.O.; Markley, J.L.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2004-06-02

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

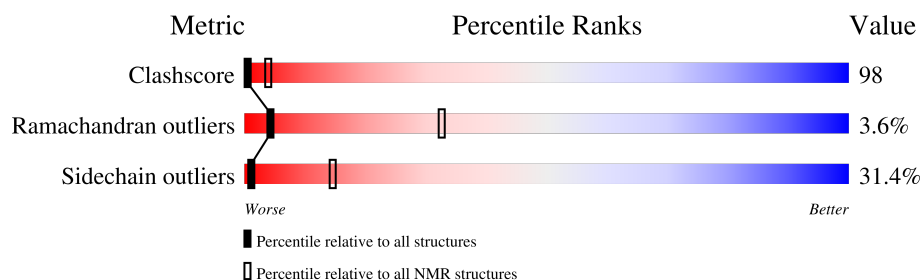
1 Overall quality at a glance

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	67	21% 48% 24% 7%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:63 (62)	0.25	2

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1061 atoms, of which 518 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called calmodulin-related protein, putative.

Mol	Chain	Residues	Atoms						Trace
1	A	67	Total	C	H	N	O	S	0
			1061	347	518	84	110	2	

There is a discrepancy between the modelled and reference sequences:

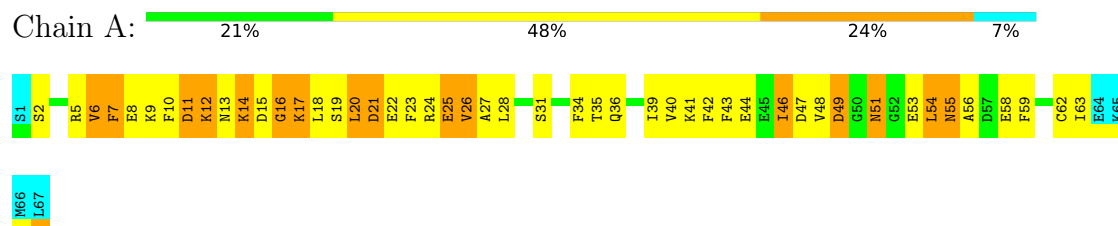
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	cloning artifact	UNP Q9SRP5

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: calmodulin-related protein, putative

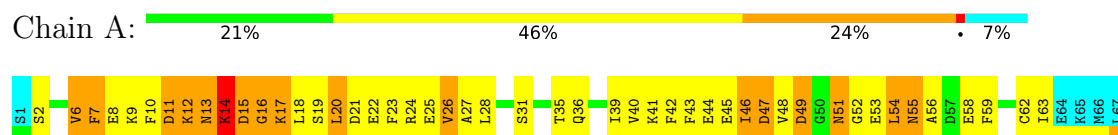


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

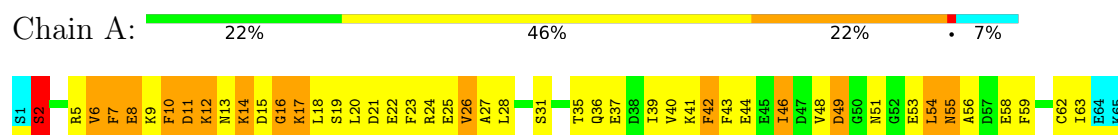
4.2.1 Score per residue for model 1

- Molecule 1: calmodulin-related protein, putative



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: calmodulin-related protein, putative



K66
L67

4.2.3 Score per residue for model 3

- Molecule 1: calmodulin-related protein, putative

Chain A: 15% 57% 19% 7%

S1 S2 A3 K4 R5 V6 F7 E8 F9 F10 D11 K12 K13 K14 D15 G16 K17 L18 L19 S19 L20 L21 D22 F23 R24 E25 V26 A27 L28 F30 A29 S31 F32 Y33 F34 T35 Q36 I39 V40 K41 F42 F43 E44 E45 I46 D47 V48 D49 G50 N51 G52 E53 L54 N55 A56 A57 E58 F59 C62

I63 E64 K65 K66 L67

4.2.4 Score per residue for model 4

- Molecule 1: calmodulin-related protein, putative

Chain A: 18% 49% 24% 7%

S1 S2 R5 V6 F7 E8 F9 F10 D11 K12 K13 K14 D15 G16 K17 L18 L19 S19 L20 D21 E22 F23 R24 E25 V26 A27 L28 A29 F30 S31 F34 T35 Q36 I39 V40 K41 F42 F43 E44 I46 D47 V48 D49 G50 N51 G52 E53 L54 N55 A56 D57 E58 F59 C62 I63 E64

K65 K66 L67

4.2.5 Score per residue for model 5

- Molecule 1: calmodulin-related protein, putative

Chain A: 18% 49% 25% 7%

S1 S2 A3 K4 R5 V6 F7 E8 F9 F10 D11 K12 K13 K14 D15 G16 K17 L18 L19 S19 L20 L21 D22 F23 R24 E25 V26 A27 L28 S31 F34 T35 Q36 I39 V40 K41 F42 F43 E44 I46 D47 V48 D49 G50 N51 G52 E53 L54 N55 A56 D57 E58 F59 C62 I63 E64

K65 K66 L67

4.2.6 Score per residue for model 6

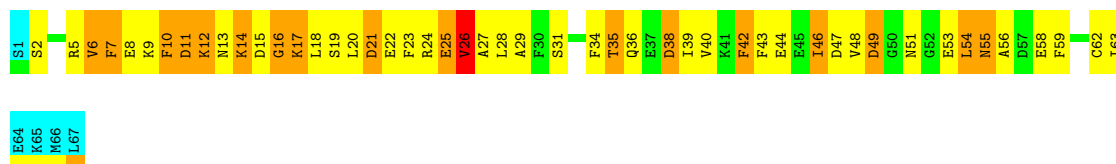
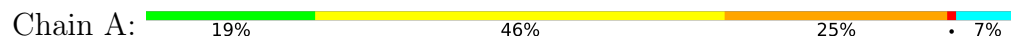
- Molecule 1: calmodulin-related protein, putative

Chain A: 18% 54% 21% 7%



4.2.7 Score per residue for model 7

- Molecule 1: calmodulin-related protein, putative



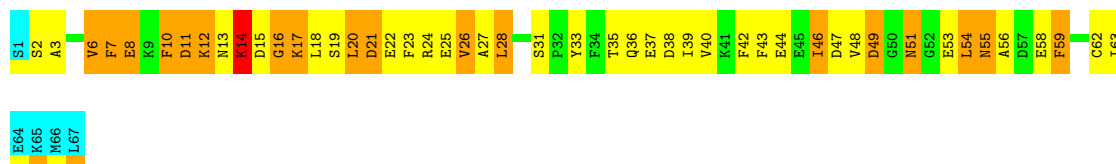
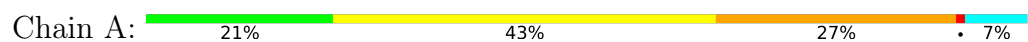
4.2.8 Score per residue for model 8

- Molecule 1: calmodulin-related protein, putative



4.2.9 Score per residue for model 9

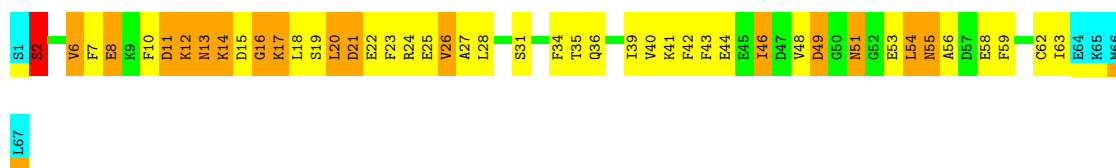
- Molecule 1: calmodulin-related protein, putative



4.2.10 Score per residue for model 10

- Molecule 1: calmodulin-related protein, putative

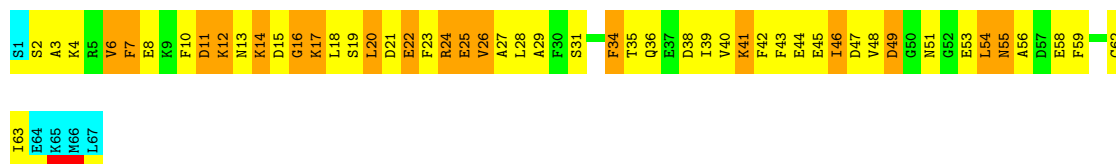




4.2.11 Score per residue for model 11

- Molecule 1: calmodulin-related protein, putative

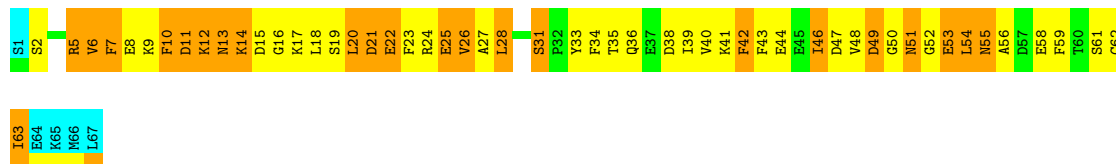
Chain A: 16% 49% 27% 7%



4.2.12 Score per residue for model 12

- Molecule 1: calmodulin-related protein, putative

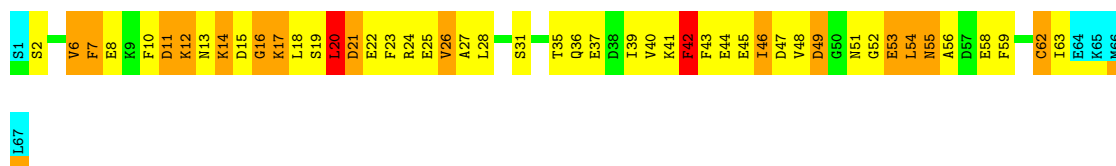
Chain A: 13% 45% 34% 7%



4.2.13 Score per residue for model 13

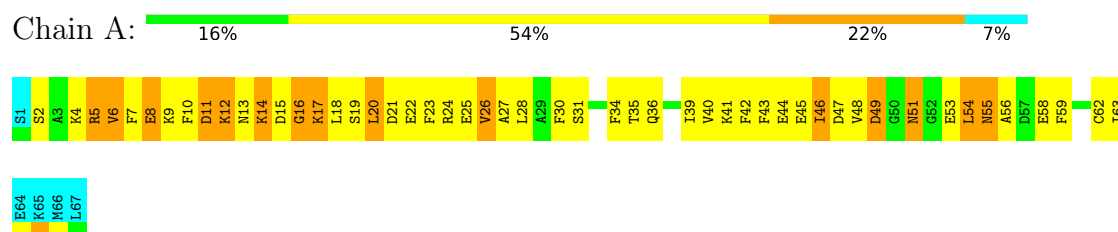
- Molecule 1: calmodulin-related protein, putative

Chain A: 21% 46% 22% 7%



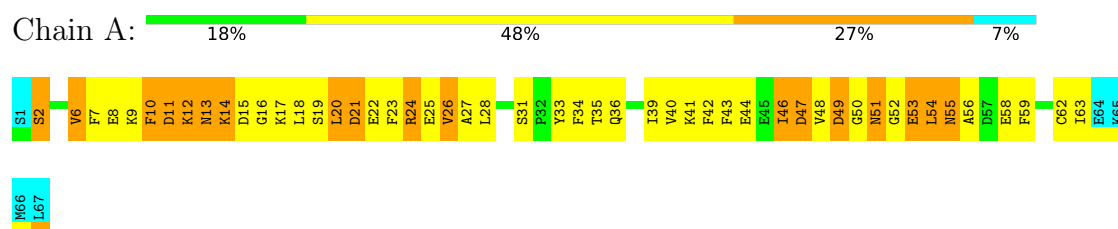
4.2.14 Score per residue for model 14

- Molecule 1: calmodulin-related protein, putative



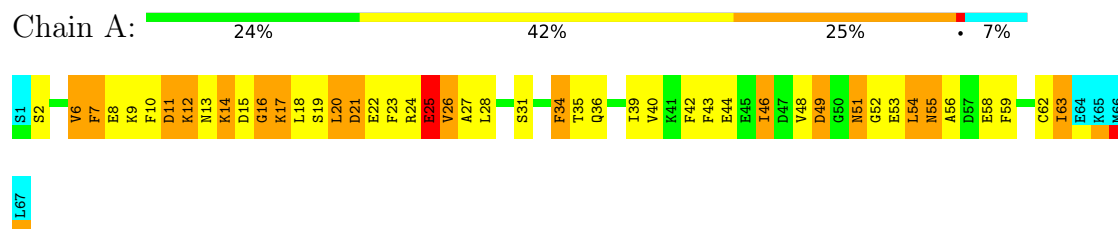
4.2.15 Score per residue for model 15

- Molecule 1: calmodulin-related protein, putative



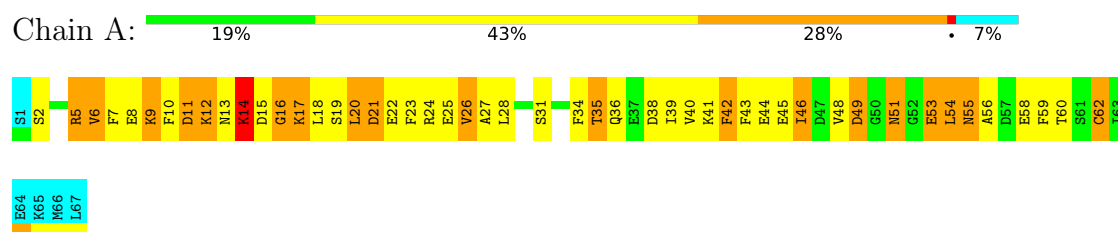
4.2.16 Score per residue for model 16

- Molecule 1: calmodulin-related protein, putative



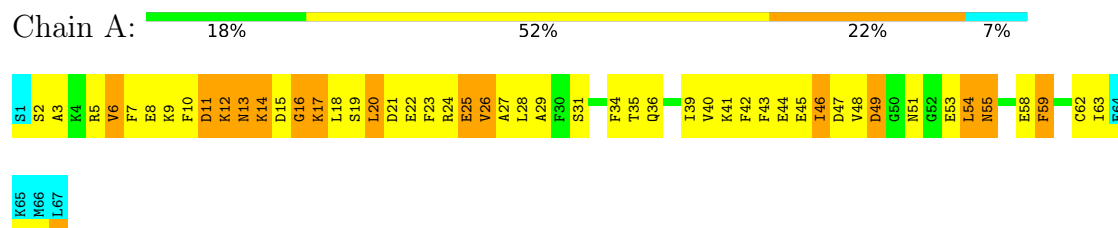
4.2.17 Score per residue for model 17

- Molecule 1: calmodulin-related protein, putative



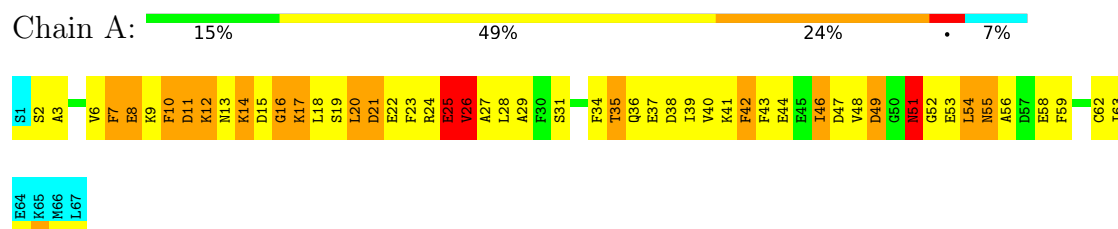
4.2.18 Score per residue for model 18

- Molecule 1: calmodulin-related protein, putative



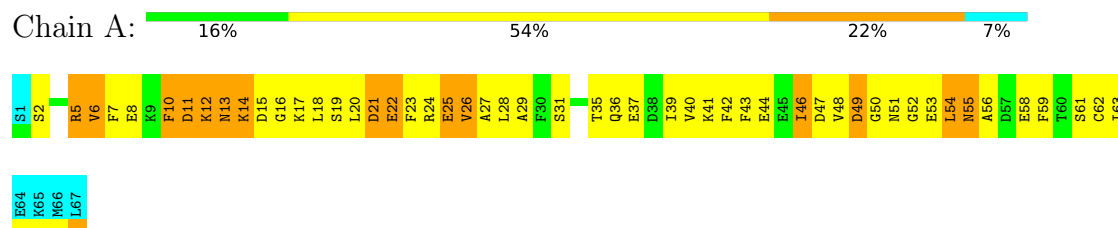
4.2.19 Score per residue for model 19

- Molecule 1: calmodulin-related protein, putative



4.2.20 Score per residue for model 20

- Molecule 1: calmodulin-related protein, putative



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
CYANA	structure solution	1.0.5
XPLOR-NIH	refinement	2.0.6

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.45±0.01	0±0/514 (0.0± 0.0%)	1.37±0.02	4±1/690 (0.6± 0.2%)
All	All	1.45	1/10280 (0.0%)	1.37	79/13800 (0.6%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	35	THR	C-N	-5.38	1.26	1.34	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	16	GLY	N-CA-C	-7.64	104.01	115.32	18	20
1	A	25	GLU	N-CA-C	-7.05	103.67	111.36	15	20
1	A	41	LYS	N-CA-C	-6.30	104.11	110.97	11	2
1	A	10	PHE	CA-CB-CG	-6.07	107.73	113.80	19	10
1	A	26	VAL	N-CA-CB	-5.66	103.93	110.55	7	2
1	A	42	PHE	CA-CB-CG	-5.46	108.34	113.80	19	6
1	A	51	ASN	N-CA-C	-5.43	106.62	113.20	4	16
1	A	20	LEU	N-CA-C	-5.09	105.72	112.34	16	2
1	A	7	PHE	CA-CB-CG	-5.07	108.73	113.80	12	1

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	504	475	475	94±22
All	All	10080	9500	9025	1874

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 98.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:PHE:CE2	1:A:18:LEU:HD13	1.19	1.73	20	3
1:A:7:PHE:CE2	1:A:59:PHE:CZ	1.12	2.36	20	9
1:A:36:GLN:NE2	1:A:40:VAL:HG11	0.99	1.73	16	1
1:A:10:PHE:O	1:A:12:LYS:N	0.98	1.95	12	19
1:A:36:GLN:O	1:A:40:VAL:HG22	0.95	1.61	19	19
1:A:7:PHE:CE2	1:A:59:PHE:CE2	0.91	2.57	11	19
1:A:18:LEU:O	1:A:54:LEU:N	0.91	2.03	18	19
1:A:7:PHE:CE1	1:A:18:LEU:CD1	0.85	2.59	11	16
1:A:18:LEU:HD13	1:A:59:PHE:HZ	0.84	1.31	18	2
1:A:20:LEU:HD13	1:A:20:LEU:O	0.83	1.72	20	4
1:A:56:ALA:HA	1:A:59:PHE:CD2	0.80	2.11	12	3
1:A:55:ASN:O	1:A:59:PHE:CD1	0.80	2.35	15	3
1:A:36:GLN:HE21	1:A:40:VAL:HG11	0.80	1.33	16	1
1:A:7:PHE:CE2	1:A:18:LEU:CD1	0.79	2.63	20	3
1:A:10:PHE:CE2	1:A:26:VAL:HG22	0.78	2.13	15	19
1:A:43:PHE:CD2	1:A:54:LEU:HD11	0.78	2.12	12	19
1:A:18:LEU:HD13	1:A:59:PHE:CZ	0.78	2.14	18	16
1:A:7:PHE:CD2	1:A:18:LEU:HD13	0.78	2.13	12	3
1:A:24:ARG:HE	1:A:36:GLN:NE2	0.77	1.76	20	2
1:A:7:PHE:CD2	1:A:59:PHE:CZ	0.76	2.74	12	4
1:A:42:PHE:CE2	1:A:62:CYS:SG	0.76	2.78	17	1
1:A:20:LEU:O	1:A:24:ARG:HB2	0.76	1.81	20	12
1:A:20:LEU:N	1:A:43:PHE:CE2	0.75	2.54	11	19
1:A:20:LEU:HD23	1:A:43:PHE:CB	0.75	2.11	20	19
1:A:24:ARG:HE	1:A:36:GLN:CD	0.74	1.90	4	2
1:A:20:LEU:HD23	1:A:43:PHE:CG	0.74	2.16	20	19
1:A:20:LEU:HD21	1:A:39:ILE:HG22	0.74	1.60	19	19
1:A:56:ALA:HA	1:A:59:PHE:CE2	0.73	2.18	12	3
1:A:24:ARG:NE	1:A:36:GLN:OE1	0.73	2.22	14	4
1:A:18:LEU:O	1:A:53:GLU:CA	0.73	2.36	4	19
1:A:55:ASN:O	1:A:59:PHE:CD2	0.72	2.42	17	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:GLN:NE2	1:A:40:VAL:HG13	0.72	1.99	10	1
1:A:7:PHE:CD2	1:A:59:PHE:CE2	0.72	2.77	15	19
1:A:7:PHE:CG	1:A:59:PHE:CZ	0.71	2.77	18	1
1:A:51:ASN:ND2	1:A:53:GLU:H	0.71	1.84	19	4
1:A:55:ASN:O	1:A:59:PHE:HB2	0.70	1.85	18	1
1:A:7:PHE:CE1	1:A:18:LEU:HD13	0.70	2.21	18	16
1:A:20:LEU:HD13	1:A:20:LEU:C	0.69	2.11	4	5
1:A:13:ASN:O	1:A:13:ASN:ND2	0.69	2.25	19	3
1:A:7:PHE:C	1:A:7:PHE:CD1	0.69	2.69	11	19
1:A:13:ASN:O	1:A:14:LYS:C	0.69	2.34	16	19
1:A:42:PHE:CE1	1:A:46:ILE:HD13	0.69	2.23	4	9
1:A:23:PHE:CE2	1:A:42:PHE:CE1	0.69	2.80	17	1
1:A:7:PHE:CE2	1:A:59:PHE:CE1	0.68	2.81	20	3
1:A:18:LEU:O	1:A:53:GLU:HA	0.68	1.89	4	19
1:A:8:GLU:O	1:A:11:ASP:OD2	0.67	2.12	13	1
1:A:47:ASP:OD2	1:A:53:GLU:N	0.67	2.27	3	5
1:A:36:GLN:HE21	1:A:40:VAL:HG13	0.67	1.50	1	4
1:A:42:PHE:CZ	1:A:62:CYS:SG	0.65	2.88	17	2
1:A:42:PHE:O	1:A:46:ILE:N	0.64	2.31	20	16
1:A:23:PHE:CZ	1:A:42:PHE:CE1	0.64	2.85	17	2
1:A:7:PHE:CD1	1:A:18:LEU:HD13	0.63	2.29	11	15
1:A:20:LEU:HD11	1:A:36:GLN:HE22	0.63	1.53	2	4
1:A:20:LEU:HD23	1:A:43:PHE:CD2	0.63	2.29	1	19
1:A:20:LEU:CA	1:A:43:PHE:CE2	0.62	2.82	20	19
1:A:24:ARG:HH11	1:A:24:ARG:HG2	0.62	1.53	10	1
1:A:24:ARG:NH1	1:A:36:GLN:OE1	0.62	2.32	10	1
1:A:24:ARG:HH11	1:A:24:ARG:CB	0.62	2.06	15	2
1:A:48:VAL:CG1	1:A:55:ASN:HD21	0.62	2.08	12	3
1:A:13:ASN:N	1:A:13:ASN:OD1	0.62	2.32	1	2
1:A:11:ASP:O	1:A:11:ASP:OD1	0.62	2.18	1	12
1:A:18:LEU:HG	1:A:22:GLU:CB	0.61	2.25	12	16
1:A:58:GLU:O	1:A:62:CYS:N	0.61	2.33	2	16
1:A:23:PHE:CE1	1:A:42:PHE:CZ	0.61	2.88	17	1
1:A:23:PHE:CZ	1:A:42:PHE:CZ	0.61	2.88	17	1
1:A:6:VAL:O	1:A:10:PHE:CD2	0.61	2.54	18	8
1:A:42:PHE:CD1	1:A:43:PHE:N	0.61	2.69	17	1
1:A:7:PHE:CD1	1:A:7:PHE:O	0.61	2.54	11	16
1:A:43:PHE:CE1	1:A:47:ASP:CG	0.60	2.79	18	2
1:A:7:PHE:CD1	1:A:18:LEU:CD1	0.60	2.85	17	15
1:A:8:GLU:O	1:A:11:ASP:OD1	0.60	2.19	1	11
1:A:19:SER:C	1:A:21:ASP:N	0.60	2.57	9	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:GLN:O	1:A:40:VAL:CG2	0.60	2.47	6	19
1:A:49:ASP:OD1	1:A:51:ASN:N	0.60	2.34	1	7
1:A:11:ASP:O	1:A:11:ASP:CG	0.60	2.44	13	12
1:A:20:LEU:O	1:A:20:LEU:HD13	0.60	1.97	2	2
1:A:23:PHE:CE1	1:A:62:CYS:SG	0.60	2.95	12	3
1:A:43:PHE:CZ	1:A:47:ASP:OD2	0.60	2.55	18	4
1:A:6:VAL:HG22	1:A:10:PHE:CE2	0.60	2.31	18	14
1:A:7:PHE:HZ	1:A:17:LYS:N	0.60	1.95	18	1
1:A:10:PHE:CD2	1:A:26:VAL:CG2	0.59	2.85	20	18
1:A:38:ASP:O	1:A:42:PHE:HB2	0.59	1.97	11	1
1:A:5:ARG:HH11	1:A:5:ARG:CG	0.59	2.10	17	5
1:A:20:LEU:O	1:A:24:ARG:CB	0.58	2.51	12	11
1:A:43:PHE:CD1	1:A:47:ASP:OD1	0.58	2.56	18	2
1:A:23:PHE:CE2	1:A:62:CYS:SG	0.58	2.96	7	4
1:A:10:PHE:CD2	1:A:26:VAL:HG22	0.58	2.32	20	19
1:A:35:THR:N	1:A:38:ASP:OD2	0.58	2.35	7	1
1:A:55:ASN:N	1:A:55:ASN:OD1	0.58	2.34	12	12
1:A:24:ARG:HG2	1:A:24:ARG:NH1	0.58	2.10	10	3
1:A:5:ARG:CG	1:A:5:ARG:NH1	0.58	2.65	20	6
1:A:7:PHE:O	1:A:11:ASP:N	0.58	2.36	4	14
1:A:27:ALA:O	1:A:31:SER:C	0.58	2.45	16	16
1:A:54:LEU:O	1:A:59:PHE:CE2	0.58	2.56	11	11
1:A:38:ASP:N	1:A:38:ASP:OD1	0.57	2.37	7	3
1:A:14:LYS:NZ	1:A:14:LYS:CB	0.57	2.67	4	1
1:A:46:ILE:O	1:A:48:VAL:N	0.57	2.37	4	19
1:A:24:ARG:CZ	1:A:36:GLN:OE1	0.57	2.53	10	2
1:A:5:ARG:HG2	1:A:5:ARG:HH11	0.57	1.58	4	2
1:A:55:ASN:OD1	1:A:55:ASN:N	0.57	2.38	6	7
1:A:23:PHE:CE1	1:A:39:ILE:HG23	0.57	2.35	11	3
1:A:56:ALA:O	1:A:59:PHE:HB2	0.57	2.00	9	15
1:A:24:ARG:HH11	1:A:24:ARG:HB3	0.57	1.59	11	1
1:A:55:ASN:O	1:A:59:PHE:CE1	0.56	2.58	15	3
1:A:7:PHE:CG	1:A:59:PHE:CE1	0.56	2.93	18	1
1:A:5:ARG:CG	1:A:5:ARG:HH11	0.56	2.13	4	1
1:A:43:PHE:CE2	1:A:54:LEU:CD1	0.56	2.88	20	6
1:A:43:PHE:CD1	1:A:43:PHE:C	0.56	2.83	5	19
1:A:27:ALA:O	1:A:31:SER:O	0.56	2.23	14	18
1:A:18:LEU:HG	1:A:22:GLU:HB2	0.56	1.78	15	7
1:A:42:PHE:CD1	1:A:42:PHE:C	0.56	2.84	17	1
1:A:36:GLN:NE2	1:A:40:VAL:CG1	0.56	2.62	16	12
1:A:23:PHE:HA	1:A:26:VAL:HB	0.55	1.78	10	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ARG:HG2	1:A:28:LEU:HD22	0.55	1.76	13	7
1:A:23:PHE:CE2	1:A:39:ILE:HG23	0.55	2.36	16	6
1:A:23:PHE:CD1	1:A:62:CYS:SG	0.55	2.99	12	2
1:A:36:GLN:NE2	1:A:36:GLN:HA	0.55	2.14	10	3
1:A:24:ARG:NE	1:A:36:GLN:CD	0.55	2.64	4	2
1:A:7:PHE:CZ	1:A:59:PHE:CE2	0.55	2.94	18	4
1:A:24:ARG:HD2	1:A:36:GLN:OE1	0.55	2.02	15	1
1:A:13:ASN:O	1:A:15:ASP:N	0.55	2.39	16	18
1:A:21:ASP:N	1:A:21:ASP:OD1	0.55	2.40	20	4
1:A:22:GLU:CD	1:A:22:GLU:N	0.54	2.65	11	4
1:A:44:GLU:O	1:A:47:ASP:OD1	0.54	2.25	13	2
1:A:20:LEU:N	1:A:43:PHE:CZ	0.54	2.75	18	19
1:A:7:PHE:CD1	1:A:59:PHE:CZ	0.54	2.95	18	1
1:A:10:PHE:CG	1:A:26:VAL:CG2	0.54	2.91	18	14
1:A:40:VAL:O	1:A:44:GLU:CG	0.54	2.55	3	18
1:A:5:ARG:HH11	1:A:5:ARG:HG2	0.54	1.61	17	2
1:A:51:ASN:HD22	1:A:52:GLY:N	0.54	2.01	5	4
1:A:7:PHE:CZ	1:A:17:LYS:N	0.54	2.76	18	1
1:A:11:ASP:OD1	1:A:13:ASN:ND2	0.54	2.41	5	2
1:A:51:ASN:N	1:A:51:ASN:ND2	0.53	2.55	1	1
1:A:8:GLU:CD	1:A:8:GLU:C	0.53	2.76	2	4
1:A:20:LEU:HA	1:A:43:PHE:CD2	0.53	2.38	20	19
1:A:42:PHE:CE2	1:A:46:ILE:HD13	0.53	2.39	19	1
1:A:51:ASN:ND2	1:A:53:GLU:OE1	0.53	2.42	12	3
1:A:7:PHE:O	1:A:7:PHE:HD1	0.53	1.86	6	16
1:A:10:PHE:O	1:A:11:ASP:C	0.53	2.50	12	4
1:A:22:GLU:N	1:A:22:GLU:OE1	0.53	2.41	11	1
1:A:31:SER:OG	1:A:31:SER:O	0.53	2.25	12	1
1:A:46:ILE:HD11	1:A:61:SER:CB	0.53	2.33	20	2
1:A:43:PHE:CG	1:A:47:ASP:OD1	0.52	2.62	18	2
1:A:36:GLN:HE21	1:A:40:VAL:CG1	0.52	2.17	12	15
1:A:49:ASP:OD1	1:A:49:ASP:O	0.52	2.27	16	11
1:A:13:ASN:HD22	1:A:13:ASN:C	0.52	2.13	20	4
1:A:46:ILE:HD11	1:A:61:SER:OG	0.52	2.04	20	2
1:A:46:ILE:O	1:A:58:GLU:OE2	0.52	2.27	20	7
1:A:25:GLU:OE1	1:A:25:GLU:N	0.52	2.42	16	2
1:A:20:LEU:O	1:A:24:ARG:N	0.52	2.43	4	12
1:A:24:ARG:HH11	1:A:24:ARG:CG	0.52	2.18	11	2
1:A:7:PHE:CD2	1:A:59:PHE:CE1	0.52	2.97	12	3
1:A:47:ASP:OD1	1:A:53:GLU:N	0.52	2.42	14	1
1:A:24:ARG:HE	1:A:36:GLN:HE22	0.52	1.47	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ASN:N	1:A:51:ASN:HD22	0.51	2.03	1	2
1:A:24:ARG:NH1	1:A:24:ARG:CG	0.51	2.72	15	2
1:A:43:PHE:CD2	1:A:54:LEU:CD1	0.51	2.92	12	13
1:A:51:ASN:ND2	1:A:53:GLU:N	0.51	2.57	16	2
1:A:18:LEU:O	1:A:53:GLU:CB	0.51	2.59	10	19
1:A:52:GLY:O	1:A:53:GLU:CD	0.51	2.54	13	1
1:A:7:PHE:CZ	1:A:59:PHE:CZ	0.51	2.96	20	2
1:A:20:LEU:C	1:A:20:LEU:CD1	0.51	2.83	4	3
1:A:18:LEU:HB2	1:A:59:PHE:CE1	0.51	2.40	19	15
1:A:49:ASP:OD2	1:A:51:ASN:CG	0.51	2.54	16	2
1:A:18:LEU:O	1:A:53:GLU:HB3	0.51	2.06	10	18
1:A:23:PHE:O	1:A:27:ALA:N	0.51	2.44	15	7
1:A:49:ASP:OD1	1:A:51:ASN:CB	0.51	2.59	14	8
1:A:23:PHE:CD1	1:A:23:PHE:C	0.51	2.88	11	3
1:A:43:PHE:CZ	1:A:47:ASP:CG	0.50	2.89	18	2
1:A:20:LEU:HD11	1:A:36:GLN:NE2	0.50	2.21	2	2
1:A:8:GLU:O	1:A:11:ASP:CG	0.50	2.53	20	10
1:A:46:ILE:O	1:A:58:GLU:OE1	0.50	2.28	12	1
1:A:23:PHE:CD1	1:A:23:PHE:O	0.50	2.64	11	5
1:A:19:SER:O	1:A:20:LEU:C	0.50	2.53	2	19
1:A:51:ASN:ND2	1:A:51:ASN:N	0.50	2.58	5	2
1:A:17:LYS:HA	1:A:54:LEU:O	0.50	2.06	18	14
1:A:54:LEU:O	1:A:59:PHE:HE1	0.50	1.89	20	3
1:A:19:SER:O	1:A:22:GLU:N	0.50	2.44	13	18
1:A:24:ARG:CG	1:A:24:ARG:NH1	0.50	2.73	11	1
1:A:5:ARG:O	1:A:8:GLU:HG2	0.49	2.07	18	1
1:A:39:ILE:O	1:A:43:PHE:CB	0.49	2.61	12	5
1:A:42:PHE:CD2	1:A:62:CYS:SG	0.49	3.05	17	1
1:A:36:GLN:HA	1:A:39:ILE:HD12	0.49	1.84	10	13
1:A:49:ASP:OD1	1:A:49:ASP:C	0.49	2.55	5	5
1:A:22:GLU:N	1:A:22:GLU:CD	0.49	2.70	13	3
1:A:47:ASP:O	1:A:47:ASP:CG	0.49	2.55	13	2
1:A:11:ASP:OD1	1:A:14:LYS:N	0.49	2.45	5	2
1:A:51:ASN:HD22	1:A:51:ASN:N	0.49	2.05	19	2
1:A:13:ASN:ND2	1:A:17:LYS:O	0.49	2.40	1	2
1:A:47:ASP:OD1	1:A:54:LEU:CD1	0.48	2.61	1	2
1:A:20:LEU:HD23	1:A:43:PHE:HB2	0.48	1.85	11	14
1:A:38:ASP:O	1:A:42:PHE:CB	0.48	2.61	11	1
1:A:42:PHE:HD1	1:A:43:PHE:N	0.48	2.06	17	1
1:A:47:ASP:OD2	1:A:53:GLU:C	0.48	2.57	1	4
1:A:10:PHE:O	1:A:22:GLU:OE1	0.48	2.31	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:VAL:HG12	1:A:55:ASN:HD21	0.48	1.68	12	4
1:A:6:VAL:CG1	1:A:7:PHE:N	0.48	2.76	17	8
1:A:14:LYS:CB	1:A:14:LYS:HZ2	0.48	2.21	4	1
1:A:36:GLN:O	1:A:40:VAL:HG13	0.48	2.07	3	3
1:A:14:LYS:HZ2	1:A:14:LYS:HB2	0.48	1.69	4	1
1:A:31:SER:O	1:A:31:SER:OG	0.48	2.31	10	4
1:A:13:ASN:ND2	1:A:22:GLU:OE2	0.48	2.46	3	3
1:A:7:PHE:O	1:A:8:GLU:C	0.48	2.56	11	16
1:A:13:ASN:O	1:A:15:ASP:OD1	0.48	2.32	1	8
1:A:48:VAL:HG12	1:A:58:GLU:HG3	0.48	1.86	11	15
1:A:7:PHE:CD2	1:A:59:PHE:CD2	0.48	3.02	11	6
1:A:13:ASN:ND2	1:A:13:ASN:H	0.48	2.07	5	2
1:A:41:LYS:O	1:A:45:GLU:CB	0.48	2.62	11	1
1:A:24:ARG:HH21	1:A:36:GLN:CD	0.48	2.16	20	1
1:A:17:LYS:HA	1:A:59:PHE:CE2	0.47	2.44	4	15
1:A:55:ASN:O	1:A:59:PHE:CG	0.47	2.67	17	5
1:A:21:ASP:O	1:A:25:GLU:CD	0.47	2.57	16	2
1:A:40:VAL:O	1:A:44:GLU:N	0.47	2.45	17	1
1:A:25:GLU:O	1:A:29:ALA:CB	0.47	2.63	4	7
1:A:22:GLU:OE1	1:A:22:GLU:CA	0.47	2.63	1	2
1:A:43:PHE:CE1	1:A:47:ASP:OD1	0.47	2.68	1	2
1:A:49:ASP:OD1	1:A:51:ASN:CG	0.47	2.57	5	2
1:A:51:ASN:ND2	1:A:51:ASN:C	0.47	2.71	16	2
1:A:55:ASN:O	1:A:59:PHE:CB	0.47	2.61	18	1
1:A:24:ARG:CD	1:A:36:GLN:OE1	0.47	2.62	14	3
1:A:56:ALA:HA	1:A:59:PHE:HD2	0.47	1.70	19	11
1:A:31:SER:OG	1:A:34:PHE:CD2	0.47	2.68	12	1
1:A:16:GLY:O	1:A:17:LYS:HG3	0.47	2.10	16	16
1:A:55:ASN:C	1:A:59:PHE:CE1	0.47	2.93	15	3
1:A:22:GLU:O	1:A:26:VAL:HG23	0.47	2.10	19	1
1:A:19:SER:O	1:A:21:ASP:N	0.46	2.48	6	15
1:A:18:LEU:HB2	1:A:59:PHE:CZ	0.46	2.46	9	12
1:A:51:ASN:ND2	1:A:51:ASN:H	0.46	2.09	1	2
1:A:47:ASP:OD2	1:A:52:GLY:CA	0.46	2.63	6	1
1:A:23:PHE:CD1	1:A:39:ILE:HG23	0.46	2.45	11	1
1:A:45:GLU:CD	1:A:45:GLU:O	0.46	2.58	17	3
1:A:8:GLU:HG3	1:A:9:LYS:N	0.46	2.25	14	1
1:A:23:PHE:CA	1:A:26:VAL:HB	0.46	2.40	13	19
1:A:18:LEU:HB3	1:A:54:LEU:HD23	0.46	1.86	9	7
1:A:55:ASN:ND2	1:A:58:GLU:CG	0.46	2.79	2	15
1:A:55:ASN:C	1:A:59:PHE:CD2	0.46	2.93	2	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:VAL:HG23	1:A:41:LYS:N	0.46	2.25	20	8
1:A:8:GLU:O	1:A:8:GLU:OE1	0.46	2.34	9	1
1:A:46:ILE:CG2	1:A:54:LEU:HD12	0.45	2.41	19	14
1:A:28:LEU:N	1:A:28:LEU:CD1	0.45	2.79	4	8
1:A:13:ASN:C	1:A:15:ASP:N	0.45	2.74	16	12
1:A:18:LEU:O	1:A:53:GLU:C	0.45	2.58	18	9
1:A:63:ILE:CD1	1:A:63:ILE:N	0.45	2.79	6	3
1:A:8:GLU:C	1:A:8:GLU:CD	0.45	2.85	9	1
1:A:44:GLU:C	1:A:47:ASP:OD1	0.45	2.60	13	2
1:A:41:LYS:CB	1:A:41:LYS:NZ	0.45	2.80	15	1
1:A:41:LYS:O	1:A:45:GLU:HB2	0.45	2.11	3	5
1:A:35:THR:OG1	1:A:38:ASP:OD2	0.45	2.34	7	2
1:A:5:ARG:NH1	1:A:5:ARG:HG2	0.45	2.26	14	1
1:A:9:LYS:CD	1:A:9:LYS:C	0.45	2.89	17	1
1:A:20:LEU:HA	1:A:43:PHE:CE2	0.45	2.46	20	7
1:A:11:ASP:OD1	1:A:13:ASN:OD1	0.45	2.35	11	1
1:A:37:GLU:CD	1:A:37:GLU:N	0.44	2.76	9	1
1:A:47:ASP:CG	1:A:53:GLU:O	0.44	2.60	20	2
1:A:34:PHE:HB3	1:A:39:ILE:HD11	0.44	1.90	16	3
1:A:52:GLY:O	1:A:53:GLU:OE2	0.44	2.36	13	1
1:A:13:ASN:OD1	1:A:15:ASP:OD2	0.44	2.35	19	1
1:A:63:ILE:N	1:A:63:ILE:HD12	0.44	2.28	6	2
1:A:63:ILE:N	1:A:63:ILE:CD1	0.44	2.80	11	3
1:A:25:GLU:OE1	1:A:25:GLU:CA	0.44	2.65	16	2
1:A:47:ASP:OD1	1:A:47:ASP:O	0.44	2.35	9	2
1:A:51:ASN:O	1:A:51:ASN:ND2	0.44	2.51	17	1
1:A:47:ASP:OD1	1:A:51:ASN:ND2	0.44	2.50	5	1
1:A:19:SER:C	1:A:21:ASP:H	0.44	2.20	17	7
1:A:8:GLU:C	1:A:8:GLU:OE1	0.44	2.61	9	2
1:A:52:GLY:C	1:A:53:GLU:CD	0.43	2.86	13	1
1:A:26:VAL:HG12	1:A:27:ALA:N	0.43	2.27	19	2
1:A:7:PHE:CG	1:A:59:PHE:CE2	0.43	3.06	20	1
1:A:47:ASP:OD1	1:A:53:GLU:O	0.43	2.35	14	7
1:A:36:GLN:NE2	1:A:36:GLN:CA	0.43	2.80	10	1
1:A:38:ASP:O	1:A:42:PHE:CG	0.43	2.71	11	1
1:A:7:PHE:CZ	1:A:16:GLY:C	0.43	2.96	18	1
1:A:47:ASP:OD1	1:A:47:ASP:C	0.43	2.61	6	1
1:A:50:GLY:C	1:A:52:GLY:H	0.43	2.20	15	3
1:A:19:SER:OG	1:A:53:GLU:OE1	0.43	2.33	13	1
1:A:37:GLU:O	1:A:41:LYS:CB	0.43	2.66	20	2
1:A:40:VAL:O	1:A:41:LYS:C	0.43	2.61	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:ARG:HG2	1:A:5:ARG:NH1	0.43	2.29	7	1
1:A:9:LYS:C	1:A:9:LYS:HD2	0.43	2.39	17	1
1:A:46:ILE:HD11	1:A:61:SER:HB3	0.43	1.90	20	1
1:A:6:VAL:HG22	1:A:10:PHE:CZ	0.42	2.49	10	7
1:A:11:ASP:OD1	1:A:11:ASP:C	0.42	2.62	1	3
1:A:7:PHE:C	1:A:7:PHE:HD1	0.42	2.20	18	1
1:A:20:LEU:HB2	1:A:43:PHE:CE1	0.42	2.49	1	3
1:A:51:ASN:ND2	1:A:53:GLU:OE2	0.42	2.52	3	1
1:A:13:ASN:O	1:A:15:ASP:CG	0.42	2.63	12	1
1:A:18:LEU:HG	1:A:22:GLU:HB3	0.42	1.90	10	1
1:A:43:PHE:CE2	1:A:54:LEU:CD2	0.42	3.02	18	6
1:A:35:THR:OG1	1:A:38:ASP:OD1	0.42	2.36	7	1
1:A:34:PHE:HB3	1:A:39:ILE:CG1	0.42	2.44	19	2
1:A:54:LEU:HG	1:A:62:CYS:SG	0.42	2.55	5	1
1:A:42:PHE:HZ	1:A:62:CYS:SG	0.42	2.34	5	1
1:A:23:PHE:CD2	1:A:62:CYS:SG	0.42	3.13	7	1
1:A:10:PHE:CZ	1:A:26:VAL:HG22	0.42	2.50	15	2
1:A:23:PHE:C	1:A:26:VAL:HB	0.42	2.40	15	1
1:A:23:PHE:CE2	1:A:42:PHE:CD1	0.42	3.08	17	1
1:A:31:SER:OG	1:A:34:PHE:CD1	0.42	2.68	3	1
1:A:42:PHE:CZ	1:A:62:CYS:O	0.42	2.72	5	1
1:A:35:THR:HG23	1:A:38:ASP:H	0.42	1.74	19	1
1:A:10:PHE:CG	1:A:26:VAL:HG22	0.41	2.50	18	3
1:A:42:PHE:CE2	1:A:62:CYS:O	0.41	2.73	5	1
1:A:7:PHE:CE2	1:A:59:PHE:CD2	0.41	3.06	18	2
1:A:51:ASN:ND2	1:A:53:GLU:CD	0.41	2.78	18	1
1:A:42:PHE:CZ	1:A:46:ILE:HD13	0.41	2.50	1	2
1:A:2:SER:O	1:A:6:VAL:HB	0.41	2.15	16	1
1:A:51:ASN:HD22	1:A:51:ASN:C	0.41	2.22	16	1
1:A:55:ASN:ND2	1:A:58:GLU:HG2	0.41	2.31	12	2
1:A:24:ARG:O	1:A:28:LEU:HB2	0.41	2.15	7	1
1:A:24:ARG:HG2	1:A:24:ARG:HH11	0.41	1.75	14	1
1:A:43:PHE:O	1:A:47:ASP:OD1	0.41	2.38	9	1
1:A:5:ARG:CD	1:A:5:ARG:C	0.41	2.93	3	1
1:A:36:GLN:OE1	1:A:36:GLN:HA	0.41	2.15	14	1
1:A:46:ILE:HG21	1:A:62:CYS:SG	0.41	2.56	17	1
1:A:55:ASN:O	1:A:59:PHE:N	0.41	2.53	18	2
1:A:6:VAL:HG13	1:A:10:PHE:CE2	0.41	2.51	17	1
1:A:23:PHE:CD1	1:A:26:VAL:HG11	0.40	2.51	6	1
1:A:24:ARG:CG	1:A:28:LEU:HD22	0.40	2.47	11	1
1:A:43:PHE:CE2	1:A:54:LEU:HD13	0.40	2.51	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:GLY:C	1:A:53:GLU:CG	0.40	2.94	16	1
1:A:20:LEU:CD2	1:A:39:ILE:HG22	0.40	2.41	19	1
1:A:40:VAL:O	1:A:44:GLU:CD	0.40	2.64	3	1
1:A:59:PHE:O	1:A:62:CYS:CB	0.40	2.69	5	1
1:A:50:GLY:C	1:A:52:GLY:N	0.40	2.79	15	1
1:A:15:ASP:O	1:A:15:ASP:OD1	0.40	2.40	6	1
1:A:40:VAL:O	1:A:44:GLU:CB	0.40	2.69	14	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	62/67 (93%)	57±1 (92±1%)	3±1 (4±1%)	2±1 (4±1%)	4	32
All	All	1240/1340 (93%)	1140 (92%)	55 (4%)	45 (4%)	4	32

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

Mol	Chain	Res	Type	Models (Total)
1	A	11	ASP	20
1	A	14	LYS	19
1	A	47	ASP	3
1	A	2	SER	3

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	55/60 (92%)	38±2 (69±4%)	17±2 (31±4%)	1	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1100/1200 (92%)	755 (69%)	345 (31%)	1 14

All 38 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	6	VAL	20
1	A	12	LYS	20
1	A	17	LYS	20
1	A	26	VAL	20
1	A	49	ASP	20
1	A	54	LEU	20
1	A	55	ASN	20
1	A	2	SER	19
1	A	35	THR	19
1	A	46	ILE	19
1	A	7	PHE	13
1	A	9	LYS	13
1	A	20	LEU	13
1	A	28	LEU	12
1	A	21	ASP	11
1	A	13	ASN	8
1	A	34	PHE	8
1	A	14	LYS	7
1	A	5	ARG	7
1	A	51	ASN	5
1	A	8	GLU	5
1	A	30	PHE	5
1	A	33	TYR	4
1	A	4	LYS	4
1	A	22	GLU	4
1	A	53	GLU	4
1	A	42	PHE	3
1	A	62	CYS	3
1	A	24	ARG	3
1	A	25	GLU	3
1	A	37	GLU	2
1	A	38	ASP	2
1	A	31	SER	2
1	A	59	PHE	2
1	A	63	ILE	2
1	A	15	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	41	LYS	1
1	A	60	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided