



Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 02:59 AM UTC

PDB ID : 1PFM / pdb_00001pfm
Title : PF4-M2 CHIMERIC MUTANT WITH THE FIRST 10 N-TERMINAL RESIDUES OF R-PF4 REPLACED BY THE N-TERMINAL RESIDUES OF THE IL8 SEQUENCE. MODELS 1-15 OF A 27-MODEL SET.
Authors : Mayo, K.H.; Roongta, V.; Ilyina, E.; Milius, R.; Barker, S.; Quinlan, C.; La Rosa, G.; Daly, T.J.
Deposited on : 1995-07-18

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

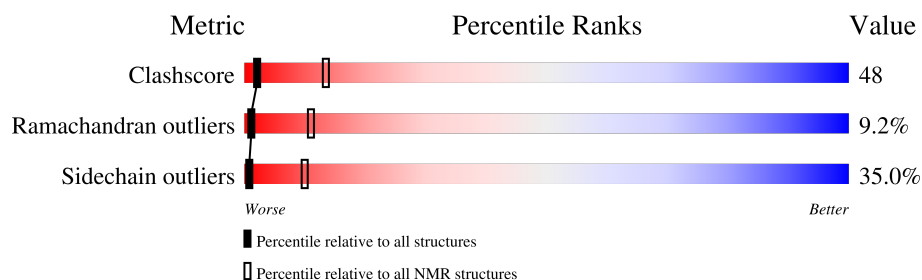
1 Overall quality at a glance

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	68	16% 53% 16% • 10%
1	B	68	16% 51% 19% • 10%
1	C	68	15% 54% 18% • 10%
1	D	68	12% 57% 19% • 9%

2 Ensemble composition and analysis

This entry contains 15 models. Model 6 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:9-A:69, B:9-B:69, C:9-C:69, D:9-D:70 (245)	0.72	6

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4460 atoms, of which 2340 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PF4-M2 CHIMERA.

Mol	Chain	Residues	Atoms						Trace
1	A	68	Total	C	H	N	O	S	0
			1115	335	585	98	92	5	
1	B	68	Total	C	H	N	O	S	0
			1115	335	585	98	92	5	
1	C	68	Total	C	H	N	O	S	0
			1115	335	585	98	92	5	
1	D	68	Total	C	H	N	O	S	0
			1115	335	585	98	92	5	

There are 8 discrepancies between the modelled and reference sequences:

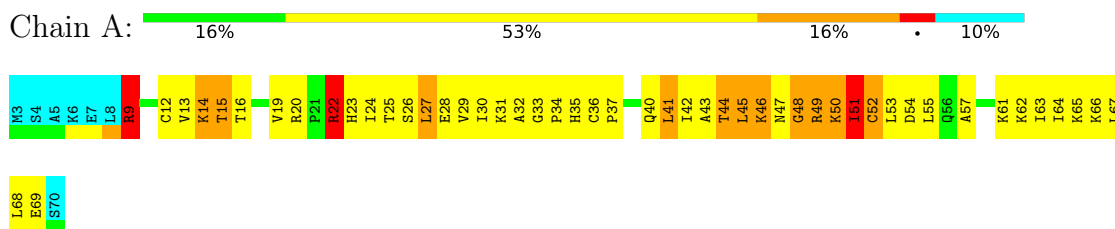
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ARG	GLN	engineered mutation	UNP P02776
A	11	GLN	LEU	engineered mutation	UNP P02776
B	9	ARG	GLN	engineered mutation	UNP P02776
B	11	GLN	LEU	engineered mutation	UNP P02776
C	9	ARG	GLN	engineered mutation	UNP P02776
C	11	GLN	LEU	engineered mutation	UNP P02776
D	9	ARG	GLN	engineered mutation	UNP P02776
D	11	GLN	LEU	engineered mutation	UNP P02776

4 Residue-property plots [i](#)

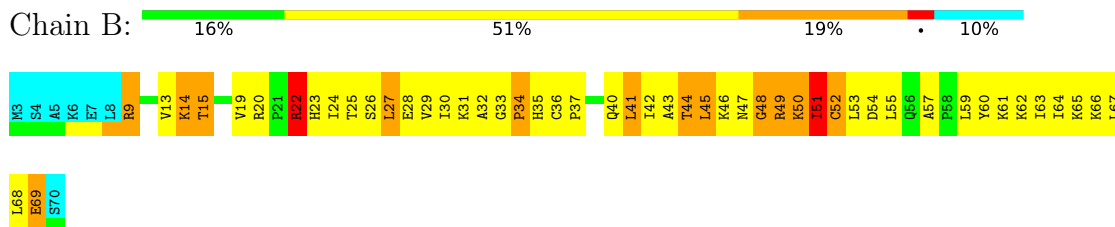
4.1 Average score per residue in the NMR ensemble

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.

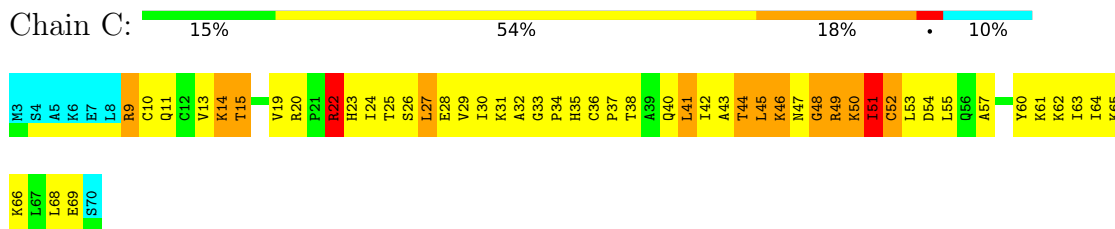
• Molecule 1: PF4-M2 CHIMERA



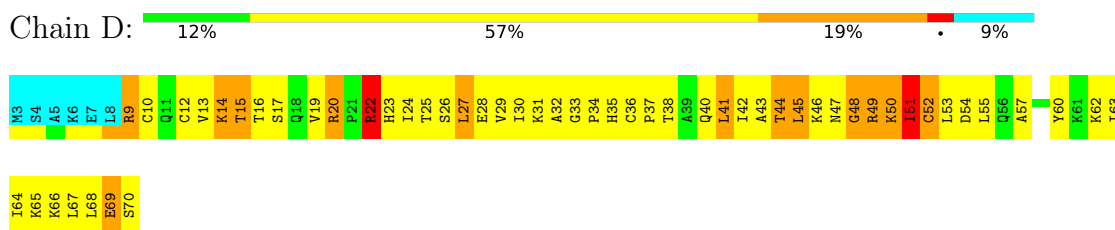
• Molecule 1: PF4-M2 CHIMERA



• Molecule 1: PF4-M2 CHIMERA



• Molecule 1: PF4-M2 CHIMERA

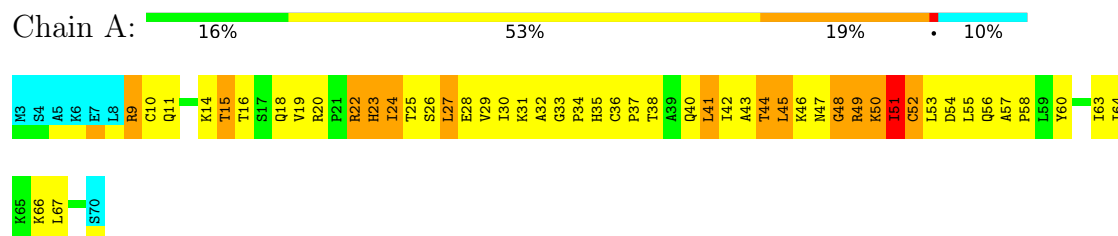


4.2 Scores per residue for each member of the ensemble

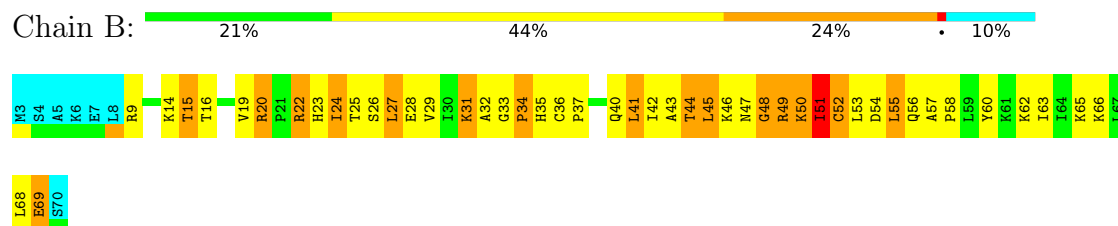
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

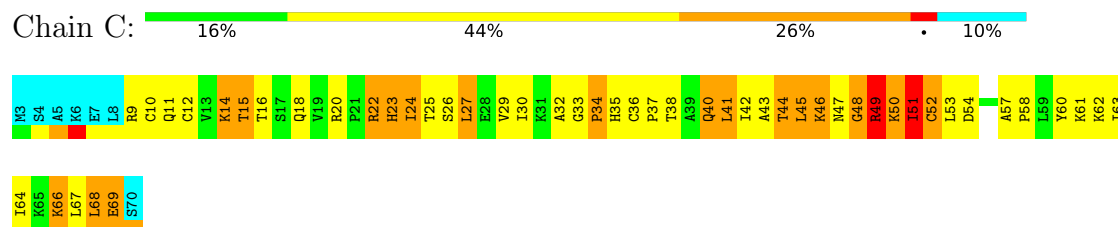
- Molecule 1: PF4-M2 CHIMERA



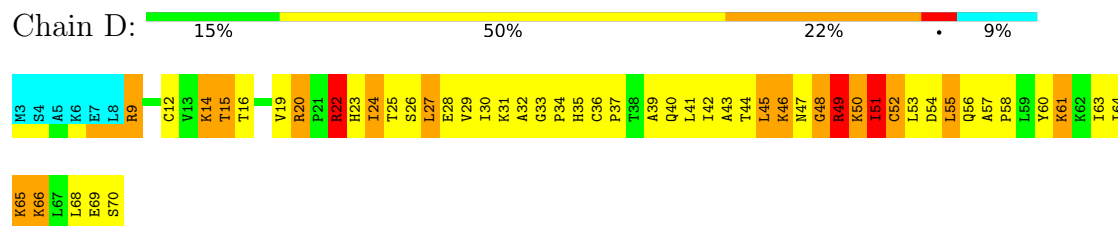
- Molecule 1: PF4-M2 CHIMERA



- Molecule 1: PF4-M2 CHIMERA

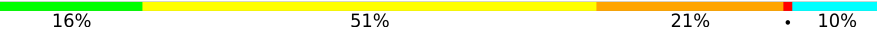


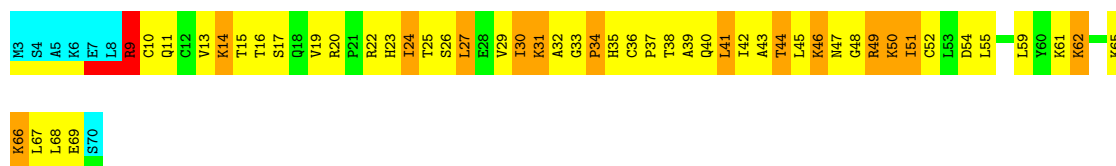
- Molecule 1: PF4-M2 CHIMERA



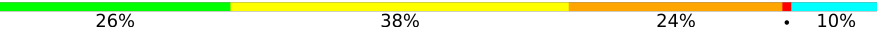
4.2.2 Score per residue for model 2

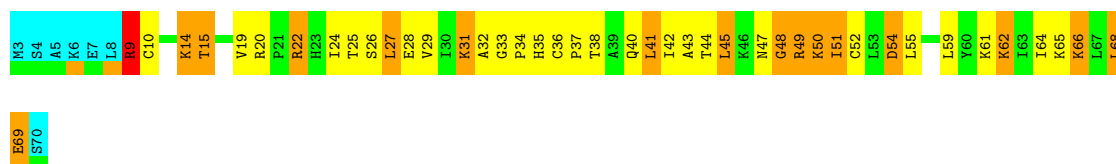
- Molecule 1: PF4-M2 CHIMERA

Chain A: 

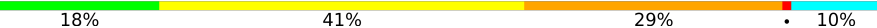


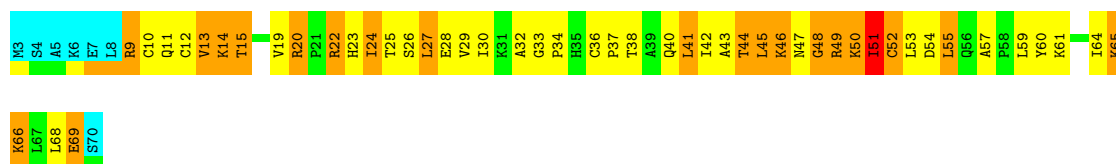
- Molecule 1: PF4-M2 CHIMERA

Chain B: 

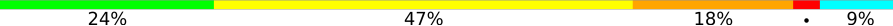


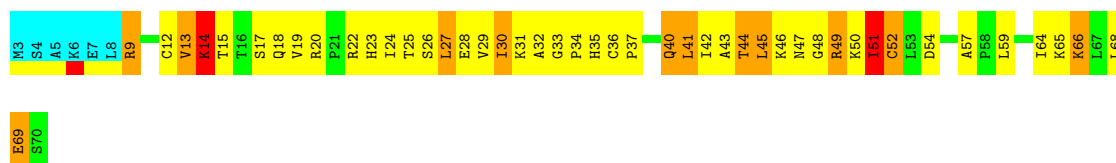
- Molecule 1: PF4-M2 CHIMERA

Chain C: 



- Molecule 1: PF4-M2 CHIMERA

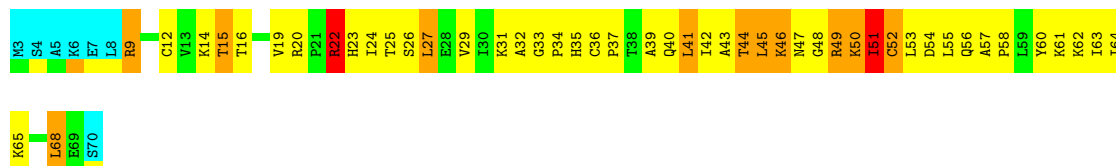
Chain D: 



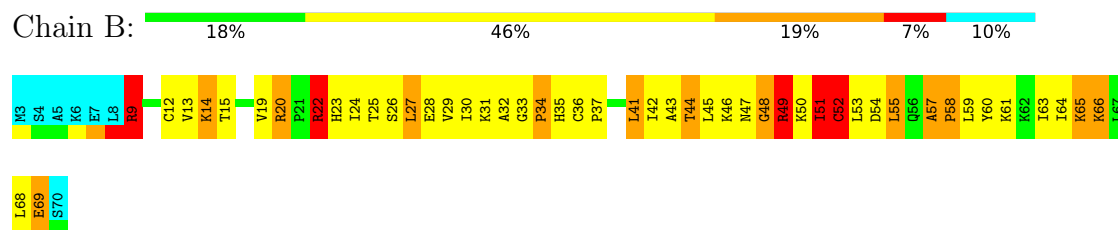
4.2.3 Score per residue for model 3

- Molecule 1: PF4-M2 CHIMERA

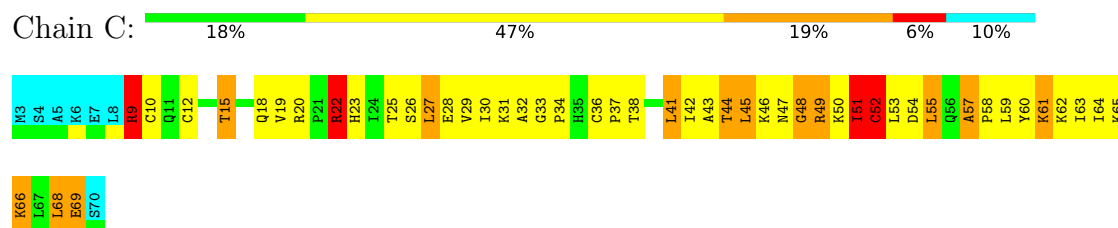
Chain A: 



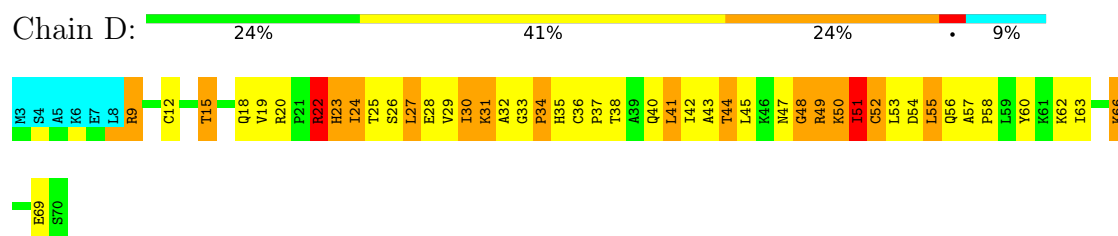
- Molecule 1: PF4-M2 CHIMERA



- Molecule 1: PF4-M2 CHIMERA

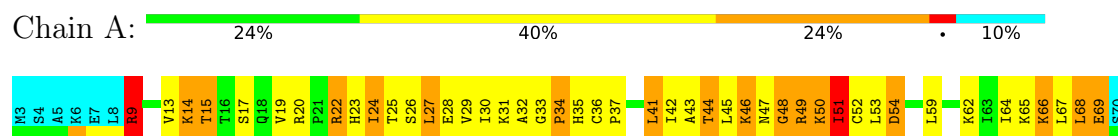


- Molecule 1: PF4-M2 CHIMERA

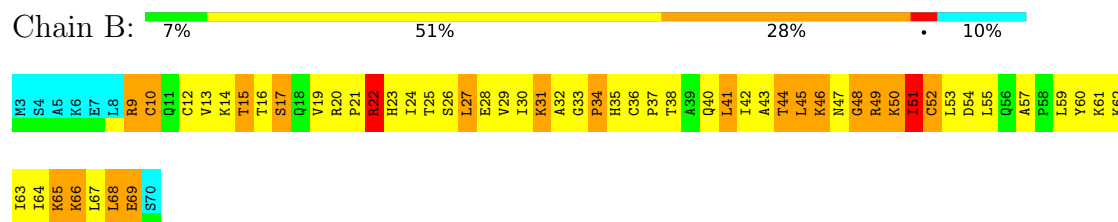


4.2.4 Score per residue for model 4

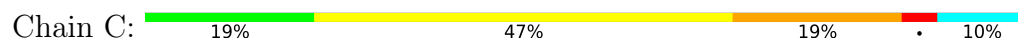
- Molecule 1: PF4-M2 CHIMERA

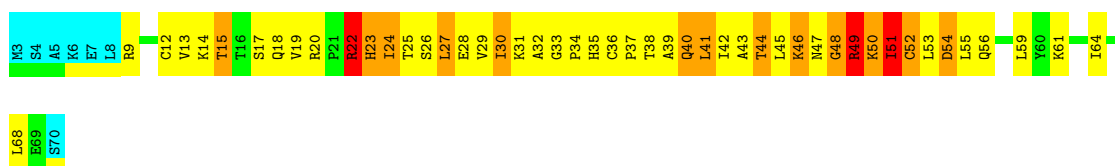


- Molecule 1: PF4-M2 CHIMERA

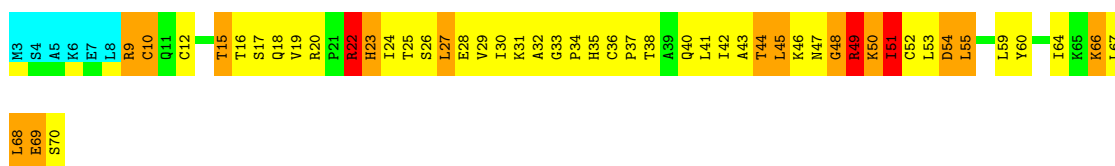
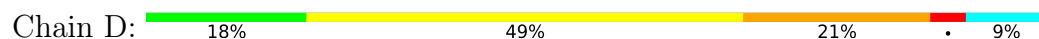


- Molecule 1: PF4-M2 CHIMERA



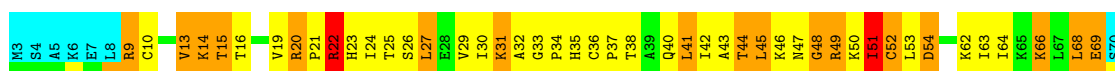
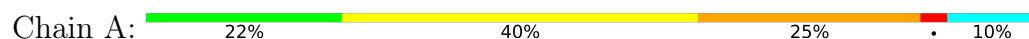


• Molecule 1: PF4-M2 CHIMERA

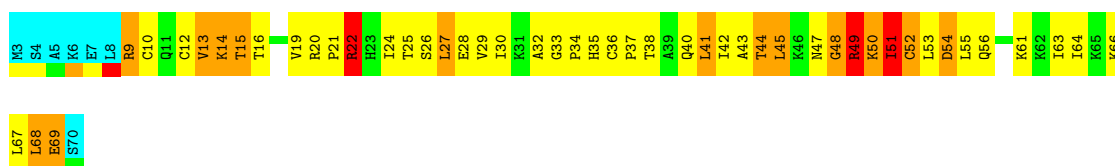
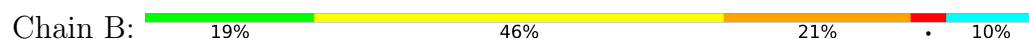


4.2.5 Score per residue for model 5

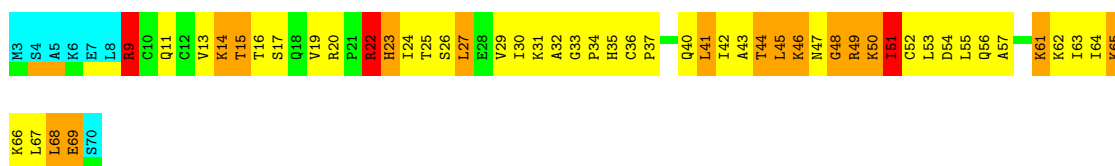
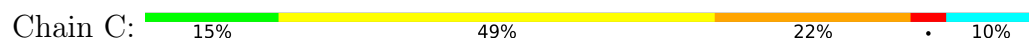
• Molecule 1: PF4-M2 CHIMERA



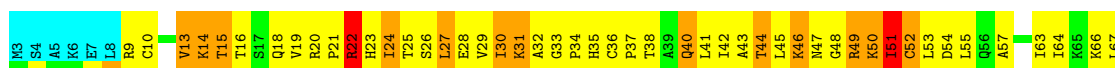
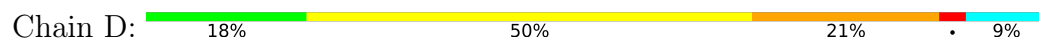
• Molecule 1: PF4-M2 CHIMERA



• Molecule 1: PF4-M2 CHIMERA



• Molecule 1: PF4-M2 CHIMERA



L68
E69
S70

4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: PF4-M2 CHIMERA

Chain A: 22% 43% 21% • 10%

M3 S4 A5 K6 E7 L8 R9 C10 Q11 K12 V13 K14 T15 V19 V20 P21 R22 H23 T24 T25 S26 L27 L30 K31 A32 G33 P34 H35 C36 P37 Q40 L41 I42 A43 T44 L45 K46 N47 G48 R49 K50 I51 C52 L53 D54 L55 Q56 A57 P58 K61 K62 T63 I64 K65 K66 L67

L68
E69
S70

- Molecule 1: PF4-M2 CHIMERA

Chain B: 22% 37% 25% 6% 10%

M3 S4 A5 K6 E7 L8 R9 V13 K14 T15 Q18 V19 R20 P21 R22 H23 T24 T25 S26 L27 E28 V29 I30 K31 A32 G33 P34 H35 C36 P37 T38 A39 Q40 L41 I42 A43 T44 L45 K46 N47 G48 R49 K50 I51 C52 L53 D54 L55 Q56 A57 P58 K62 K66 L67 E69

S70

- Molecule 1: PF4-M2 CHIMERA

Chain C: 15% 47% 24% • 10%

M3 S4 A5 K6 E7 L8 R9 C10 Q11 K12 V13 K14 T15 V19 V20 P21 R22 H23 T24 T25 S26 L27 E28 V29 I30 K31 A32 G33 P34 H35 C36 P37 T38 A39 Q40 L41 I42 A43 T44 L45 K46 N47 G48 R49 K50 I51 C52 L53 D54 L55 Q56 A57 P58 L59 Y60 K61 K62 T63 I64

K65
K66
L67
L68
E69
S70

- Molecule 1: PF4-M2 CHIMERA

Chain D: 16% 51% 19% • 9%

M3 S4 A5 K6 E7 L8 R9 C10 Q11 K12 V13 K14 T15 T16 S17 Q18 R19 V20 P21 R22 H23 T24 T25 S26 L27 E28 K31 A32 G33 P34 H35 C36 P37 T38 A39 Q40 L41 I42 A43 T44 L45 K46 N47 G48 R49 K50 I51 C52 L53 D54 L55 Q56 A57 P58 L59 Y60 K61 K62

K65
K66
L67
L68
E69
S70

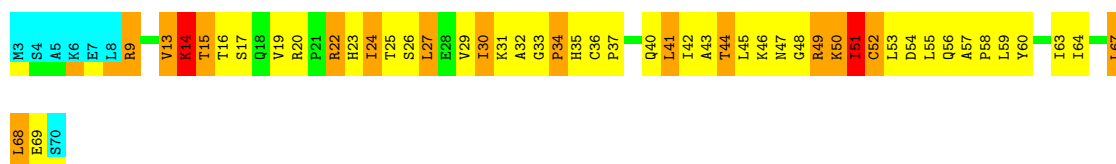
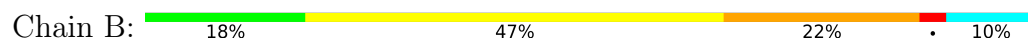
4.2.7 Score per residue for model 7

- Molecule 1: PF4-M2 CHIMERA

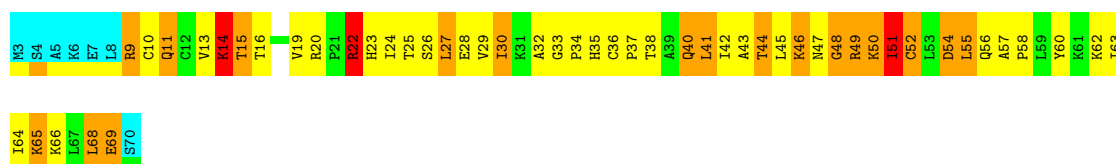
Chain A: 24% 40% 21% 6% 10%



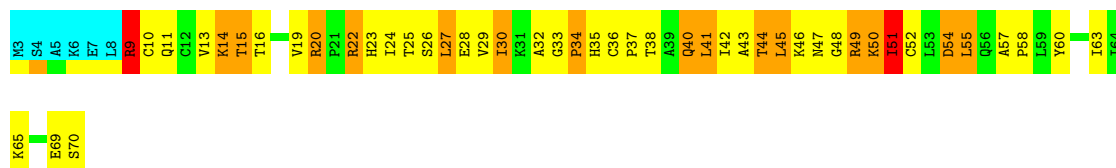
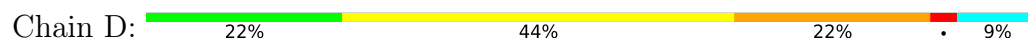
• Molecule 1: PF4-M2 CHIMERA



• Molecule 1: PF4-M2 CHIMERA

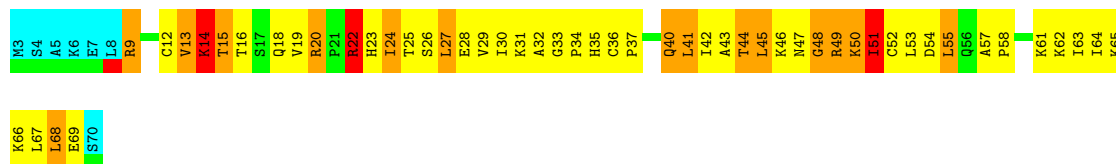
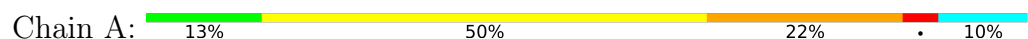


• Molecule 1: PF4-M2 CHIMERA

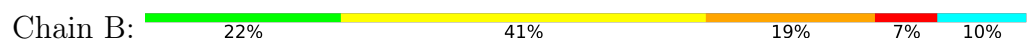


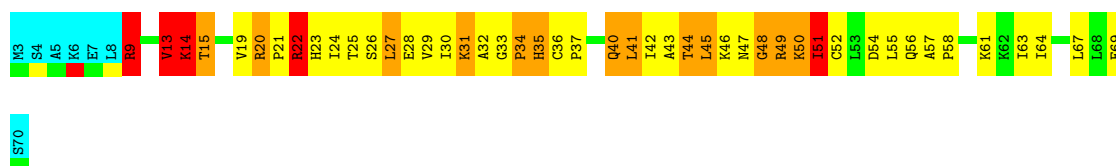
4.2.8 Score per residue for model 8

• Molecule 1: PF4-M2 CHIMERA

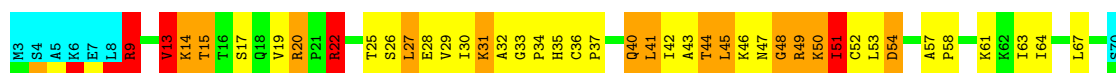


• Molecule 1: PF4-M2 CHIMERA

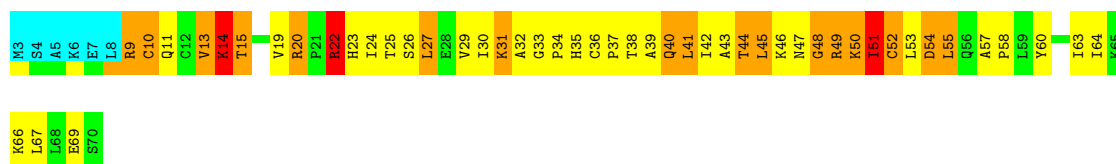
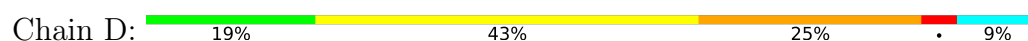




- Molecule 1: PF4-M2 CHIMERA

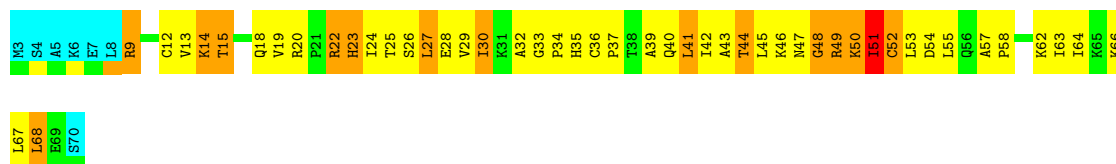
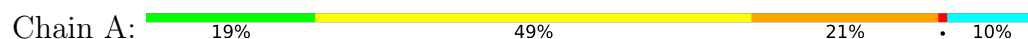


- Molecule 1: PF4-M2 CHIMERA

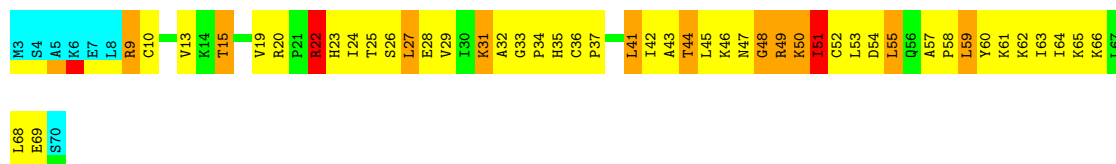
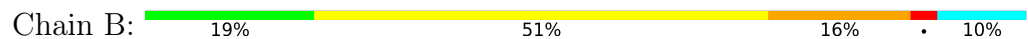


4.2.9 Score per residue for model 9

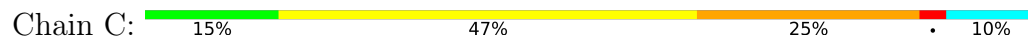
- Molecule 1: PF4-M2 CHIMERA



- Molecule 1: PF4-M2 CHIMERA



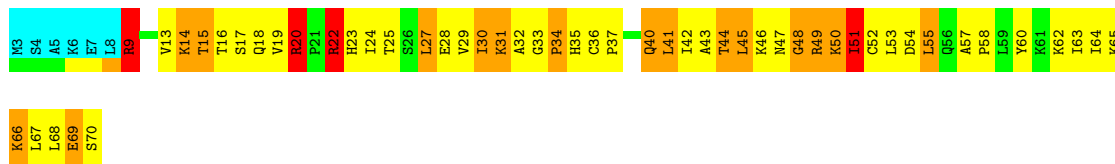
- Molecule 1: PF4-M2 CHIMERA





- Molecule 1: PF4-M2 CHIMERA

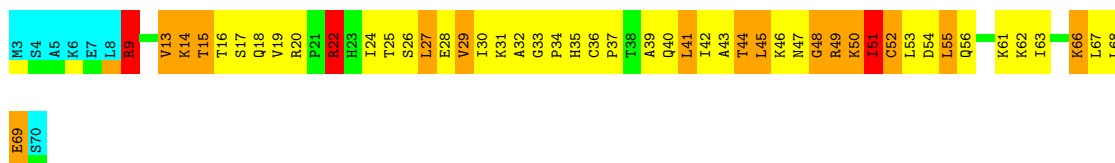
Chain D: 15% 47% 24% 6% 9%



4.2.10 Score per residue for model 10

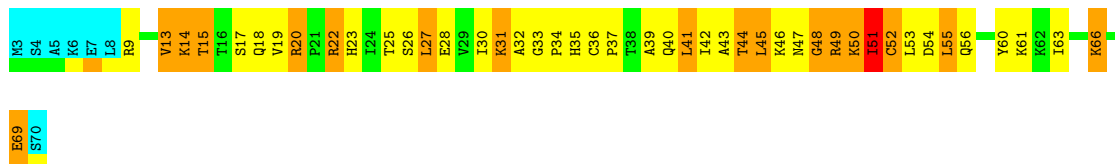
- Molecule 1: PF4-M2 CHIMERA

Chain A: 18% 46% 22% • 10%



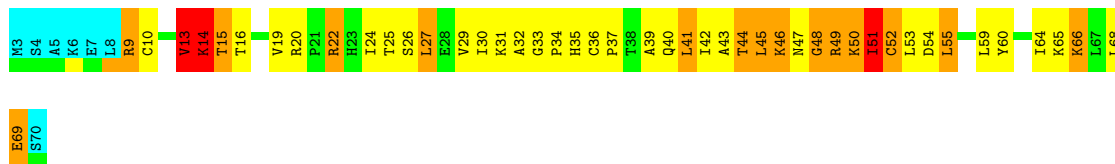
- Molecule 1: PF4-M2 CHIMERA

Chain B: 24% 40% 25% • 10%



- Molecule 1: PF4-M2 CHIMERA

Chain C: 22% 41% 22% • 10%



- Molecule 1: PF4-M2 CHIMERA

Chain D: 19% 41% 28% • 9%



E69
S70

4.2.11 Score per residue for model 11

- Molecule 1: PF4-M2 CHIMERA

Chain A: 15% 54% 16% • 10%

M3 S4 A5 K6 E7 L8 R9 C12 V13 K14 K15 T15 T16 V19 R20 P21 R22 H23 T24 T25 S26 L27 L28 E28 V29 T30 K31 A32 G33 P34 H35 C36 P37 T38 A39 Q40 L41 L42 I43 A43 T44 L45 K46 K47 N47 G48 R49 K50 I51 C52 L53 D54 L55 Q56 A57 Y60 K61 K62 I63 I64 K65 K66

K66 L67 L68 E69 S70

- Molecule 1: PF4-M2 CHIMERA

Chain B: 19% 46% 19% 6% 10%

M3 S4 A5 K6 E7 L8 R9 V13 K14 T15 Q18 V19 R20 P21 R22 H23 T24 T25 S26 L27 L28 E28 V29 T30 K31 A32 G33 P34 H35 C36 P37 T38 A39 Q40 L41 L42 I43 A43 T44 L45 K46 N47 G48 R49 K50 I51 C52 L53 D54 L55 Q56 Y60 K61 K62 I63 I64 K65 K66 L67

L68 E69 S70

- Molecule 1: PF4-M2 CHIMERA

Chain C: 21% 38% 26% • 10%

M3 S4 A5 K6 E7 L8 R9 C10 Q11 C12 V13 K14 K15 T15 V19 R20 P21 R22 H23 T24 T25 S26 L27 L28 E28 V29 T30 K31 A32 G33 P34 H35 C36 P37 T38 A39 Q40 L41 L42 I43 A43 T44 L45 K46 N47 G48 R49 K50 I51 C52 L53 D54 L55 Q56 Y60 K61 K62 I63 I64 K65 K66

L67 L68 E69 S70

- Molecule 1: PF4-M2 CHIMERA

Chain D: 13% 49% 24% 6% 9%

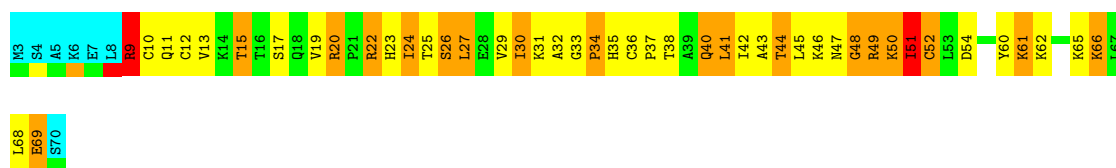
M3 S4 A5 K6 E7 L8 R9 C10 V13 K14 T15 T16 S17 Q18 V19 R20 P21 R22 H23 T24 T25 S26 L27 L28 E28 V29 T30 K31 A32 G33 P34 H35 C36 P37 T38 A39 Q40 L41 L42 I43 A43 T44 L45 K46 K47 N47 G48 R49 K50 I51 C52 L53 D54 L55 Q56 Y60 K61 K62 I63 I64 K65 K66

K65 K66 L67 L68 E69 S70

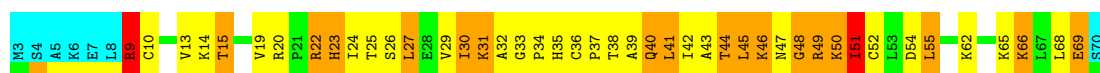
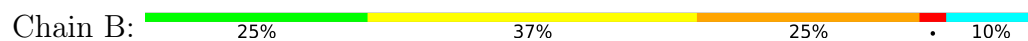
4.2.12 Score per residue for model 12

- Molecule 1: PF4-M2 CHIMERA

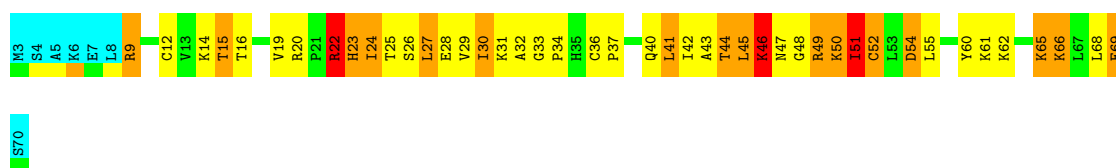
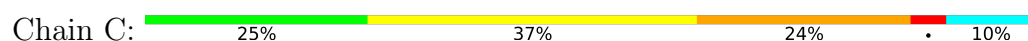
Chain A: 22% 38% 26% • 10%



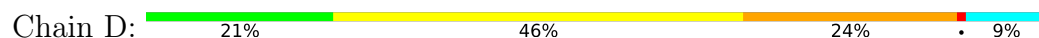
- Molecule 1: PF4-M2 CHIMERA



- Molecule 1: PF4-M2 CHIMERA

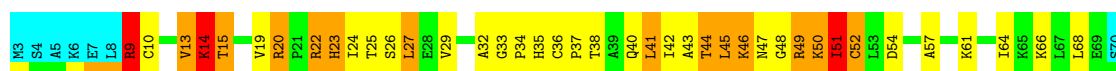


- Molecule 1: PF4-M2 CHIMERA

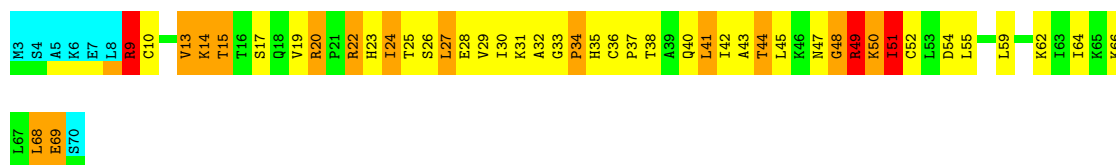
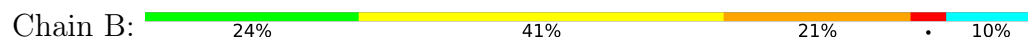


4.2.13 Score per residue for model 13

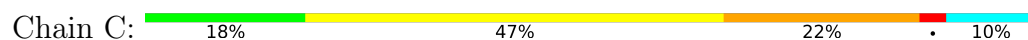
- Molecule 1: PF4-M2 CHIMERA

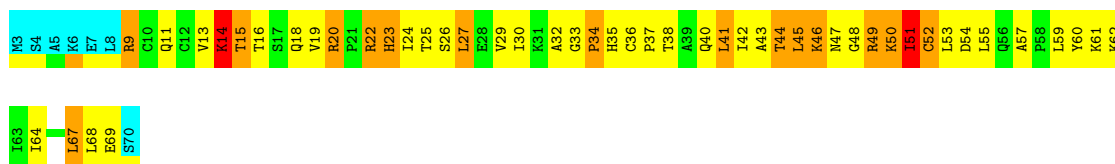


- Molecule 1: PF4-M2 CHIMERA

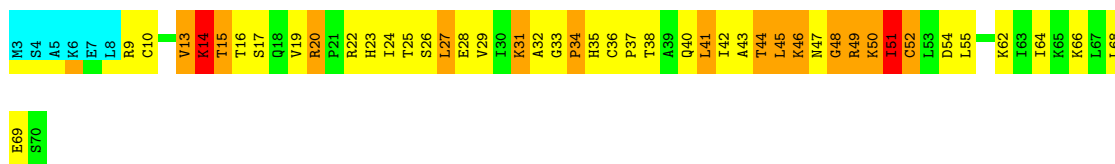
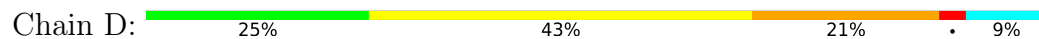


- Molecule 1: PF4-M2 CHIMERA



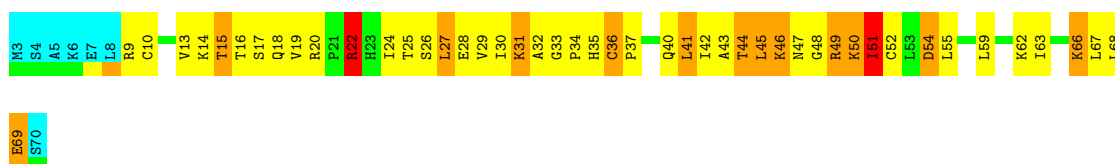
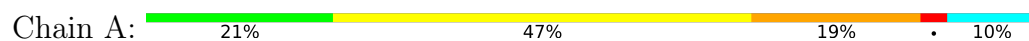


• Molecule 1: PF4-M2 CHIMERA

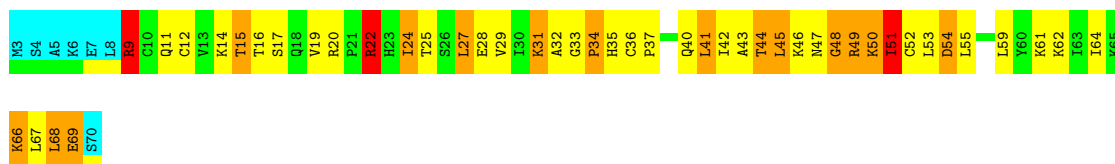
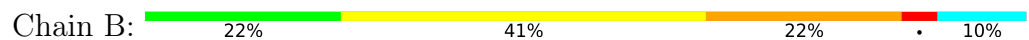


4.2.14 Score per residue for model 14

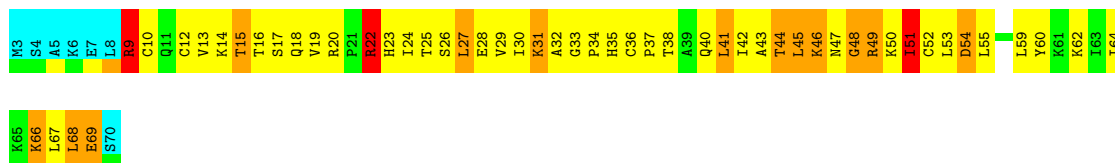
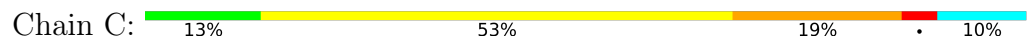
• Molecule 1: PF4-M2 CHIMERA



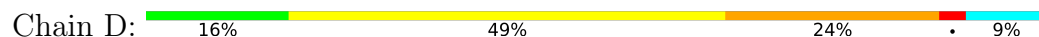
• Molecule 1: PF4-M2 CHIMERA

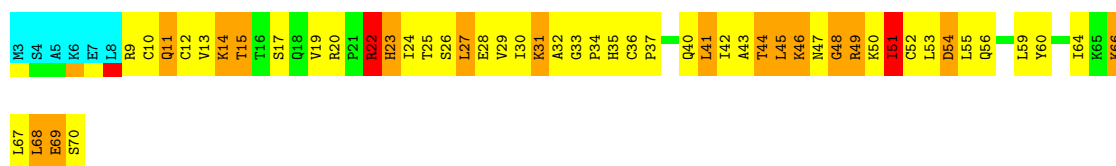


• Molecule 1: PF4-M2 CHIMERA



• Molecule 1: PF4-M2 CHIMERA





4.2.15 Score per residue for model 15

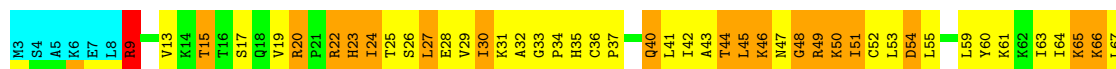
- Molecule 1: PF4-M2 CHIMERA

Chain A: 25% 40% 19% 6% 10%



- Molecule 1: PF4-M2 CHIMERA

Chain B: 19% 41% 28% 10%



- Molecule 1: PF4-M2 CHIMERA

Chain C: 26% 41% 19% 10%



- Molecule 1: PF4-M2 CHIMERA

Chain D: 22% 47% 18% 9%



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 15 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	

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	1.41±0.01	0±0/485 (0.0± 0.0%)	1.32±0.01	0±0/654 (0.0± 0.1%)
1	B	1.41±0.02	0±0/485 (0.0± 0.1%)	1.33±0.02	0±0/654 (0.0± 0.1%)
1	C	1.42±0.01	0±0/485 (0.0± 0.1%)	1.33±0.01	0±0/654 (0.0± 0.1%)
1	D	1.41±0.01	0±0/491 (0.0± 0.0%)	1.32±0.01	0±1/659 (0.0± 0.1%)
All	All	1.41	2/29190 (0.0%)	1.32	12/39315 (0.0%)

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	4.0±0.0
1	B	0.0±0.0	4.0±0.0
1	C	0.0±0.0	4.0±0.0
1	D	0.0±0.0	4.0±0.0
All	All	0	240

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	C	52	CYS	C-N	-5.38	1.28	1.33	3	1
1	B	52	CYS	C-N	-5.15	1.28	1.33	3	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	D	23	HIS	CA-CB-CG	-5.51	108.28	113.80	11	1
1	C	46	LYS	N-CA-C	-5.42	105.45	111.36	12	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	46	LYS	N-CA-C	-5.26	105.62	111.36	11	4
1	D	46	LYS	N-CA-C	-5.16	105.74	111.36	11	1
1	D	62	LYS	N-CA-C	-5.12	106.88	113.23	11	1
1	B	46	LYS	N-CA-C	-5.04	105.86	111.36	3	2

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	9	ARG	Sidechain	15
1	A	20	ARG	Sidechain	15
1	A	22	ARG	Sidechain	15
1	A	49	ARG	Sidechain	15
1	B	9	ARG	Sidechain	15
1	B	20	ARG	Sidechain	15
1	B	22	ARG	Sidechain	15
1	B	49	ARG	Sidechain	15
1	C	9	ARG	Sidechain	15
1	C	20	ARG	Sidechain	15
1	C	22	ARG	Sidechain	15
1	C	49	ARG	Sidechain	15
1	D	9	ARG	Sidechain	15
1	D	20	ARG	Sidechain	15
1	D	22	ARG	Sidechain	15
1	D	49	ARG	Sidechain	15

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	478	529	529	47±6
1	B	478	529	529	49±7
1	C	478	529	529	51±6
1	D	485	534	534	51±7
All	All	28785	31815	31815	2886

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 48.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:19:VAL:HG21	1:B:51:ILE:HG21	1.09	1.18	2	13
1:A:39:ALA:HB1	1:A:55:LEU:HD21	1.07	1.21	9	3
1:A:19:VAL:HG21	1:A:51:ILE:HG21	1.02	1.31	2	12
1:D:19:VAL:HG21	1:D:51:ILE:HG21	1.00	1.32	14	13
1:C:19:VAL:HG21	1:C:51:ILE:HG21	1.00	1.30	14	11
1:A:27:LEU:HD11	1:A:41:LEU:HD21	0.97	1.35	15	5
1:C:41:LEU:HD13	1:C:55:LEU:HD21	0.97	1.34	6	2
1:C:43:ALA:HB3	1:C:51:ILE:CD1	0.96	1.91	8	15
1:A:43:ALA:HB3	1:A:51:ILE:CD1	0.95	1.91	11	15
1:B:43:ALA:HB3	1:B:51:ILE:CD1	0.95	1.92	8	15
1:D:43:ALA:HB3	1:D:51:ILE:CD1	0.94	1.93	5	15
1:B:19:VAL:HG21	1:B:51:ILE:CG2	0.90	1.96	2	3
1:D:23:HIS:NE2	1:D:45:LEU:HD21	0.89	1.83	1	1
1:A:19:VAL:HG21	1:A:51:ILE:CG2	0.88	1.98	2	2
1:B:42:ILE:HD13	1:B:52:CYS:HB2	0.87	1.47	5	15
1:A:41:LEU:HD22	1:A:55:LEU:HD23	0.87	1.45	9	1
1:C:19:VAL:HG21	1:C:51:ILE:CG2	0.87	2.00	2	3
1:B:23:HIS:CD2	1:B:45:LEU:HD12	0.87	2.05	7	1
1:D:19:VAL:HG21	1:D:51:ILE:CG2	0.86	2.01	2	2
1:D:39:ALA:HB3	1:D:55:LEU:HD13	0.84	1.47	11	1
1:A:27:LEU:HD11	1:A:41:LEU:HD11	0.84	1.48	7	5
1:A:42:ILE:HD13	1:A:52:CYS:HB2	0.84	1.48	5	15
1:C:39:ALA:HB3	1:C:55:LEU:HD13	0.83	1.49	11	1
1:C:43:ALA:HB3	1:C:51:ILE:HD11	0.83	1.51	5	15
1:D:43:ALA:HB3	1:D:51:ILE:HD11	0.83	1.50	11	15
1:D:57:ALA:HB1	1:D:58:PRO:HD2	0.82	1.51	3	6
1:C:42:ILE:HD13	1:C:52:CYS:HB2	0.82	1.50	1	15
1:D:42:ILE:HD13	1:D:52:CYS:HB2	0.82	1.50	2	15
1:A:57:ALA:HB1	1:A:58:PRO:HD2	0.82	1.52	3	6
1:D:24:ILE:HD12	1:D:45:LEU:HD22	0.82	1.52	11	1
1:A:43:ALA:HB3	1:A:51:ILE:HD11	0.82	1.50	11	14
1:B:43:ALA:HB3	1:B:51:ILE:HD11	0.81	1.52	5	14
1:B:39:ALA:HB1	1:B:55:LEU:HD13	0.80	1.54	11	1
1:B:24:ILE:HD13	1:B:44:THR:O	0.80	1.77	14	2
1:B:23:HIS:CE1	1:B:45:LEU:HD21	0.80	2.11	15	1
1:C:41:LEU:HD11	1:C:54:ASP:O	0.80	1.76	7	5
1:B:42:ILE:HD13	1:B:52:CYS:CB	0.79	2.07	10	13
1:D:39:ALA:CB	1:D:55:LEU:HD13	0.79	2.06	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:24:ILE:HD13	1:D:44:THR:O	0.79	1.77	5	2
1:A:39:ALA:CB	1:A:55:LEU:HD21	0.78	2.08	9	3
1:A:24:ILE:HD13	1:A:44:THR:O	0.78	1.79	4	1
1:C:39:ALA:CB	1:C:55:LEU:HD13	0.78	2.08	11	1
1:A:57:ALA:HB1	1:A:58:PRO:CD	0.77	2.10	3	4
1:D:29:VAL:HA	1:D:41:LEU:HD12	0.77	1.56	1	7
1:C:39:ALA:HB3	1:C:55:LEU:HD22	0.77	1.56	11	1
1:D:57:ALA:HB1	1:D:58:PRO:CD	0.77	2.09	3	4
1:D:32:ALA:HB1	1:D:37:PRO:O	0.77	1.80	10	15
1:C:24:ILE:HD13	1:C:44:THR:O	0.77	1.80	4	1
1:A:42:ILE:HD13	1:A:52:CYS:CB	0.77	2.10	5	14
1:C:40:GLN:C	1:C:41:LEU:HD23	0.77	2.05	7	2
1:C:32:ALA:HB1	1:C:37:PRO:O	0.76	1.80	14	15
1:D:42:ILE:HD13	1:D:52:CYS:CB	0.76	2.09	2	15
1:D:39:ALA:HB3	1:D:55:LEU:HD22	0.76	1.57	11	1
1:C:57:ALA:HB3	1:C:58:PRO:HD3	0.76	1.55	3	1
1:B:32:ALA:HB1	1:B:37:PRO:O	0.76	1.81	10	15
1:A:30:ILE:HG23	1:B:26:SER:OG	0.75	1.81	9	4
1:D:29:VAL:HG23	1:D:41:LEU:HD12	0.75	1.56	3	2
1:B:55:LEU:HD22	1:B:55:LEU:O	0.75	1.81	9	1
1:D:29:VAL:HG13	1:D:41:LEU:HD12	0.75	1.56	2	2
1:C:67:LEU:HD12	1:C:67:LEU:O	0.75	1.82	13	1
1:A:32:ALA:HB1	1:A:37:PRO:O	0.75	1.82	15	15
1:A:31:LYS:HG3	1:B:67:LEU:HD23	0.75	1.58	8	2
1:A:29:VAL:HG23	1:A:41:LEU:HD12	0.75	1.59	3	1
1:A:55:LEU:HD13	1:A:55:LEU:N	0.75	1.97	8	1
1:D:54:ASP:C	1:D:55:LEU:HD22	0.75	2.06	10	1
1:D:24:ILE:HA	1:D:45:LEU:HD13	0.75	1.59	6	2
1:B:24:ILE:HA	1:B:45:LEU:HD13	0.74	1.59	13	3
1:C:55:LEU:O	1:C:55:LEU:HD22	0.74	1.82	7	1
1:C:30:ILE:HG22	1:D:26:SER:OG	0.74	1.81	8	1
1:A:64:ILE:HA	1:A:67:LEU:HD12	0.74	1.59	9	4
1:A:41:LEU:HD11	1:A:54:ASP:O	0.74	1.82	9	5
1:B:44:THR:HG23	1:B:50:LYS:HG3	0.73	1.59	3	13
1:B:27:LEU:HD11	1:B:41:LEU:HD11	0.73	1.59	14	10
1:B:67:LEU:O	1:B:67:LEU:HD12	0.73	1.83	11	2
1:C:27:LEU:O	1:C:27:LEU:HD23	0.73	1.83	1	4
1:A:67:LEU:HD23	1:B:31:LYS:CD	0.73	2.14	9	1
1:C:42:ILE:HD13	1:C:52:CYS:CB	0.73	2.13	13	13
1:A:27:LEU:CD1	1:A:41:LEU:HD21	0.72	2.12	15	3
1:D:27:LEU:HD11	1:D:41:LEU:HD11	0.72	1.59	1	11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:LEU:HD13	1:B:31:LYS:HD3	0.72	1.59	1	1
1:A:26:SER:OG	1:B:30:ILE:HG23	0.72	1.85	13	4
1:D:55:LEU:HD12	1:D:60:TYR:CE2	0.72	2.20	3	1
1:A:44:THR:HG23	1:A:50:LYS:HG3	0.71	1.62	8	15
1:A:29:VAL:HG13	1:A:41:LEU:HB3	0.71	1.62	5	3
1:C:44:THR:HG23	1:C:50:LYS:HG3	0.71	1.62	8	14
1:B:40:GLN:C	1:B:41:LEU:HD23	0.71	2.11	10	2
1:B:57:ALA:HB1	1:B:58:PRO:HD2	0.71	1.61	1	5
1:D:32:ALA:HB1	1:D:37:PRO:C	0.70	2.10	7	15
1:D:39:ALA:CB	1:D:55:LEU:HD21	0.70	2.15	1	2
1:B:19:VAL:CG2	1:B:51:ILE:HG21	0.70	2.10	2	9
1:C:27:LEU:HD11	1:C:41:LEU:HD11	0.70	1.63	14	8
1:A:30:ILE:HD13	1:A:30:ILE:N	0.70	2.01	9	1
1:C:23:HIS:CD2	1:C:45:LEU:HD12	0.70	2.21	7	1
1:C:57:ALA:HB1	1:C:58:PRO:HD2	0.70	1.60	1	5
1:C:26:SER:OG	1:D:30:ILE:HG23	0.70	1.85	1	2
1:A:32:ALA:HB1	1:A:37:PRO:C	0.69	2.11	2	15
1:D:23:HIS:CE1	1:D:45:LEU:HD21	0.69	2.22	1	1
1:C:19:VAL:CG2	1:C:51:ILE:HG21	0.69	2.17	2	6
1:B:29:VAL:HA	1:B:41:LEU:HD12	0.69	1.62	14	8
1:D:39:ALA:HB1	1:D:55:LEU:HD21	0.69	1.62	1	2
1:B:19:VAL:HG21	1:B:51:ILE:HG12	0.69	1.63	4	2
1:D:23:HIS:CE1	1:D:45:LEU:HD12	0.69	2.23	6	1
1:C:32:ALA:HB1	1:C:37:PRO:C	0.69	2.13	1	15
1:D:44:THR:HG23	1:D:50:LYS:HG3	0.69	1.64	9	14
1:D:16:THR:HG23	1:D:52:CYS:SG	0.69	2.28	7	1
1:B:41:LEU:HD13	1:B:55:LEU:CD2	0.69	2.16	1	1
1:C:29:VAL:HG22	1:C:41:LEU:HD12	0.69	1.65	10	3
1:A:27:LEU:CD1	1:A:41:LEU:HD11	0.68	2.18	7	4
1:A:10:CYS:HB2	1:A:13:VAL:HG22	0.68	1.63	12	1
1:C:30:ILE:HD13	1:C:30:ILE:N	0.68	2.03	7	1
1:C:39:ALA:HB3	1:C:55:LEU:CD1	0.68	2.18	11	1
1:B:32:ALA:HB1	1:B:37:PRO:C	0.68	2.12	1	14
1:D:24:ILE:HD12	1:D:45:LEU:HG	0.68	1.65	13	7
1:C:29:VAL:HG13	1:C:41:LEU:HB3	0.68	1.64	13	2
1:D:40:GLN:C	1:D:41:LEU:HD23	0.68	2.13	12	1
1:A:41:LEU:N	1:A:41:LEU:HD23	0.68	2.04	9	2
1:D:39:ALA:HB3	1:D:55:LEU:CD1	0.68	2.19	11	1
1:D:55:LEU:HD13	1:D:60:TYR:CZ	0.67	2.23	4	1
1:A:65:LYS:HA	1:A:68:LEU:HD12	0.67	1.66	12	1
1:C:41:LEU:N	1:C:41:LEU:HD23	0.67	2.05	3	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:29:VAL:HG23	1:C:41:LEU:HD12	0.67	1.66	4	1
1:A:41:LEU:HD22	1:A:55:LEU:HD12	0.67	1.65	10	1
1:B:27:LEU:HD11	1:B:41:LEU:HD21	0.67	1.64	7	3
1:B:54:ASP:OD1	1:B:57:ALA:HB3	0.67	1.89	4	1
1:B:41:LEU:HD13	1:B:55:LEU:HD21	0.67	1.64	2	3
1:A:29:VAL:HA	1:A:41:LEU:HD12	0.67	1.65	1	3
1:B:27:LEU:HD23	1:B:27:LEU:O	0.67	1.89	3	5
1:B:41:LEU:HD23	1:B:41:LEU:N	0.67	2.04	3	3
1:D:19:VAL:HG21	1:D:51:ILE:HG12	0.67	1.66	4	2
1:A:67:LEU:HD23	1:B:31:LYS:HD3	0.67	1.66	9	2
1:D:41:LEU:HD11	1:D:54:ASP:O	0.66	1.90	12	1
1:D:64:ILE:HA	1:D:67:LEU:HD12	0.66	1.68	10	3
1:C:30:ILE:HD13	1:C:40:GLN:NE2	0.66	2.05	9	1
1:D:15:THR:HG21	1:D:54:ASP:HB2	0.66	1.67	4	5
1:C:30:ILE:HD12	1:C:30:ILE:N	0.66	2.06	14	2
1:B:41:LEU:HD11	1:B:54:ASP:O	0.66	1.90	12	2
1:A:41:LEU:HD23	1:A:41:LEU:N	0.66	2.06	5	3
1:B:55:LEU:HD13	1:B:60:TYR:CZ	0.66	2.25	4	2
1:D:19:VAL:CG2	1:D:51:ILE:HG21	0.66	2.20	9	8
1:A:15:THR:HG21	1:A:54:ASP:HB2	0.66	1.67	4	3
1:C:59:LEU:HD12	1:C:60:TYR:N	0.65	2.06	13	3
1:C:15:THR:HG21	1:C:54:ASP:HB2	0.65	1.67	4	7
1:B:30:ILE:N	1:B:30:ILE:HD13	0.65	2.07	7	1
1:B:15:THR:HG21	1:B:54:ASP:HB2	0.65	1.66	15	5
1:D:29:VAL:O	1:D:29:VAL:HG13	0.65	1.92	7	2
1:D:41:LEU:HD23	1:D:41:LEU:N	0.65	2.06	12	1
1:C:30:ILE:N	1:C:30:ILE:HD13	0.65	2.06	12	1
1:D:30:ILE:HD12	1:D:30:ILE:N	0.65	2.06	14	1
1:B:65:LYS:HA	1:B:68:LEU:HD12	0.65	1.65	12	3
1:D:29:VAL:HG22	1:D:41:LEU:HD11	0.65	1.69	4	5
1:C:13:VAL:HG22	1:C:14:LYS:N	0.65	2.07	10	3
1:C:30:ILE:HG23	1:D:26:SER:OG	0.65	1.92	3	4
1:C:65:LYS:HA	1:C:68:LEU:HD12	0.65	1.67	12	3
1:C:29:VAL:HG22	1:C:41:LEU:CD1	0.65	2.22	5	6
1:C:55:LEU:HD22	1:C:55:LEU:C	0.65	2.16	7	1
1:A:67:LEU:HD13	1:B:31:LYS:CD	0.65	2.22	1	1
1:C:43:ALA:HB3	1:C:51:ILE:HD12	0.65	1.69	2	15
1:B:59:LEU:HD12	1:B:60:TYR:N	0.65	2.07	3	1
1:A:23:HIS:CD2	1:A:45:LEU:HD12	0.65	2.26	9	1
1:C:41:LEU:HD23	1:C:41:LEU:N	0.64	2.07	7	2
1:D:41:LEU:HD23	1:D:53:LEU:HB2	0.64	1.68	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:HIS:CD2	1:A:45:LEU:HD21	0.64	2.28	1	1
1:A:64:ILE:O	1:A:68:LEU:HD12	0.64	1.91	11	10
1:A:67:LEU:HD13	1:B:31:LYS:CG	0.64	2.21	14	1
1:A:27:LEU:O	1:A:27:LEU:HD23	0.64	1.92	10	2
1:A:60:TYR:HA	1:A:63:ILE:HD12	0.64	1.69	11	1
1:B:27:LEU:CD1	1:B:41:LEU:HD21	0.64	2.23	7	1
1:A:24:ILE:HD12	1:A:45:LEU:HG	0.64	1.69	10	8
1:A:43:ALA:HB3	1:A:51:ILE:HD12	0.64	1.70	14	14
1:C:29:VAL:HA	1:C:41:LEU:HD12	0.64	1.68	14	3
1:B:27:LEU:CD1	1:B:41:LEU:HD11	0.64	2.23	5	9
1:D:43:ALA:HB3	1:D:51:ILE:HD12	0.64	1.69	8	15
1:A:26:SER:HG	1:B:30:ILE:HG23	0.64	1.53	3	1
1:D:27:LEU:HD11	1:D:41:LEU:HD21	0.64	1.70	8	3
1:C:41:LEU:HD23	1:C:53:LEU:HB2	0.64	1.70	11	1
1:D:10:CYS:SG	1:D:38:THR:HG22	0.63	2.34	4	8
1:A:59:LEU:HD12	1:A:62:LYS:CD	0.63	2.23	15	1
1:C:15:THR:HG21	1:C:54:ASP:HB3	0.63	1.70	11	4
1:C:31:LYS:HG3	1:D:67:LEU:HD23	0.63	1.69	9	2
1:A:27:LEU:HD11	1:A:41:LEU:CD2	0.63	2.19	15	3
1:B:30:ILE:HD11	1:B:40:GLN:HB3	0.63	1.71	10	1
1:A:27:LEU:CD2	1:A:63:ILE:HG21	0.63	2.23	5	5
1:D:27:LEU:CD1	1:D:41:LEU:HD11	0.63	2.24	7	10
1:C:30:ILE:HD11	1:C:40:GLN:HB3	0.63	1.71	8	1
1:D:27:LEU:CD1	1:D:41:LEU:HD21	0.63	2.23	8	1
1:C:41:LEU:CD1	1:C:55:LEU:HD21	0.63	2.18	6	1
1:B:43:ALA:HB3	1:B:51:ILE:HD12	0.62	1.70	2	14
1:C:27:LEU:CD1	1:C:41:LEU:HD11	0.62	2.24	15	6
1:B:57:ALA:HB3	1:B:58:PRO:HD3	0.62	1.70	3	1
1:C:13:VAL:HG13	1:C:14:LYS:N	0.62	2.08	6	3
1:B:64:ILE:O	1:B:68:LEU:HD12	0.62	1.93	7	9
1:D:55:LEU:HD22	1:D:55:LEU:N	0.62	2.10	10	1
1:C:53:LEU:CD1	1:C:63:ILE:HD11	0.62	2.25	1	5
1:C:19:VAL:HG11	1:C:45:LEU:HD11	0.62	1.71	9	3
1:B:53:LEU:CD1	1:B:63:ILE:HD11	0.62	2.25	1	5
1:D:29:VAL:HG23	1:D:41:LEU:CD1	0.62	2.25	7	2
1:C:29:VAL:O	1:C:29:VAL:HG13	0.62	1.94	4	1
1:C:39:ALA:HB3	1:C:55:LEU:CD2	0.62	2.23	11	2
1:B:64:ILE:HA	1:B:67:LEU:HD12	0.62	1.71	8	1
1:B:13:VAL:HG22	1:B:14:LYS:N	0.62	2.08	11	1
1:B:55:LEU:HD22	1:B:55:LEU:C	0.61	2.19	9	1
1:C:39:ALA:HB3	1:C:55:LEU:HD21	0.61	1.72	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:19:VAL:CG1	1:C:53:LEU:HD21	0.61	2.25	15	2
1:A:42:ILE:HD12	1:C:11:GLN:NE2	0.61	2.10	5	2
1:D:39:ALA:HB3	1:D:55:LEU:CD2	0.61	2.25	11	1
1:A:15:THR:HG21	1:A:54:ASP:HB3	0.61	1.71	11	8
1:A:26:SER:OG	1:B:30:ILE:HG22	0.61	1.95	10	1
1:B:30:ILE:HD12	1:B:30:ILE:C	0.61	2.21	10	1
1:C:30:ILE:HD13	1:C:40:GLN:HE22	0.61	1.54	9	1
1:D:27:LEU:CD2	1:D:63:ILE:HG21	0.61	2.25	10	4
1:A:29:VAL:HG13	1:A:29:VAL:O	0.61	1.95	3	1
1:D:27:LEU:HD23	1:D:27:LEU:O	0.61	1.95	8	3
1:A:19:VAL:CG2	1:A:51:ILE:HG21	0.61	2.17	2	5
1:C:59:LEU:HD12	1:C:59:LEU:C	0.61	2.20	13	3
1:A:53:LEU:CD1	1:A:63:ILE:HD11	0.61	2.25	1	5
1:D:47:ASN:O	1:D:49:ARG:N	0.61	2.34	2	15
1:D:54:ASP:OD1	1:D:57:ALA:HB3	0.61	1.95	5	2
1:C:24:ILE:HD12	1:C:45:LEU:HG	0.61	1.71	10	7
1:B:59:LEU:HD12	1:B:59:LEU:C	0.61	2.20	3	1
1:C:41:LEU:HD13	1:C:55:LEU:CD2	0.61	2.20	6	1
1:D:53:LEU:CD1	1:D:63:ILE:HD11	0.61	2.26	1	3
1:D:30:ILE:HD11	1:D:40:GLN:NE2	0.61	2.10	7	2
1:D:19:VAL:CG1	1:D:53:LEU:HD21	0.61	2.26	15	1
1:D:29:VAL:CG2	1:D:41:LEU:HD12	0.61	2.25	3	2
1:A:63:ILE:O	1:A:67:LEU:HD23	0.60	1.96	7	2
1:B:10:CYS:SG	1:B:38:THR:HG22	0.60	2.36	4	5
1:C:60:TYR:HA	1:C:63:ILE:HD12	0.60	1.72	11	3
1:C:30:ILE:C	1:C:30:ILE:HD12	0.60	2.20	8	1
1:B:63:ILE:O	1:B:67:LEU:HD23	0.60	1.97	15	1
1:A:44:THR:HG23	1:A:50:LYS:CG	0.60	2.27	8	13
1:C:47:ASN:O	1:C:49:ARG:N	0.60	2.34	4	15
1:C:41:LEU:HD13	1:C:55:LEU:CD1	0.60	2.26	9	1
1:A:47:ASN:O	1:A:49:ARG:N	0.60	2.35	2	15
1:D:29:VAL:HG22	1:D:41:LEU:CD1	0.60	2.27	4	8
1:B:24:ILE:HD12	1:B:45:LEU:HD13	0.60	1.73	3	2
1:B:19:VAL:CG1	1:B:53:LEU:HD21	0.60	2.27	15	1
1:B:47:ASN:O	1:B:49:ARG:N	0.59	2.35	8	15
1:A:67:LEU:HD21	1:B:29:VAL:CG1	0.59	2.27	15	1
1:B:27:LEU:CD2	1:B:63:ILE:HG21	0.59	2.26	1	4
1:B:23:HIS:ND1	1:B:45:LEU:HD21	0.59	2.11	15	1
1:D:17:SER:OG	1:D:59:LEU:HD22	0.59	1.97	4	1
1:C:41:LEU:HD13	1:C:55:LEU:HD13	0.59	1.72	9	1
1:B:29:VAL:HG22	1:B:41:LEU:CD1	0.59	2.27	5	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HD11	1:A:54:ASP:C	0.59	2.21	2	2
1:B:59:LEU:C	1:B:59:LEU:HD12	0.59	2.21	9	1
1:A:41:LEU:HD22	1:A:55:LEU:CD1	0.59	2.28	10	1
1:A:54:ASP:OD1	1:A:57:ALA:HB3	0.59	1.98	11	3
1:A:23:HIS:NE2	1:A:45:LEU:HD21	0.59	2.11	1	1
1:A:31:LYS:CG	1:B:67:LEU:HD23	0.59	2.27	8	1
1:A:55:LEU:C	1:A:55:LEU:HD12	0.59	2.22	9	1
1:C:31:LYS:CG	1:D:67:LEU:HD13	0.59	2.28	14	2
1:B:41:LEU:HD23	1:B:53:LEU:HB2	0.59	1.73	15	2
1:B:15:THR:HG21	1:B:54:ASP:HB3	0.59	1.74	11	7
1:C:41:LEU:HD11	1:C:54:ASP:C	0.59	2.22	1	5
1:B:29:VAL:HG13	1:B:55:LEU:CD1	0.59	2.28	3	1
1:A:19:VAL:HG21	1:A:51:ILE:HG12	0.59	1.75	15	2
1:D:39:ALA:CB	1:D:55:LEU:HD11	0.58	2.28	6	3
1:C:43:ALA:O	1:C:50:LYS:CG	0.58	2.51	4	3
1:A:27:LEU:HD23	1:A:27:LEU:O	0.58	1.98	12	3
1:A:67:LEU:HD21	1:B:29:VAL:HG12	0.58	1.75	15	1
1:A:24:ILE:HD12	1:A:45:LEU:HD13	0.58	1.75	15	4
1:D:23:HIS:CE1	1:D:45:LEU:HD23	0.58	2.34	13	1
1:B:24:ILE:HD12	1:B:45:LEU:HG	0.58	1.74	4	6
1:C:10:CYS:SG	1:C:38:THR:HG22	0.58	2.38	15	7
1:D:39:ALA:O	1:D:55:LEU:HD22	0.58	1.98	11	1
1:B:44:THR:HG23	1:B:50:LYS:CG	0.58	2.28	3	13
1:D:19:VAL:HG21	1:D:51:ILE:CG1	0.58	2.29	4	1
1:C:27:LEU:CD2	1:C:63:ILE:HG21	0.58	2.29	8	1
1:C:30:ILE:HG22	1:D:26:SER:CB	0.58	2.28	8	1
1:B:60:TYR:HA	1:B:63:ILE:HD12	0.58	1.75	7	6
1:C:27:LEU:C	1:C:27:LEU:HD12	0.58	2.24	6	10
1:C:30:ILE:HG23	1:D:26:SER:HG	0.58	1.59	3	1
1:C:30:ILE:HD12	1:C:31:LYS:O	0.58	1.98	8	1
1:B:42:ILE:HG22	1:B:43:ALA:N	0.57	2.14	15	15
1:D:27:LEU:HD12	1:D:27:LEU:C	0.57	2.24	7	5
1:C:39:ALA:O	1:C:55:LEU:HD22	0.57	1.99	11	1
1:D:41:LEU:HD13	1:D:55:LEU:CD1	0.57	2.29	7	1
1:A:29:VAL:HG22	1:A:41:LEU:CD1	0.57	2.29	4	4
1:B:27:LEU:C	1:B:27:LEU:HD12	0.57	2.24	6	10
1:A:40:GLN:C	1:A:41:LEU:HD23	0.57	2.23	10	1
1:A:27:LEU:HD12	1:A:27:LEU:C	0.57	2.25	1	9
1:A:53:LEU:HD12	1:A:63:ILE:CD1	0.57	2.28	8	4
1:B:57:ALA:HB1	1:B:58:PRO:CD	0.57	2.29	1	2
1:B:19:VAL:HG21	1:B:51:ILE:CG1	0.57	2.29	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:55:LEU:HD21	1:D:67:LEU:O	0.57	1.98	5	1
1:D:27:LEU:C	1:D:27:LEU:HD12	0.57	2.24	15	7
1:B:39:ALA:HB3	1:B:55:LEU:HD21	0.57	1.74	10	3
1:C:67:LEU:HD13	1:D:31:LYS:CG	0.57	2.29	14	1
1:A:42:ILE:HG22	1:A:43:ALA:N	0.57	2.14	6	15
1:B:29:VAL:HG22	1:B:41:LEU:HD11	0.57	1.76	5	8
1:C:42:ILE:HG22	1:C:43:ALA:N	0.57	2.14	10	15
1:D:19:VAL:HG21	1:D:51:ILE:CB	0.57	2.30	4	1
1:B:43:ALA:O	1:B:50:LYS:CG	0.57	2.53	2	8
1:D:42:ILE:HG22	1:D:43:ALA:N	0.56	2.15	6	15
1:D:29:VAL:HG22	1:D:41:LEU:HD12	0.56	1.77	5	3
1:C:41:LEU:HB2	1:C:55:LEU:HD11	0.56	1.76	6	1
1:D:43:ALA:O	1:D:50:LYS:CG	0.56	2.53	1	7
1:B:39:ALA:CB	1:B:55:LEU:HD21	0.56	2.31	6	1
1:A:26:SER:CB	1:B:30:ILE:HG22	0.56	2.30	10	1
1:B:30:ILE:HD12	1:B:31:LYS:O	0.56	1.99	10	1
1:D:64:ILE:O	1:D:68:LEU:HD23	0.56	1.99	12	1
1:A:19:VAL:HG21	1:A:51:ILE:CG1	0.56	2.31	15	1
1:C:27:LEU:HD11	1:C:29:VAL:CG2	0.56	2.30	13	4
1:C:54:ASP:OD1	1:C:57:ALA:HB3	0.56	2.00	5	3
1:C:26:SER:HB3	1:D:30:ILE:HG22	0.56	1.77	5	1
1:D:15:THR:HG21	1:D:54:ASP:OD1	0.56	2.01	11	1
1:C:64:ILE:O	1:C:68:LEU:HD12	0.56	1.99	13	6
1:A:19:VAL:HG21	1:A:51:ILE:CB	0.56	2.31	15	1
1:C:26:SER:CB	1:D:30:ILE:HG22	0.56	2.29	5	1
1:D:41:LEU:HB2	1:D:55:LEU:HD21	0.56	1.76	10	1
1:C:44:THR:HG23	1:C:50:LYS:CG	0.56	2.31	10	12
1:A:27:LEU:HD12	1:A:28:GLU:O	0.56	2.01	7	6
1:C:27:LEU:HD12	1:C:28:GLU:O	0.56	2.01	6	9
1:A:16:THR:HG23	1:A:52:CYS:SG	0.56	2.40	3	1
1:C:23:HIS:CE1	1:C:45:LEU:HD22	0.56	2.36	3	1
1:B:24:ILE:CD1	1:B:45:LEU:HD22	0.55	2.31	9	2
1:D:27:LEU:HD23	1:D:27:LEU:C	0.55	2.26	8	3
1:C:64:ILE:HA	1:C:67:LEU:HD12	0.55	1.78	8	1
1:C:57:ALA:HB1	1:C:58:PRO:CD	0.55	2.30	1	3
1:C:53:LEU:HD13	1:C:59:LEU:CD1	0.55	2.32	10	2
1:B:27:LEU:HD23	1:B:27:LEU:C	0.55	2.27	7	5
1:D:54:ASP:C	1:D:60:TYR:CZ	0.55	2.85	11	1
1:B:53:LEU:HD12	1:B:63:ILE:CD1	0.55	2.32	7	4
1:C:27:LEU:HD23	1:C:27:LEU:C	0.55	2.27	3	4
1:C:27:LEU:HD21	1:C:29:VAL:HG23	0.55	1.79	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:23:HIS:CE1	1:D:45:LEU:CD2	0.55	2.90	13	2
1:D:44:THR:HG23	1:D:50:LYS:CG	0.54	2.32	8	11
1:C:30:ILE:HD11	1:C:40:GLN:CD	0.54	2.27	11	1
1:A:31:LYS:HD3	1:B:67:LEU:HD13	0.54	1.77	4	1
1:A:23:HIS:CD2	1:A:45:LEU:CD1	0.54	2.90	9	1
1:C:30:ILE:HD11	1:C:40:GLN:NE2	0.54	2.17	11	1
1:D:10:CYS:HB2	1:D:13:VAL:HG22	0.54	1.80	8	1
1:D:45:LEU:HD13	1:D:49:ARG:HH11	0.54	1.62	9	1
1:D:27:LEU:HD12	1:D:28:GLU:O	0.54	2.03	5	12
1:A:24:ILE:CD1	1:A:45:LEU:HD22	0.54	2.33	15	2
1:C:23:HIS:CE1	1:C:45:LEU:CD2	0.54	2.91	3	1
1:A:67:LEU:HD12	1:A:67:LEU:O	0.54	2.02	15	1
1:D:64:ILE:O	1:D:68:LEU:HD12	0.54	2.03	4	8
1:A:55:LEU:N	1:A:55:LEU:CD1	0.54	2.71	8	1
1:A:41:LEU:CD2	1:A:55:LEU:HD23	0.54	2.26	9	1
1:A:67:LEU:HD13	1:B:31:LYS:HG3	0.54	1.78	14	1
1:B:41:LEU:HD13	1:B:55:LEU:HD23	0.53	1.79	1	1
1:B:27:LEU:HD12	1:B:28:GLU:O	0.53	2.03	6	9
1:B:39:ALA:CB	1:B:55:LEU:HD11	0.53	2.33	6	3
1:D:29:VAL:HG13	1:D:41:LEU:CD1	0.53	2.33	1	2
1:D:39:ALA:HB1	1:D:55:LEU:HD11	0.53	1.79	6	2
1:A:41:LEU:HD13	1:A:55:LEU:HD21	0.53	1.79	15	1
1:A:27:LEU:HD23	1:A:27:LEU:C	0.53	2.29	12	4
1:C:55:LEU:C	1:C:55:LEU:HD12	0.53	2.29	3	1
1:C:27:LEU:HD11	1:C:41:LEU:HD21	0.53	1.79	11	3
1:A:29:VAL:HG23	1:A:41:LEU:CD1	0.53	2.32	3	1
1:B:19:VAL:HG11	1:B:45:LEU:HD11	0.53	1.80	10	1
1:B:23:HIS:CD2	1:B:45:LEU:CD2	0.53	2.91	12	1
1:B:41:LEU:HD11	1:B:54:ASP:C	0.53	2.28	12	2
1:C:60:TYR:CE2	1:C:64:ILE:CD1	0.53	2.92	2	8
1:A:45:LEU:HD13	1:A:49:ARG:HE	0.53	1.64	8	1
1:A:53:LEU:HD12	1:A:63:ILE:HD11	0.53	1.79	8	2
1:B:29:VAL:HG13	1:B:41:LEU:CD1	0.53	2.34	5	1
1:B:42:ILE:HD12	1:D:11:GLN:HE22	0.53	1.64	7	1
1:D:19:VAL:HG12	1:D:53:LEU:HD21	0.53	1.81	15	1
1:A:23:HIS:CE1	1:A:45:LEU:CD2	0.53	2.91	3	1
1:C:24:ILE:HA	1:C:45:LEU:HD13	0.53	1.79	7	1
1:B:23:HIS:CD2	1:B:45:LEU:HD21	0.53	2.39	12	1
1:A:59:LEU:HD12	1:A:62:LYS:HD2	0.53	1.80	15	1
1:A:31:LYS:CD	1:B:67:LEU:HD13	0.52	2.34	4	2
1:B:53:LEU:HD12	1:B:63:ILE:HD11	0.52	1.80	1	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:60:TYR:CE2	1:D:64:ILE:CD1	0.52	2.92	4	4
1:A:60:TYR:CE2	1:A:64:ILE:CD1	0.52	2.92	1	3
1:C:41:LEU:HD21	1:C:54:ASP:HA	0.52	1.82	3	1
1:C:57:ALA:HB3	1:C:58:PRO:CD	0.52	2.29	3	1
1:A:57:ALA:CB	1:A:58:PRO:CD	0.52	2.82	3	2
1:C:27:LEU:HD21	1:C:29:VAL:CG2	0.52	2.35	11	3
1:C:27:LEU:HD11	1:C:29:VAL:HG23	0.52	1.82	7	2
1:B:27:LEU:HD21	1:B:29:VAL:HG23	0.52	1.80	3	1
1:A:27:LEU:HD11	1:A:29:VAL:HG23	0.52	1.80	9	2
1:A:29:VAL:HG22	1:A:41:LEU:HD12	0.52	1.80	12	1
1:A:67:LEU:HD23	1:B:31:LYS:HG3	0.52	1.81	8	3
1:A:42:ILE:HD12	1:C:11:GLN:HE22	0.52	1.62	5	2
1:D:53:LEU:HD22	1:D:59:LEU:HD23	0.52	1.82	14	1
1:B:30:ILE:HD11	1:B:40:GLN:NE2	0.52	2.20	15	1
1:D:12:CYS:HB2	1:D:42:ILE:HD11	0.51	1.82	1	2
1:D:15:THR:CG2	1:D:54:ASP:N	0.51	2.73	11	13
1:D:41:LEU:HD11	1:D:54:ASP:C	0.51	2.31	12	1
1:B:60:TYR:CE2	1:B:64:ILE:CD1	0.51	2.93	9	2
1:A:19:VAL:HG11	1:A:45:LEU:HD11	0.51	1.81	10	3
1:A:43:ALA:HB3	1:A:51:ILE:HG12	0.51	1.82	8	1
1:B:19:VAL:HG21	1:B:51:ILE:CB	0.51	2.35	4	1
1:D:24:ILE:HD12	1:D:45:LEU:CD2	0.51	2.30	11	1
1:C:19:VAL:HG12	1:C:53:LEU:HD21	0.51	1.82	15	3
1:B:30:ILE:CD1	1:B:40:GLN:NE2	0.51	2.74	15	1
1:D:23:HIS:CD2	1:D:46:LYS:HB2	0.51	2.41	11	1
1:D:64:ILE:O	1:D:68:LEU:CD2	0.51	2.58	12	1
1:D:10:CYS:HB2	1:D:13:VAL:HG12	0.51	1.83	14	1
1:B:55:LEU:HD23	1:B:60:TYR:CE2	0.51	2.41	15	2
1:A:30:ILE:HD13	1:A:40:GLN:NE2	0.51	2.20	7	1
1:D:55:LEU:CD1	1:D:60:TYR:CE2	0.51	2.93	3	2
1:A:27:LEU:HD11	1:A:29:VAL:CG2	0.51	2.36	5	4
1:D:23:HIS:CD2	1:D:46:LYS:CB	0.51	2.94	11	1
1:C:55:LEU:HD13	1:C:60:TYR:CZ	0.51	2.41	12	1
1:A:29:VAL:HG22	1:A:41:LEU:HD11	0.51	1.83	1	3
1:D:25:THR:HG23	1:D:26:SER:N	0.51	2.21	1	12
1:B:29:VAL:CG1	1:B:55:LEU:HD11	0.51	2.35	3	1
1:A:41:LEU:HD23	1:A:53:LEU:HB2	0.51	1.81	11	3
1:C:10:CYS:HB2	1:C:13:VAL:HG12	0.51	1.81	14	1
1:C:13:VAL:O	1:C:14:LYS:O	0.50	2.29	6	8
1:D:19:VAL:HG11	1:D:45:LEU:HD11	0.50	1.82	9	2
1:A:30:ILE:HD11	1:A:40:GLN:NE2	0.50	2.21	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:67:LEU:HD13	1:D:31:LYS:HD3	0.50	1.82	5	1
1:A:51:ILE:CG1	1:A:52:CYS:N	0.50	2.74	8	1
1:C:68:LEU:HD21	1:D:55:LEU:O	0.50	2.07	11	1
1:B:19:VAL:HG12	1:B:53:LEU:HD21	0.50	1.82	15	1
1:D:29:VAL:O	1:D:29:VAL:CG1	0.50	2.58	7	2
1:D:60:TYR:O	1:D:63:ILE:HG22	0.50	2.06	11	1
1:B:55:LEU:CD2	1:B:60:TYR:CE2	0.50	2.94	3	1
1:A:41:LEU:HD13	1:A:55:LEU:HD12	0.50	1.82	6	1
1:B:57:ALA:O	1:B:61:LYS:CG	0.50	2.60	3	1
1:B:25:THR:HG23	1:B:45:LEU:C	0.50	2.32	6	3
1:A:25:THR:HG23	1:A:45:LEU:C	0.50	2.32	10	5
1:A:29:VAL:O	1:A:29:VAL:CG1	0.50	2.59	3	1
1:B:43:ALA:HB3	1:B:51:ILE:HG12	0.50	1.82	7	1
1:D:55:LEU:HD12	1:D:60:TYR:CD2	0.50	2.42	9	1
1:D:25:THR:HG23	1:D:45:LEU:C	0.50	2.32	13	3
1:C:25:THR:HG23	1:C:26:SER:N	0.49	2.22	4	13
1:D:41:LEU:HD13	1:D:55:LEU:HD21	0.49	1.84	4	1
1:A:39:ALA:HB1	1:A:55:LEU:CD2	0.49	2.36	2	1
1:B:28:GLU:O	1:B:29:VAL:HG23	0.49	2.07	3	1
1:C:39:ALA:CB	1:C:55:LEU:HD22	0.49	2.34	11	1
1:C:12:CYS:HB3	1:C:42:ILE:HD11	0.49	1.84	1	1
1:B:41:LEU:HD21	1:B:54:ASP:HA	0.49	1.83	3	1
1:A:30:ILE:N	1:A:30:ILE:CD1	0.49	2.71	9	1
1:C:45:LEU:HD13	1:C:49:ARG:HE	0.49	1.67	13	1
1:D:51:ILE:HD12	1:D:51:ILE:C	0.49	2.32	5	15
1:C:67:LEU:CD1	1:D:31:LYS:CD	0.49	2.90	5	1
1:D:13:VAL:HG13	1:D:14:LYS:N	0.49	2.23	9	1
1:C:31:LYS:HG3	1:D:67:LEU:HD13	0.49	1.84	12	2
1:D:24:ILE:CD1	1:D:45:LEU:HD22	0.49	2.37	12	1
1:C:51:ILE:HD12	1:C:51:ILE:C	0.49	2.32	5	15
1:C:13:VAL:HG23	1:C:14:LYS:N	0.49	2.22	14	2
1:C:39:ALA:HB2	1:D:70:SER:O	0.49	2.06	10	1
1:A:35:HIS:CD2	1:A:35:HIS:C	0.49	2.91	4	1
1:A:10:CYS:SG	1:A:38:THR:HG22	0.49	2.47	12	5
1:B:25:THR:HG23	1:B:26:SER:N	0.49	2.23	1	12
1:A:13:VAL:HG13	1:A:14:LYS:N	0.49	2.23	4	3
1:D:30:ILE:CD1	1:D:40:GLN:NE2	0.49	2.75	7	2
1:B:51:ILE:CG1	1:B:52:CYS:N	0.49	2.74	7	1
1:C:29:VAL:HG22	1:C:41:LEU:HD11	0.49	1.84	14	3
1:D:13:VAL:HG23	1:D:14:LYS:N	0.49	2.23	14	1
1:A:25:THR:HG23	1:A:26:SER:N	0.49	2.23	9	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ILE:HD12	1:A:51:ILE:C	0.49	2.33	15	14
1:B:51:ILE:HD12	1:B:51:ILE:C	0.49	2.33	5	14
1:C:52:CYS:O	1:C:53:LEU:HD23	0.49	2.08	4	5
1:B:13:VAL:HG13	1:B:14:LYS:N	0.49	2.23	12	3
1:A:19:VAL:CG1	1:A:53:LEU:HD21	0.49	2.38	4	1
1:D:24:ILE:HD12	1:D:45:LEU:HD13	0.49	1.84	12	1
1:C:16:THR:HG22	1:C:16:THR:O	0.49	2.08	14	1
1:A:13:VAL:O	1:A:14:LYS:C	0.48	2.55	11	2
1:C:28:GLU:O	1:C:29:VAL:HG23	0.48	2.08	3	1
1:D:28:GLU:OE1	1:D:30:ILE:HD11	0.48	2.08	4	1
1:C:45:LEU:HD13	1:C:49:ARG:NH1	0.48	2.23	15	1
1:C:29:VAL:O	1:C:29:VAL:CG1	0.48	2.60	4	1
1:A:27:LEU:HD12	1:A:28:GLU:N	0.48	2.23	7	1
1:D:55:LEU:N	1:D:55:LEU:CD2	0.48	2.76	10	1
1:C:63:ILE:O	1:C:67:LEU:HD23	0.48	2.08	1	2
1:C:67:LEU:HD13	1:D:31:LYS:CD	0.48	2.38	5	2
1:A:29:VAL:CG1	1:B:67:LEU:CD2	0.48	2.91	11	2
1:B:15:THR:CG2	1:B:54:ASP:N	0.48	2.76	11	13
1:C:15:THR:CG2	1:C:54:ASP:N	0.48	2.76	4	11
1:C:67:LEU:HD13	1:D:31:LYS:HG3	0.48	1.84	14	2
1:A:10:CYS:O	1:A:13:VAL:HG13	0.48	2.08	14	1
1:C:31:LYS:CG	1:D:67:LEU:CD1	0.48	2.92	14	1
1:B:52:CYS:O	1:B:53:LEU:HD23	0.48	2.09	7	5
1:D:23:HIS:HB3	1:D:45:LEU:CD1	0.48	2.38	11	1
1:C:61:LYS:CD	1:C:61:LYS:C	0.48	2.87	3	1
1:B:24:ILE:HD11	1:B:45:LEU:HD22	0.48	1.86	3	1
1:A:67:LEU:HD23	1:B:31:LYS:HD2	0.48	1.84	9	1
1:C:39:ALA:CB	1:C:55:LEU:HD11	0.48	2.39	10	1
1:B:39:ALA:CB	1:B:55:LEU:CD1	0.48	2.91	12	2
1:B:23:HIS:CG	1:B:23:HIS:O	0.48	2.66	3	1
1:B:59:LEU:CD1	1:B:60:TYR:N	0.48	2.77	3	1
1:D:29:VAL:CB	1:D:41:LEU:HD12	0.48	2.39	3	2
1:A:60:TYR:OH	1:B:68:LEU:HD21	0.48	2.09	12	1
1:A:15:THR:CG2	1:A:54:ASP:N	0.48	2.77	7	13
1:C:25:THR:HG23	1:C:45:LEU:C	0.48	2.33	1	2
1:D:57:ALA:CB	1:D:58:PRO:CD	0.48	2.81	3	2
1:B:29:VAL:CG1	1:B:55:LEU:CD1	0.47	2.92	3	1
1:A:55:LEU:CD2	1:A:55:LEU:C	0.47	2.87	8	1
1:A:67:LEU:CD2	1:B:29:VAL:CG1	0.47	2.92	15	1
1:D:32:ALA:CB	1:D:37:PRO:O	0.47	2.61	5	14
1:D:53:LEU:HD12	1:D:63:ILE:CD1	0.47	2.39	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:67:LEU:CD1	1:D:31:LYS:CG	0.47	2.91	14	1
1:A:32:ALA:CB	1:A:37:PRO:O	0.47	2.62	5	14
1:A:35:HIS:N	1:A:35:HIS:CD2	0.47	2.83	10	4
1:A:23:HIS:CE1	1:A:45:LEU:HD22	0.47	2.44	3	1
1:A:53:LEU:CD1	1:A:63:ILE:CD1	0.47	2.92	15	2
1:C:60:TYR:CE2	1:C:64:ILE:HD12	0.47	2.45	3	1
1:A:9:ARG:O	1:A:35:HIS:CD2	0.47	2.67	4	1
1:C:43:ALA:O	1:C:50:LYS:HG2	0.47	2.09	4	1
1:D:64:ILE:HG22	1:D:68:LEU:CD2	0.47	2.39	12	1
1:B:9:ARG:CB	1:B:35:HIS:CB	0.47	2.92	15	1
1:A:15:THR:HG21	1:A:54:ASP:CB	0.47	2.38	8	10
1:B:42:ILE:CG2	1:B:43:ALA:N	0.47	2.77	10	15
1:A:13:VAL:HG12	1:A:14:LYS:N	0.47	2.24	5	3
1:C:29:VAL:CG1	1:D:67:LEU:HD13	0.47	2.39	6	1
1:B:55:LEU:CD1	1:B:55:LEU:N	0.47	2.78	9	1
1:C:27:LEU:HD23	1:C:63:ILE:HG21	0.47	1.86	8	1
1:A:13:VAL:HG23	1:A:14:LYS:N	0.47	2.23	14	1
1:B:32:ALA:CB	1:B:37:PRO:O	0.47	2.62	5	12
1:D:13:VAL:O	1:D:14:LYS:O	0.47	2.33	2	7
1:C:13:VAL:CG2	1:C:14:LYS:N	0.47	2.78	8	1
1:A:33:GLY:N	1:A:36:CYS:O	0.47	2.48	14	15
1:A:42:ILE:CG2	1:A:43:ALA:N	0.47	2.78	5	15
1:B:41:LEU:N	1:B:41:LEU:CD2	0.47	2.77	10	3
1:C:13:VAL:HG13	1:C:14:LYS:H	0.47	1.69	6	3
1:C:30:ILE:N	1:C:30:ILE:CD1	0.47	2.78	14	4
1:D:30:ILE:HD11	1:D:40:GLN:CD	0.47	2.34	7	1
1:D:55:LEU:CD1	1:D:60:TYR:CD2	0.47	2.98	9	1
1:C:30:ILE:CD1	1:C:40:GLN:NE2	0.47	2.78	11	1
1:C:42:ILE:CG2	1:C:43:ALA:N	0.47	2.77	1	15
1:B:13:VAL:HG12	1:B:14:LYS:N	0.47	2.24	5	3
1:A:30:ILE:HD11	1:A:40:GLN:HE21	0.47	1.70	10	1
1:A:24:ILE:HA	1:A:45:LEU:HD13	0.47	1.86	12	2
1:C:41:LEU:N	1:C:41:LEU:CD2	0.47	2.76	2	3
1:C:53:LEU:HD22	1:C:59:LEU:HD23	0.47	1.87	2	2
1:D:52:CYS:O	1:D:53:LEU:HD23	0.47	2.09	15	7
1:C:27:LEU:HD21	1:C:29:VAL:HG22	0.47	1.87	11	1
1:C:15:THR:HG21	1:C:54:ASP:CB	0.47	2.40	11	7
1:B:23:HIS:CE1	1:B:45:LEU:HD12	0.47	2.44	3	1
1:C:23:HIS:CG	1:C:23:HIS:O	0.47	2.67	3	2
1:A:27:LEU:HG	1:A:42:ILE:O	0.47	2.10	11	3
1:D:54:ASP:O	1:D:60:TYR:CZ	0.47	2.68	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:32:ALA:CB	1:C:37:PRO:O	0.46	2.63	11	14
1:A:27:LEU:C	1:A:27:LEU:HD23	0.46	2.35	6	2
1:D:33:GLY:N	1:D:36:CYS:O	0.46	2.48	4	15
1:D:13:VAL:HG12	1:D:14:LYS:N	0.46	2.24	5	3
1:B:30:ILE:CD1	1:B:31:LYS:O	0.46	2.63	10	3
1:C:30:ILE:CD1	1:C:40:GLN:CD	0.46	2.88	11	1
1:D:25:THR:CG2	1:D:26:SER:N	0.46	2.79	11	9
1:D:27:LEU:HD23	1:D:63:ILE:HG21	0.46	1.87	10	2
1:D:42:ILE:CG2	1:D:43:ALA:N	0.46	2.79	1	15
1:C:67:LEU:HD23	1:D:31:LYS:HD3	0.46	1.87	8	1
1:D:15:THR:HG21	1:D:54:ASP:CB	0.46	2.41	15	8
1:A:25:THR:CG2	1:A:46:LYS:HA	0.46	2.41	15	3
1:C:30:ILE:CD1	1:C:31:LYS:O	0.46	2.64	8	2
1:C:9:ARG:CB	1:C:35:HIS:HB2	0.46	2.41	6	1
1:D:13:VAL:O	1:D:14:LYS:C	0.46	2.58	8	2
1:D:41:LEU:HD13	1:D:55:LEU:HD11	0.46	1.87	10	1
1:C:27:LEU:C	1:C:27:LEU:HD23	0.46	2.35	11	1
1:B:29:VAL:HG22	1:B:41:LEU:CB	0.46	2.40	12	1
1:B:51:ILE:CD1	1:B:51:ILE:C	0.46	2.88	5	14
1:D:15:THR:HG21	1:D:54:ASP:HB3	0.46	1.86	1	6
1:D:51:ILE:CD1	1:D:51:ILE:C	0.46	2.89	5	15
1:C:35:HIS:CD2	1:C:35:HIS:N	0.46	2.84	14	1
1:A:52:CYS:O	1:A:53:LEU:HD23	0.46	2.10	4	4
1:B:53:LEU:CD1	1:B:63:ILE:CD1	0.46	2.94	11	3
1:B:55:LEU:HD23	1:B:60:TYR:CZ	0.46	2.46	15	2
1:B:13:VAL:O	1:B:14:LYS:O	0.46	2.33	6	6
1:A:30:ILE:HD13	1:A:40:GLN:HE21	0.46	1.70	7	1
1:A:67:LEU:CD1	1:B:31:LYS:CG	0.46	2.93	14	1
1:C:35:HIS:CG	1:C:36:CYS:N	0.46	2.84	15	1
1:B:33:GLY:N	1:B:36:CYS:O	0.46	2.49	4	15
1:C:33:GLY:N	1:C:36:CYS:O	0.46	2.49	2	15
1:C:27:LEU:CD1	1:C:29:VAL:HG23	0.46	2.41	7	2
1:C:39:ALA:HB1	1:C:55:LEU:HD13	0.46	1.87	4	1
1:A:42:ILE:HD12	1:C:11:GLN:OE1	0.46	2.10	7	1
1:B:39:ALA:HB3	1:B:55:LEU:CD2	0.46	2.39	12	2
1:A:51:ILE:CD1	1:A:51:ILE:C	0.46	2.89	10	14
1:C:51:ILE:CD1	1:C:51:ILE:C	0.46	2.89	10	15
1:B:57:ALA:O	1:B:61:LYS:HG3	0.46	2.11	3	1
1:C:27:LEU:HG	1:C:42:ILE:O	0.46	2.11	11	1
1:C:35:HIS:CE1	1:C:36:CYS:HB2	0.46	2.46	13	1
1:A:41:LEU:N	1:A:41:LEU:CD2	0.46	2.78	14	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:59:LEU:CD1	1:C:60:TYR:N	0.46	2.79	3	2
1:D:35:HIS:N	1:D:35:HIS:CD2	0.46	2.83	6	7
1:A:31:LYS:CG	1:B:67:LEU:HD13	0.46	2.41	6	1
1:C:19:VAL:CG1	1:C:45:LEU:HD11	0.46	2.40	9	1
1:A:13:VAL:HG22	1:A:14:LYS:N	0.46	2.26	11	1
1:B:23:HIS:CG	1:B:45:LEU:HD21	0.46	2.46	15	1
1:B:40:GLN:OE1	1:B:41:LEU:N	0.46	2.49	15	1
1:D:43:ALA:O	1:D:50:LYS:HG2	0.45	2.11	1	1
1:D:16:THR:O	1:D:16:THR:HG22	0.45	2.11	15	3
1:B:60:TYR:CD2	1:B:64:ILE:CD1	0.45	2.99	9	1
1:A:19:VAL:HG21	1:A:51:ILE:HB	0.45	1.87	15	1
1:B:24:ILE:CD1	1:B:44:THR:O	0.45	2.62	15	1
1:A:31:LYS:HD2	1:B:67:LEU:HD13	0.45	1.86	5	1
1:C:13:VAL:HG12	1:C:14:LYS:N	0.45	2.27	11	1
1:C:53:LEU:CD1	1:C:63:ILE:CD1	0.45	2.94	11	2
1:B:15:THR:HG21	1:B:54:ASP:CB	0.45	2.40	4	9
1:A:16:THR:HG22	1:A:16:THR:O	0.45	2.12	8	2
1:A:25:THR:CG2	1:A:26:SER:N	0.45	2.80	12	6
1:D:30:ILE:CD1	1:D:31:LYS:O	0.45	2.65	3	3
1:D:39:ALA:CB	1:D:55:LEU:HD22	0.45	2.36	11	1
1:D:60:TYR:CD1	1:D:60:TYR:N	0.45	2.85	11	1
1:D:64:ILE:C	1:D:68:LEU:HD23	0.45	2.36	12	1
1:B:53:LEU:HD22	1:B:59:LEU:HD23	0.45	1.89	14	1
1:B:25:THR:CG2	1:B:26:SER:N	0.45	2.79	7	7
1:D:10:CYS:SG	1:D:38:THR:CG2	0.45	3.05	10	8
1:A:13:VAL:O	1:A:14:LYS:O	0.45	2.35	7	6
1:B:13:VAL:CG2	1:B:14:LYS:N	0.45	2.79	11	1
1:D:54:ASP:O	1:D:60:TYR:CE1	0.45	2.69	11	1
1:D:25:THR:CG2	1:D:45:LEU:O	0.45	2.65	11	7
1:D:23:HIS:O	1:D:46:LYS:CG	0.45	2.64	4	5
1:D:39:ALA:HB1	1:D:55:LEU:CD2	0.45	2.38	1	1
1:D:41:LEU:HD22	1:D:53:LEU:HB2	0.45	1.88	5	1
1:D:27:LEU:HG	1:D:42:ILE:O	0.45	2.12	11	2
1:C:67:LEU:HD23	1:D:31:LYS:CD	0.45	2.42	8	1
1:D:27:LEU:C	1:D:27:LEU:CD2	0.45	2.90	8	1
1:B:10:CYS:HB3	1:B:13:VAL:HG22	0.45	1.88	9	1
1:C:23:HIS:O	1:C:46:LYS:CG	0.45	2.64	11	8
1:B:42:ILE:HD12	1:D:11:GLN:NE2	0.45	2.26	7	1
1:A:30:ILE:HD12	1:A:40:GLN:HB3	0.45	1.89	12	1
1:D:66:LYS:HA	1:D:69:GLU:HG3	0.45	1.89	1	2
1:A:29:VAL:CG2	1:A:41:LEU:HD12	0.45	2.38	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:27:LEU:C	1:B:27:LEU:CD2	0.45	2.89	7	4
1:C:53:LEU:HD12	1:C:63:ILE:HD11	0.45	1.89	3	2
1:B:23:HIS:O	1:B:46:LYS:CG	0.45	2.64	11	3
1:A:40:GLN:OE1	1:A:41:LEU:N	0.45	2.50	10	1
1:D:41:LEU:CB	1:D:55:LEU:HD21	0.45	2.42	10	1
1:D:65:LYS:O	1:D:69:GLU:HG3	0.45	2.12	6	3
1:B:43:ALA:O	1:B:50:LYS:HG2	0.45	2.11	2	2
1:A:55:LEU:C	1:A:55:LEU:HD22	0.45	2.37	8	1
1:C:39:ALA:CB	1:C:55:LEU:CD1	0.45	2.95	10	1
1:A:23:HIS:CD2	1:A:45:LEU:CD2	0.45	3.00	1	1
1:C:57:ALA:CB	1:C:58:PRO:CD	0.45	2.94	3	3
1:C:17:SER:OG	1:C:59:LEU:HD23	0.44	2.11	4	1
1:D:29:VAL:CA	1:D:41:LEU:HD12	0.44	2.34	1	3
1:D:17:SER:OG	1:D:59:LEU:HD23	0.44	2.12	2	1
1:A:23:HIS:O	1:A:23:HIS:CG	0.44	2.70	3	1
1:B:35:HIS:CD2	1:B:35:HIS:N	0.44	2.85	4	1
1:D:13:VAL:HG12	1:D:14:LYS:H	0.44	1.72	8	2
1:C:53:LEU:HD12	1:C:63:ILE:CD1	0.44	2.42	3	2
1:C:25:THR:CG2	1:C:45:LEU:O	0.44	2.65	7	6
1:C:55:LEU:C	1:C:55:LEU:CD2	0.44	2.88	7	1
1:A:30:ILE:HG22	1:B:26:SER:CB	0.44	2.41	10	1
1:B:27:LEU:CD1	1:B:29:VAL:HG23	0.44	2.43	12	1
1:A:24:ILE:HD12	1:A:45:LEU:CD1	0.44	2.43	15	1
1:C:25:THR:CG2	1:C:26:SER:N	0.44	2.80	11	9
1:C:65:LYS:CG	1:C:66:LYS:N	0.44	2.81	7	1
1:B:61:LYS:O	1:B:65:LYS:HB3	0.44	2.12	3	1
1:D:15:THR:CG2	1:D:54:ASP:CG	0.44	2.91	3	1
1:A:23:HIS:O	1:A:46:LYS:CG	0.44	2.66	6	3
1:A:19:VAL:HG11	1:A:51:ILE:HG12	0.44	1.90	15	1
1:A:25:THR:CG2	1:A:45:LEU:O	0.44	2.66	12	6
1:B:27:LEU:HA	1:B:43:ALA:HA	0.44	1.88	2	1
1:B:29:VAL:HG13	1:B:41:LEU:HD12	0.44	1.88	5	1
1:B:35:HIS:CD2	1:B:35:HIS:C	0.44	2.96	12	1
1:B:9:ARG:CB	1:B:35:HIS:HB2	0.44	2.43	15	1
1:B:45:LEU:HD23	1:B:46:LYS:H	0.44	1.73	15	1
1:B:25:THR:CG2	1:B:45:LEU:O	0.44	2.66	12	6
1:C:35:HIS:N	1:C:35:HIS:CD2	0.44	2.85	7	2
1:C:13:VAL:O	1:C:14:LYS:C	0.44	2.59	5	2
1:D:27:LEU:CD1	1:D:27:LEU:C	0.44	2.91	7	4
1:B:27:LEU:HD23	1:B:63:ILE:HG21	0.44	1.90	8	1
1:A:27:LEU:HD21	1:A:29:VAL:HG23	0.44	1.88	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ILE:N	1:A:30:ILE:HD12	0.44	2.28	11	1
1:B:55:LEU:CD1	1:B:60:TYR:CE2	0.44	3.01	1	1
1:C:27:LEU:C	1:C:27:LEU:CD2	0.44	2.90	3	4
1:D:60:TYR:CE2	1:D:64:ILE:HD11	0.44	2.48	15	3
1:D:27:LEU:HD12	1:D:28:GLU:N	0.44	2.28	15	2
1:C:27:LEU:HD23	1:C:27:LEU:O	0.44	2.13	11	1
1:B:66:LYS:O	1:B:69:GLU:CG	0.43	2.66	2	10
1:C:15:THR:CG2	1:C:54:ASP:CG	0.43	2.91	1	1
1:D:66:LYS:O	1:D:69:GLU:CG	0.43	2.66	2	9
1:A:66:LYS:O	1:A:69:GLU:CG	0.43	2.66	5	7
1:C:30:ILE:O	1:C:40:GLN:O	0.43	2.35	7	3
1:B:29:VAL:HG22	1:B:41:LEU:HD12	0.43	1.90	7	1
1:C:69:GLU:OE1	1:C:69:GLU:N	0.43	2.51	7	1
1:A:9:ARG:CB	1:A:35:HIS:HB2	0.43	2.43	15	2
1:B:24:ILE:HD12	1:B:45:LEU:CD1	0.43	2.42	3	2
1:B:39:ALA:HB1	1:B:55:LEU:HD11	0.43	1.90	6	1
1:A:27:LEU:CD1	1:A:29:VAL:HG23	0.43	2.43	14	2
1:C:28:GLU:C	1:C:29:VAL:HG23	0.43	2.38	11	1
1:A:65:LYS:O	1:A:69:GLU:HG2	0.43	2.13	2	1
1:C:65:LYS:O	1:C:69:GLU:HG2	0.43	2.13	7	1
1:A:35:HIS:CG	1:A:36:CYS:N	0.43	2.87	9	1
1:A:55:LEU:C	1:A:55:LEU:CD1	0.43	2.92	9	1
1:A:28:GLU:O	1:A:29:VAL:CG2	0.43	2.66	10	1
1:A:30:ILE:HG22	1:B:26:SER:OG	0.43	2.13	10	1
1:A:24:ILE:HD12	1:A:45:LEU:HD22	0.43	1.89	15	1
1:B:66:LYS:HA	1:B:69:GLU:HG3	0.43	1.90	15	1
1:C:66:LYS:O	1:C:69:GLU:CG	0.43	2.67	10	9
1:D:65:LYS:O	1:D:69:GLU:CG	0.43	2.66	1	3
1:D:30:ILE:CD1	1:D:40:GLN:HB3	0.43	2.44	2	2
1:A:27:LEU:C	1:A:27:LEU:CD2	0.43	2.92	10	2
1:A:28:GLU:O	1:A:29:VAL:HG23	0.43	2.13	10	1
1:D:23:HIS:C	1:D:45:LEU:CD1	0.43	2.92	11	1
1:B:25:THR:C	1:B:26:SER:HG	0.43	2.20	12	1
1:C:27:LEU:CD1	1:C:29:VAL:CG2	0.43	2.96	13	1
1:D:17:SER:HB2	1:D:59:LEU:HD22	0.43	1.88	14	1
1:D:56:GLN:N	1:D:60:TYR:CE1	0.43	2.86	3	1
1:C:9:ARG:CB	1:C:35:HIS:CB	0.43	2.96	6	1
1:A:27:LEU:C	1:A:27:LEU:CD1	0.43	2.91	9	5
1:C:30:ILE:CG1	1:D:26:SER:OG	0.43	2.67	1	3
1:D:65:LYS:HA	1:D:68:LEU:HD12	0.43	1.89	1	2
1:A:30:ILE:CD1	1:A:31:LYS:O	0.43	2.67	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:SER:OG	1:B:30:ILE:CG2	0.43	2.66	7	3
1:B:55:LEU:HG	1:B:60:TYR:CE2	0.43	2.49	3	1
1:B:27:LEU:CD1	1:B:27:LEU:C	0.43	2.91	8	3
1:C:12:CYS:HB2	1:C:42:ILE:HD11	0.43	1.90	6	1
1:B:27:LEU:HG	1:B:42:ILE:O	0.43	2.14	11	2
1:D:60:TYR:O	1:D:64:ILE:HD12	0.43	2.14	11	1
1:A:60:TYR:CD2	1:A:64:ILE:CD1	0.43	3.02	1	1
1:C:15:THR:CG2	1:C:53:LEU:C	0.43	2.92	1	2
1:A:59:LEU:O	1:A:62:LYS:CG	0.43	2.66	2	1
1:A:11:GLN:CG	1:A:12:CYS:N	0.43	2.81	6	1
1:C:11:GLN:N	1:C:40:GLN:OE1	0.43	2.52	7	2
1:C:47:ASN:O	1:C:49:ARG:HG3	0.43	2.13	6	2
1:C:30:ILE:C	1:C:30:ILE:CD1	0.43	2.92	8	1
1:D:30:ILE:N	1:D:30:ILE:CD1	0.43	2.78	14	1
1:C:11:GLN:CB	1:C:40:GLN:OE1	0.43	2.67	1	1
1:D:60:TYR:HA	1:D:63:ILE:HD12	0.43	1.91	1	2
1:B:21:PRO:O	1:B:22:ARG:CG	0.43	2.67	8	3
1:C:64:ILE:HG22	1:C:68:LEU:HD11	0.43	1.90	4	1
1:C:27:LEU:CD1	1:C:28:GLU:O	0.43	2.67	6	1
1:C:19:VAL:HG21	1:C:51:ILE:HG12	0.43	1.90	9	1
1:D:35:HIS:CG	1:D:36:CYS:N	0.43	2.87	9	1
1:D:41:LEU:N	1:D:41:LEU:CD2	0.43	2.76	12	1
1:B:57:ALA:CB	1:B:58:PRO:CD	0.43	2.95	1	1
1:C:49:ARG:C	1:C:50:LYS:CE	0.43	2.91	1	1
1:B:10:CYS:SG	1:B:38:THR:CG2	0.43	3.07	4	4
1:C:27:LEU:C	1:C:27:LEU:CD1	0.43	2.92	2	4
1:B:65:LYS:CD	1:B:65:LYS:C	0.43	2.92	4	1
1:C:30:ILE:HA	1:D:26:SER:HG	0.43	1.74	5	1
1:D:21:PRO:O	1:D:22:ARG:CG	0.43	2.67	5	1
1:B:30:ILE:CD1	1:B:40:GLN:HB3	0.43	2.44	6	1
1:C:27:LEU:CD1	1:C:27:LEU:C	0.43	2.92	9	2
1:A:26:SER:HB3	1:B:30:ILE:HG22	0.43	1.91	10	1
1:A:27:LEU:HG	1:A:28:GLU:N	0.43	2.28	11	1
1:A:49:ARG:C	1:A:50:LYS:CD	0.43	2.92	14	1
1:B:28:GLU:C	1:B:29:VAL:CG2	0.43	2.91	15	1
1:A:32:ALA:CA	1:A:36:CYS:O	0.42	2.67	1	1
1:A:43:ALA:O	1:A:50:LYS:CG	0.42	2.67	5	3
1:C:10:CYS:SG	1:C:38:THR:CG2	0.42	3.07	7	5
1:C:27:LEU:HA	1:C:43:ALA:HA	0.42	1.90	4	1
1:D:47:ASN:O	1:D:49:ARG:HG3	0.42	2.13	5	1
1:C:60:TYR:CE2	1:C:64:ILE:HD11	0.42	2.48	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:23:HIS:ND1	1:D:45:LEU:HD12	0.42	2.28	6	1
1:A:67:LEU:HD23	1:B:31:LYS:CG	0.42	2.44	10	1
1:A:10:CYS:SG	1:A:38:THR:CG2	0.42	3.07	1	3
1:C:41:LEU:HD23	1:C:41:LEU:H	0.42	1.74	1	1
1:D:27:LEU:C	1:D:27:LEU:CD1	0.42	2.91	10	3
1:D:40:GLN:OE1	1:D:41:LEU:N	0.42	2.52	5	1
1:B:15:THR:CG2	1:B:54:ASP:CG	0.42	2.92	9	1
1:D:19:VAL:HG12	1:D:20:ARG:N	0.42	2.29	9	1
1:C:40:GLN:OE1	1:C:40:GLN:C	0.42	2.62	11	1
1:A:27:LEU:HD21	1:A:41:LEU:HD11	0.42	1.91	15	1
1:B:65:LYS:O	1:B:69:GLU:HG3	0.42	2.14	15	1
1:A:15:THR:CG2	1:A:53:LEU:C	0.42	2.92	3	1
1:A:26:SER:OG	1:B:30:ILE:CG1	0.42	2.68	3	2
1:A:27:LEU:CD1	1:A:27:LEU:C	0.42	2.92	8	3
1:A:21:PRO:O	1:A:22:ARG:CG	0.42	2.67	7	2
1:C:30:ILE:HD12	1:C:30:ILE:O	0.42	2.15	8	1
1:D:46:LYS:HG3	1:D:47:ASN:N	0.42	2.29	8	2
1:C:21:PRO:O	1:C:22:ARG:CG	0.42	2.67	9	1
1:D:63:ILE:O	1:D:67:LEU:CD1	0.42	2.68	11	1
1:C:25:THR:C	1:C:26:SER:HG	0.42	2.20	12	1
1:A:65:LYS:CG	1:A:66:LYS:N	0.42	2.82	15	1
1:A:47:ASN:O	1:A:48:GLY:C	0.42	2.62	15	8
1:D:32:ALA:CA	1:D:36:CYS:O	0.42	2.68	1	1
1:D:47:ASN:O	1:D:48:GLY:C	0.42	2.63	15	12
1:A:49:ARG:O	1:A:50:LYS:CD	0.42	2.68	2	1
1:B:17:SER:CB	1:B:59:LEU:CD2	0.42	2.97	4	1
1:C:13:VAL:HG22	1:C:14:LYS:H	0.42	1.74	6	2
1:D:9:ARG:HB3	1:D:35:HIS:CB	0.42	2.45	15	2
1:C:55:LEU:HD21	1:D:64:ILE:HG23	0.42	1.89	2	1
1:D:27:LEU:HG	1:D:28:GLU:N	0.42	2.30	11	2
1:B:27:LEU:HG	1:B:28:GLU:N	0.42	2.30	11	1
1:D:55:LEU:N	1:D:60:TYR:OH	0.42	2.53	11	1
1:D:56:GLN:N	1:D:60:TYR:OH	0.42	2.52	11	1
1:A:61:LYS:O	1:A:65:LYS:CG	0.42	2.68	12	1
1:B:9:ARG:O	1:B:35:HIS:CD2	0.42	2.72	12	1
1:A:23:HIS:CD2	1:A:23:HIS:N	0.42	2.86	13	1
1:B:63:ILE:O	1:B:67:LEU:CD2	0.42	2.66	15	1
1:C:25:THR:CG2	1:C:46:LYS:HA	0.42	2.44	1	1
1:A:27:LEU:CD1	1:A:28:GLU:O	0.42	2.68	7	1
1:B:17:SER:HB3	1:B:59:LEU:HD22	0.42	1.91	14	2
1:C:49:ARG:C	1:C:50:LYS:CD	0.42	2.92	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ILE:CB	1:B:26:SER:OG	0.42	2.68	10	1
1:B:47:ASN:O	1:B:48:GLY:C	0.42	2.63	1	14
1:C:47:ASN:O	1:C:48:GLY:C	0.42	2.63	4	12
1:D:42:ILE:HG23	1:D:50:LYS:HD3	0.42	1.90	1	1
1:A:11:GLN:NE2	1:C:11:GLN:O	0.42	2.53	2	1
1:C:57:ALA:O	1:C:61:LYS:CG	0.42	2.68	3	1
1:C:27:LEU:HD12	1:C:28:GLU:N	0.42	2.30	6	5
1:C:23:HIS:NE2	1:C:45:LEU:HD12	0.42	2.29	7	1
1:C:46:LYS:HG3	1:C:47:ASN:N	0.42	2.30	10	3
1:D:46:LYS:CG	1:D:47:ASN:N	0.42	2.82	9	1
1:A:27:LEU:HD21	1:A:29:VAL:CG2	0.42	2.45	11	2
1:C:27:LEU:HG	1:C:28:GLU:N	0.42	2.29	11	1
1:D:65:LYS:HA	1:D:68:LEU:HD23	0.42	1.92	12	1
1:D:23:HIS:CD2	1:D:23:HIS:N	0.42	2.86	3	2
1:C:42:ILE:HG23	1:C:50:LYS:HD3	0.42	1.91	4	1
1:B:27:LEU:HD13	1:B:41:LEU:HD21	0.42	1.91	14	1
1:B:32:ALA:CA	1:B:36:CYS:O	0.42	2.68	1	1
1:A:49:ARG:O	1:A:50:LYS:CG	0.42	2.68	2	1
1:B:24:ILE:CD1	1:B:45:LEU:CD2	0.42	2.98	3	1
1:D:53:LEU:CD1	1:D:63:ILE:CD1	0.42	2.98	3	1
1:A:23:HIS:O	1:A:46:LYS:N	0.42	2.53	4	1
1:A:30:ILE:CG1	1:B:26:SER:OG	0.42	2.67	4	1
1:C:55:LEU:HA	1:C:60:TYR:CE1	0.42	2.49	6	1
1:B:17:SER:OG	1:B:59:LEU:HD22	0.42	2.15	13	2
1:B:56:GLN:CG	1:B:56:GLN:O	0.42	2.67	1	1
1:D:45:LEU:HD23	1:D:46:LYS:H	0.42	1.75	1	1
1:C:53:LEU:HD22	1:C:59:LEU:CD2	0.42	2.44	2	1
1:A:31:LYS:HG3	1:B:67:LEU:HD13	0.42	1.90	6	1
1:D:16:THR:O	1:D:16:THR:OG1	0.42	2.37	7	1
1:B:62:LYS:O	1:B:66:LYS:CB	0.42	2.68	11	1
1:C:28:GLU:C	1:C:29:VAL:CG2	0.42	2.93	11	1
1:D:9:ARG:CB	1:D:35:HIS:HB3	0.42	2.45	15	1
1:B:9:ARG:NH2	1:D:18:GLN:OE1	0.41	2.53	5	1
1:A:30:ILE:O	1:A:40:GLN:O	0.41	2.38	8	2
1:A:60:TYR:CE2	1:A:64:ILE:HD11	0.41	2.50	7	1
1:C:47:ASN:OD1	1:C:47:ASN:N	0.41	2.53	7	1
1:A:47:ASN:O	1:A:49:ARG:HG3	0.41	2.15	11	1
1:B:25:THR:CG2	1:B:46:LYS:HA	0.41	2.45	14	1
1:D:27:LEU:HA	1:D:43:ALA:HA	0.41	1.91	1	1
1:B:59:LEU:O	1:B:62:LYS:CG	0.41	2.67	2	1
1:C:55:LEU:O	1:C:55:LEU:CD1	0.41	2.68	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:SER:CB	1:A:59:LEU:CD2	0.41	2.98	4	1
1:C:46:LYS:CE	1:C:47:ASN:OD1	0.41	2.68	6	1
1:C:24:ILE:HD12	1:C:45:LEU:HD13	0.41	1.90	7	1
1:A:43:ALA:HB3	1:A:51:ILE:CG1	0.41	2.45	8	1
1:D:59:LEU:HD12	1:D:62:LYS:HE3	0.41	1.90	11	1
1:B:11:GLN:CB	1:D:11:GLN:OE1	0.41	2.68	14	1
1:A:27:LEU:HD23	1:A:63:ILE:HG21	0.41	1.93	8	2
1:B:27:LEU:C	1:B:27:LEU:CD1	0.41	2.93	12	2
1:A:16:THR:OG1	1:A:16:THR:O	0.41	2.37	3	1
1:A:55:LEU:HA	1:A:60:TYR:CD1	0.41	2.51	3	1
1:C:67:LEU:HD23	1:D:31:LYS:HG3	0.41	1.90	9	1
1:A:16:THR:O	1:A:16:THR:HG22	0.41	2.15	14	1
1:B:55:LEU:HD13	1:B:60:TYR:CE2	0.41	2.50	1	1
1:C:55:LEU:C	1:C:55:LEU:CD1	0.41	2.93	3	1
1:D:25:THR:CG2	1:D:46:LYS:HA	0.41	2.46	5	3
1:D:30:ILE:O	1:D:40:GLN:O	0.41	2.39	8	1
1:B:60:TYR:CE2	1:B:64:ILE:HD11	0.41	2.49	9	1
1:A:12:CYS:O	1:A:12:CYS:SG	0.41	2.78	11	1
1:C:39:ALA:O	1:C:55:LEU:CD2	0.41	2.69	11	1
1:B:23:HIS:CD2	1:B:23:HIS:N	0.41	2.88	4	1
1:C:23:HIS:O	1:C:46:LYS:N	0.41	2.52	4	1
1:B:43:ALA:HB3	1:B:51:ILE:CG1	0.41	2.45	7	1
1:A:30:ILE:CD1	1:A:40:GLN:HB3	0.41	2.44	12	1
1:B:17:SER:OG	1:B:59:LEU:CD2	0.41	2.68	13	1
1:D:49:ARG:O	1:D:50:LYS:CG	0.41	2.68	2	1
1:D:55:LEU:HA	1:D:60:TYR:CE1	0.41	2.51	3	3
1:C:27:LEU:O	1:D:29:VAL:HG12	0.41	2.16	7	1
1:B:59:LEU:C	1:B:59:LEU:CD1	0.41	2.90	9	1
1:C:62:LYS:O	1:C:66:LYS:CG	0.41	2.69	11	1
1:D:27:LEU:HD21	1:D:29:VAL:CG2	0.41	2.46	11	1
1:B:23:HIS:ND1	1:B:45:LEU:CD2	0.41	2.84	15	1
1:A:66:LYS:HA	1:A:69:GLU:HG2	0.41	1.93	2	1
1:D:49:ARG:O	1:D:50:LYS:CD	0.41	2.68	2	1
1:D:55:LEU:HA	1:D:60:TYR:CD1	0.41	2.50	3	1
1:D:55:LEU:CD1	1:D:60:TYR:CZ	0.41	3.02	4	1
1:B:16:THR:O	1:B:16:THR:HG22	0.41	2.15	7	1
1:A:39:ALA:HB1	1:A:55:LEU:HD13	0.41	1.92	11	1
1:D:23:HIS:C	1:D:45:LEU:HD13	0.41	2.41	11	1
1:D:61:LYS:O	1:D:65:LYS:CG	0.41	2.69	1	1
1:A:30:ILE:CD1	1:A:40:GLN:NE2	0.41	2.83	10	1
1:C:24:ILE:HG12	1:C:44:THR:O	0.41	2.15	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:23:HIS:CD2	1:D:23:HIS:H	0.41	2.34	1	1
1:C:12:CYS:O	1:C:13:VAL:O	0.41	2.38	6	2
1:C:57:ALA:O	1:C:61:LYS:HG2	0.41	2.16	3	1
1:D:15:THR:HG21	1:D:54:ASP:CG	0.41	2.40	3	1
1:C:30:ILE:CD1	1:C:40:GLN:HB3	0.41	2.45	4	1
1:C:36:CYS:SG	1:C:38:THR:CG2	0.41	3.09	4	2
1:C:61:LYS:O	1:C:65:LYS:HB3	0.41	2.16	5	1
1:B:9:ARG:N	1:B:35:HIS:HB2	0.41	2.31	14	2
1:B:30:ILE:O	1:B:40:GLN:O	0.41	2.39	8	1
1:B:60:TYR:CD2	1:B:64:ILE:HD11	0.41	2.51	9	1
1:A:23:HIS:O	1:A:46:LYS:HG2	0.41	2.15	11	1
1:B:35:HIS:CD2	1:B:36:CYS:HB2	0.41	2.51	12	1
1:A:17:SER:HB3	1:A:59:LEU:HD22	0.41	1.92	14	1
1:B:11:GLN:CB	1:D:11:GLN:CD	0.41	2.94	14	1
1:B:65:LYS:O	1:B:69:GLU:CG	0.41	2.68	15	1
1:D:56:GLN:O	1:D:56:GLN:CG	0.41	2.69	15	1
1:C:59:LEU:C	1:C:59:LEU:CD1	0.41	2.90	3	1
1:D:28:GLU:HG3	1:D:42:ILE:HB	0.41	1.93	3	1
1:A:30:ILE:CG1	1:B:26:SER:HB3	0.41	2.46	5	1
1:B:27:LEU:HD21	1:B:29:VAL:CG2	0.40	2.46	3	2
1:D:36:CYS:SG	1:D:38:THR:CG2	0.40	3.09	3	1
1:B:12:CYS:HB2	1:B:42:ILE:HD11	0.40	1.93	5	1
1:B:23:HIS:CD2	1:B:45:LEU:CD1	0.40	2.93	7	1
1:B:27:LEU:HD12	1:B:28:GLU:N	0.40	2.30	8	1
1:C:56:GLN:O	1:C:56:GLN:CG	0.40	2.69	9	1
1:D:27:LEU:CD1	1:D:29:VAL:HG23	0.40	2.47	12	1
1:D:9:ARG:CB	1:D:35:HIS:CB	0.40	2.99	15	1
1:A:69:GLU:OE1	1:A:69:GLU:HA	0.40	2.16	2	1
1:D:24:ILE:CD1	1:D:44:THR:O	0.40	2.62	3	1
1:C:66:LYS:HA	1:C:69:GLU:HG2	0.40	1.92	7	1
1:B:30:ILE:HD12	1:B:30:ILE:O	0.40	2.16	10	1
1:C:31:LYS:HG2	1:D:67:LEU:HD13	0.40	1.91	14	1
1:D:27:LEU:HB2	1:D:43:ALA:HA	0.40	1.92	1	1
1:A:35:HIS:CD2	1:A:36:CYS:HB2	0.40	2.51	5	2
1:D:41:LEU:HD23	1:D:53:LEU:H	0.40	1.77	5	1
1:B:13:VAL:HG13	1:B:14:LYS:H	0.40	1.74	11	1
1:D:29:VAL:HG22	1:D:41:LEU:CB	0.40	2.46	12	1
1:C:23:HIS:CD2	1:C:23:HIS:N	0.40	2.87	13	1
1:C:15:THR:CG2	1:C:54:ASP:HB3	0.40	2.47	2	1
1:C:30:ILE:N	1:C:30:ILE:HD12	0.40	2.31	2	1
1:A:55:LEU:HA	1:A:60:TYR:CE1	0.40	2.50	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:27:LEU:HB2	1:C:43:ALA:HA	0.40	1.92	4	1
1:D:63:ILE:O	1:D:67:LEU:HD23	0.40	2.17	8	1
1:B:28:GLU:HG3	1:B:42:ILE:HB	0.40	1.94	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	61/68 (90%)	49±2 (80±4%)	7±3 (11±5%)	6±1 (9±2%)	1	11
1	B	61/68 (90%)	49±2 (80±4%)	7±2 (11±3%)	6±1 (9±2%)	1	11
1	C	61/68 (90%)	48±2 (79±4%)	7±3 (11±4%)	6±1 (10±2%)	1	10
1	D	61/68 (90%)	49±2 (80±3%)	7±2 (11±3%)	5±1 (9±2%)	1	11
All	All	3660/4080 (90%)	2920 (80%)	404 (11%)	336 (9%)	1	11

All 37 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	34	PRO	15
1	A	48	GLY	15
1	B	34	PRO	15
1	B	48	GLY	15
1	C	34	PRO	15
1	C	48	GLY	15
1	C	51	ILE	15
1	D	34	PRO	15
1	D	48	GLY	15
1	D	51	ILE	15
1	A	22	ARG	13
1	A	51	ILE	13
1	B	22	ARG	13
1	B	51	ILE	13
1	C	22	ARG	13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	D	22	ARG	13
1	C	9	ARG	11
1	A	14	LYS	9
1	C	14	LYS	9
1	D	14	LYS	9
1	A	9	ARG	9
1	B	9	ARG	8
1	B	14	LYS	8
1	B	13	VAL	7
1	D	9	ARG	6
1	D	13	VAL	6
1	C	13	VAL	5
1	A	13	VAL	5
1	A	24	ILE	4
1	C	24	ILE	3
1	B	24	ILE	2
1	D	24	ILE	2
1	B	57	ALA	1
1	B	58	PRO	1
1	C	57	ALA	1
1	A	29	VAL	1
1	C	29	VAL	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	55/61 (90%)	36±2 (66±4%)	19±2 (34±4%)	1	11
1	B	55/61 (90%)	36±2 (65±3%)	19±2 (35±3%)	1	10
1	C	55/61 (90%)	35±2 (64±4%)	20±2 (36±4%)	1	9
1	D	56/61 (92%)	36±2 (65±4%)	20±2 (35±4%)	1	9
All	All	3315/3660 (91%)	2154 (65%)	1161 (35%)	1	10

All 147 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	15	THR	15
1	A	27	LEU	15
1	A	44	THR	15
1	A	51	ILE	15
1	B	15	THR	15
1	B	27	LEU	15
1	B	44	THR	15
1	B	51	ILE	15
1	C	15	THR	15
1	C	27	LEU	15
1	C	44	THR	15
1	C	51	ILE	15
1	D	15	THR	15
1	D	27	LEU	15
1	D	40	GLN	15
1	D	44	THR	15
1	D	51	ILE	15
1	A	50	LYS	14
1	B	50	LYS	14
1	B	69	GLU	14
1	C	41	LEU	14
1	C	45	LEU	14
1	A	41	LEU	13
1	A	46	LYS	13
1	A	66	LYS	13
1	B	31	LYS	13
1	B	41	LEU	13
1	C	46	LYS	13
1	C	50	LYS	13
1	D	50	LYS	13
1	D	55	LEU	13
1	D	31	LYS	13
1	A	40	GLN	12
1	B	40	GLN	12
1	B	55	LEU	12
1	C	40	GLN	12
1	D	45	LEU	12
1	A	62	LYS	12
1	C	22	ARG	12
1	A	23	HIS	11
1	B	45	LEU	11
1	C	69	GLU	11
1	D	66	LYS	11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	68	LEU	11
1	D	69	GLU	11
1	A	9	ARG	10
1	A	31	LYS	10
1	A	45	LEU	10
1	B	46	LYS	10
1	D	22	ARG	10
1	D	46	LYS	10
1	B	22	ARG	10
1	D	41	LEU	10
1	D	23	HIS	10
1	B	23	HIS	9
1	C	23	HIS	9
1	C	52	CYS	9
1	C	61	LYS	9
1	C	62	LYS	9
1	C	66	LYS	9
1	D	14	LYS	9
1	D	52	CYS	9
1	A	61	LYS	9
1	B	9	ARG	9
1	B	66	LYS	9
1	C	55	LEU	9
1	C	65	LYS	9
1	A	22	ARG	9
1	C	31	LYS	9
1	A	52	CYS	8
1	B	62	LYS	8
1	D	20	ARG	8
1	D	70	SER	8
1	B	61	LYS	8
1	B	14	LYS	7
1	B	20	ARG	7
1	B	52	CYS	7
1	C	14	LYS	7
1	C	68	LEU	7
1	B	68	LEU	7
1	D	9	ARG	7
1	A	14	LYS	7
1	C	9	ARG	7
1	A	69	GLU	7
1	C	16	THR	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	C	18	GLN	6
1	D	16	THR	6
1	D	12	CYS	6
1	D	30	ILE	6
1	A	12	CYS	6
1	A	65	LYS	6
1	D	62	LYS	6
1	C	54	ASP	6
1	D	54	ASP	6
1	B	56	GLN	6
1	A	55	LEU	5
1	D	24	ILE	5
1	B	54	ASP	5
1	B	65	LYS	5
1	C	20	ARG	5
1	D	18	GLN	5
1	A	20	ARG	5
1	C	17	SER	5
1	D	17	SER	5
1	A	16	THR	4
1	A	56	GLN	4
1	B	16	THR	4
1	D	65	LYS	4
1	A	30	ILE	4
1	C	12	CYS	4
1	C	24	ILE	4
1	C	30	ILE	4
1	C	56	GLN	4
1	D	10	CYS	4
1	D	68	LEU	4
1	B	30	ILE	4
1	B	24	ILE	4
1	A	18	GLN	4
1	D	56	GLN	3
1	A	17	SER	3
1	B	12	CYS	3
1	B	49	ARG	3
1	A	54	ASP	3
1	B	18	GLN	3
1	A	11	GLN	2
1	C	49	ARG	2
1	D	49	ARG	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	24	ILE	2
1	B	17	SER	2
1	C	35	HIS	2
1	B	67	LEU	2
1	C	11	GLN	2
1	B	13	VAL	2
1	B	35	HIS	2
1	C	13	VAL	2
1	D	11	GLN	2
1	D	35	HIS	2
1	D	61	LYS	1
1	B	10	CYS	1
1	B	59	LEU	1
1	C	10	CYS	1
1	D	60	TYR	1
1	D	63	ILE	1
1	A	26	SER	1
1	C	67	LEU	1
1	A	36	CYS	1
1	A	49	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers [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