



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 08:28 PM UTC

PDB ID : 2L4T / pdb_00002l4t
Title : GIP/Glutaminase L peptide complex
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Deposited on : 2010-10-13

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

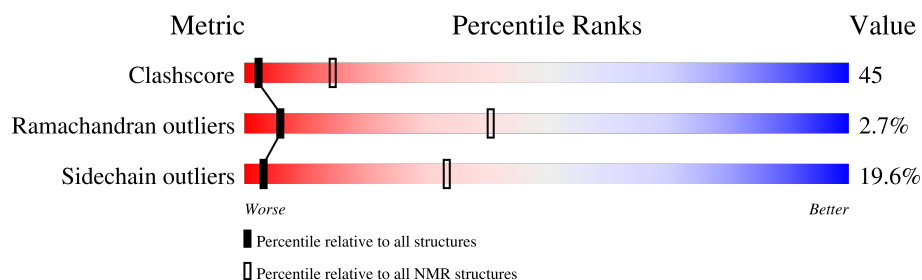
1 Overall quality at a glance

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	124	
2	B	8	

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 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:11-A:19, A:31-A:35, A:54-A:112, B:166-B:168 (76)	0.84	9

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 4 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2075 atoms, of which 1049 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tax1-binding protein 3.

Mol	Chain	Residues	Atoms						Trace
1	A	124	Total	C	H	N	O	S	0
			1945	596	984	175	185	5	

- Molecule 2 is a protein called Glutaminase L peptide.

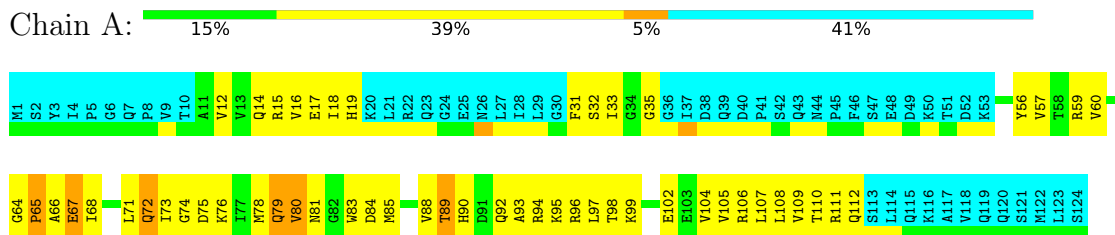
Mol	Chain	Residues	Atoms						Trace
2	B	8	Total	C	H	N	O	S	0
			130	39	65	10	15	1	

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: Tax1-binding protein 3



- Molecule 2: Glutaminase L peptide

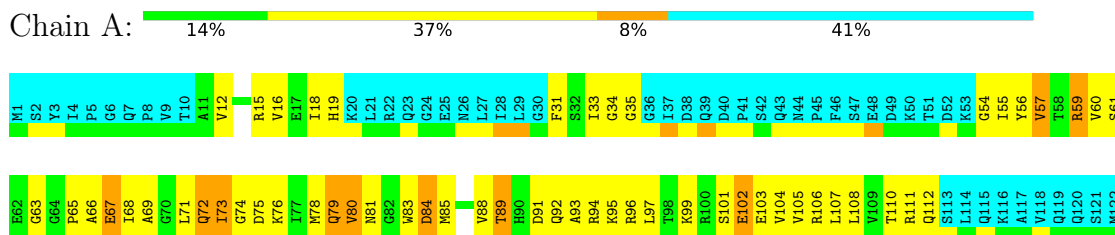


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Tax1-binding protein 3



L123
S124

- Molecule 2: Glutaminase L peptide

Chain B: 12% 12% 12% 62%

K161
E162
M163
L164
E165
S166
M167
V168

4.2.2 Score per residue for model 2

- Molecule 1: Tax1-binding protein 3

Chain A: 22% 27% 10% 41%

M1 S2 Y3 I4 P5 G6 Q7 P8 V9 A11 V12 V13 Q14 R15 V16 E17 D84 I18 H19 K20 L21 L22 R22 Q23 G24 E25 N26 L27 R94 L28 L29 G30 F31 S32 I33 G36 I37 D38 Q39 D40 P41 S42 Q43 N44 P45 F46 S47 E48 D49 K50 T51 D52 K53 Y56 V57 T58 R59 V60 P65

A66 E67 L71 Q72 I73 G74 D75 K76 M77 M78 Q79 W80 N81 G82 W83 D84 M85 T86 M87 V88 T89 H90 Q91 Q92 A93 K94 R95 R96 L97 T98 K99 R100 E101 V105 R106 L107 L108 V109 T110 R111 Q112 S113 L114 Q115 K116 A117 V118 Q119 M120 M121 M122 L123 S124

- Molecule 2: Glutaminase L peptide

Chain B: 12% 25% 62%

K161
E162
M163
L164
E165
S166
M167
V168

4.2.3 Score per residue for model 3

- Molecule 1: Tax1-binding protein 3

Chain A: 21% 27% 11% 41%

M1 S2 Y3 I4 P5 G6 Q7 P8 V9 A11 V12 R15 V16 E17 I18 H19 K20 L21 L22 R22 Q23 G24 E25 N26 L27 R94 L28 L29 G30 F31 S32 I33 G36 I37 D38 Q39 D40 P41 S42 Q43 N44 P45 F46 S47 E48 D49 K50 T51 D52 K53 Y56 V57 T58 R59 V60

G64 P65 A66 E67 I68 L71 Q72 I73 G74 D75 K76 M77 M78 Q79 W80 N81 G82 W83 D84 M85 T86 V88 T89 H90 Q91 Q92 R96 L97 T98 K99 R100 E101 V105 R106 L107 L108 V109 T110 R111 Q112 S113 L114 Q115 K116 A117 V118 Q119 M120 M121 M122 L123 S124

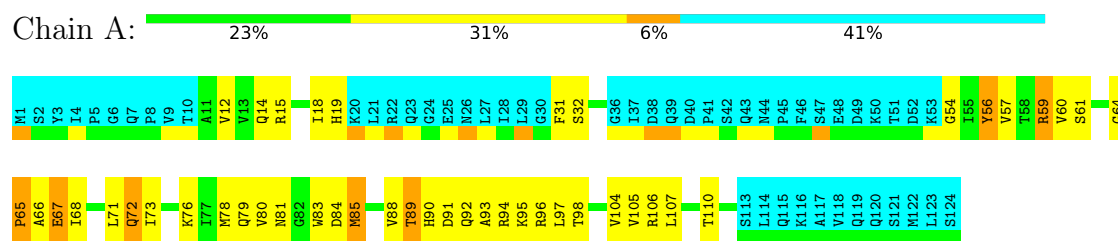
- Molecule 2: Glutaminase L peptide

Chain B: 12% 25% 62%

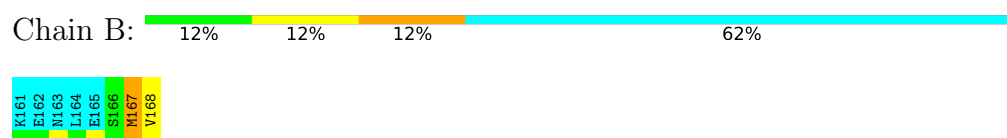
K161
E162
M163
L164
E165
S166
M167
V168

4.2.4 Score per residue for model 4

- Molecule 1: Tax1-binding protein 3

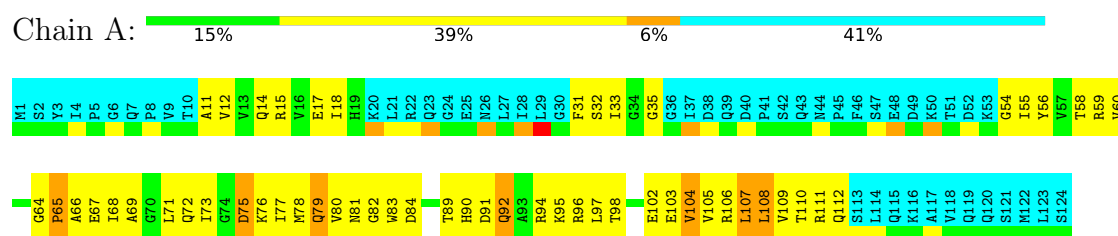


- Molecule 2: Glutaminase L peptide

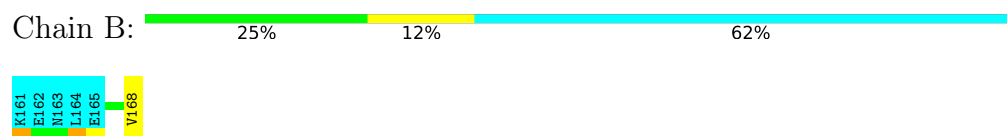


4.2.5 Score per residue for model 5

- Molecule 1: Tax1-binding protein 3

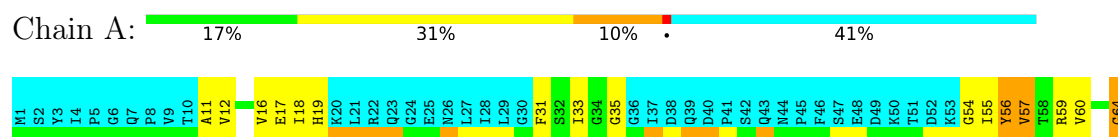


- Molecule 2: Glutaminase L peptide



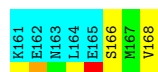
4.2.6 Score per residue for model 6

- Molecule 1: Tax1-binding protein 3





- Molecule 2: Glutaminase L peptide

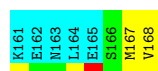


4.2.7 Score per residue for model 7

- Molecule 1: Tax1-binding protein 3



- Molecule 2: Glutaminase L peptide

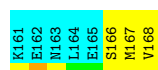


4.2.8 Score per residue for model 8

- Molecule 1: Tax1-binding protein 3

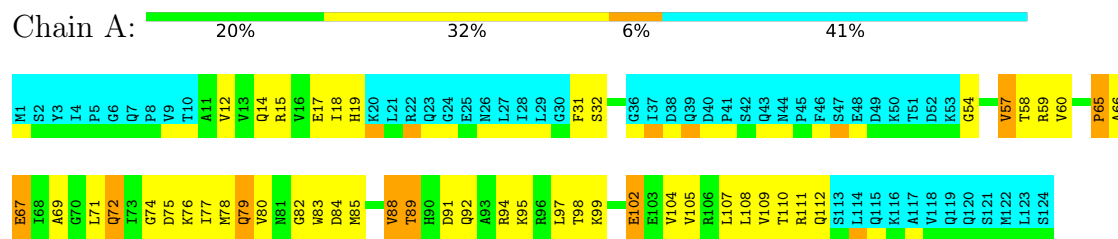


- Molecule 2: Glutaminase L peptide

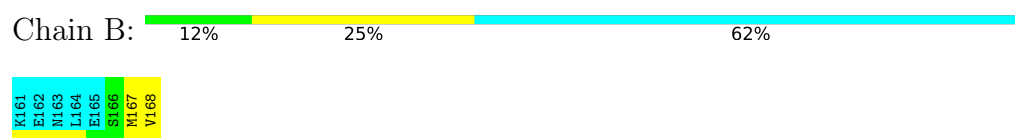


4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Tax1-binding protein 3

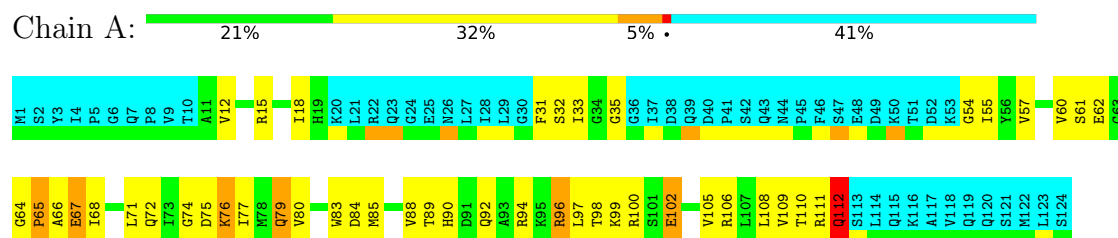


- Molecule 2: Glutaminase L peptide

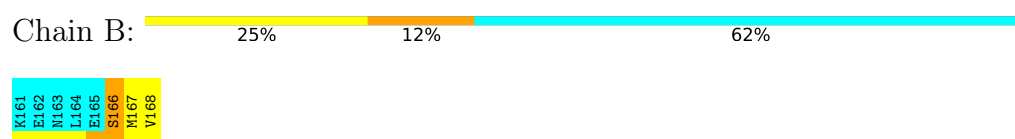


4.2.10 Score per residue for model 10

- Molecule 1: Tax1-binding protein 3

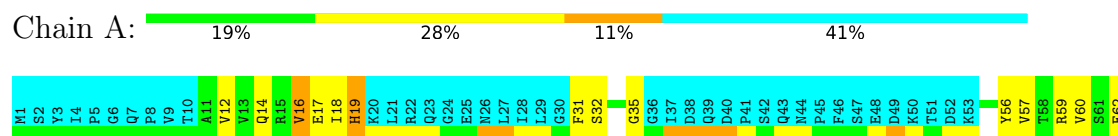


- Molecule 2: Glutaminase L peptide



4.2.11 Score per residue for model 11

- Molecule 1: Tax1-binding protein 3





- Molecule 2: Glutaminase L peptide



4.2.12 Score per residue for model 12

- Molecule 1: Tax1-binding protein 3

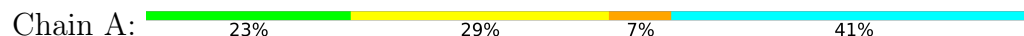


- Molecule 2: Glutaminase L peptide

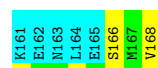


4.2.13 Score per residue for model 13

- Molecule 1: Tax1-binding protein 3

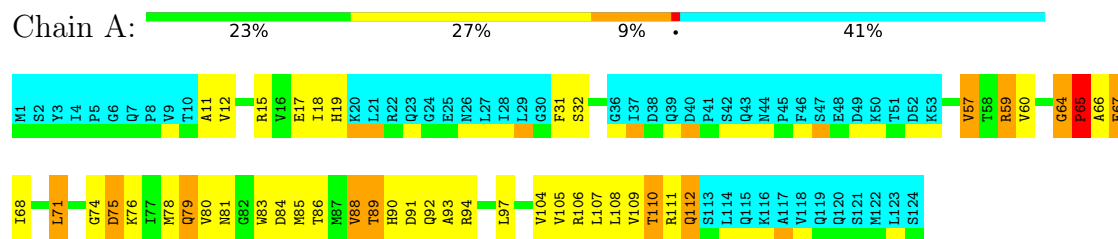


- Molecule 2: Glutaminase L peptide

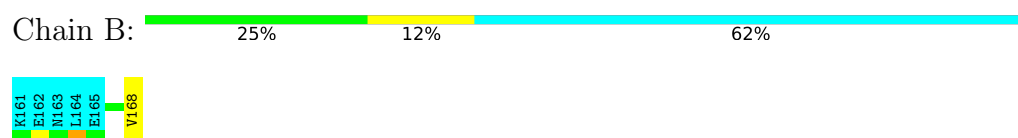


4.2.14 Score per residue for model 14

- Molecule 1: Tax1-binding protein 3

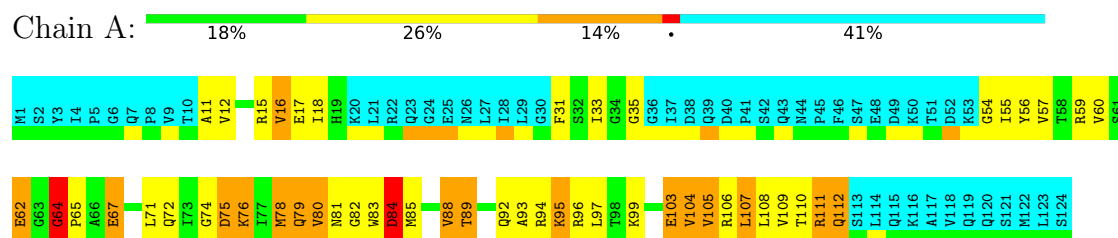


- Molecule 2: Glutaminase L peptide

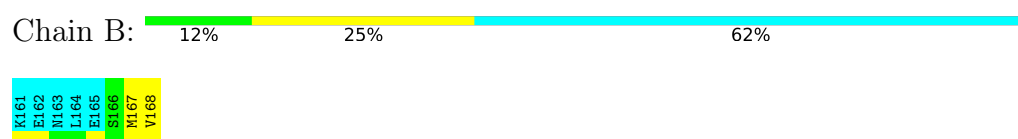


4.2.15 Score per residue for model 15

- Molecule 1: Tax1-binding protein 3

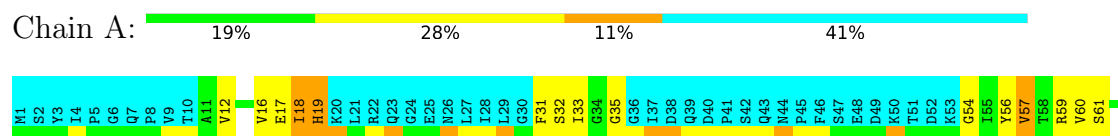


- Molecule 2: Glutaminase L peptide



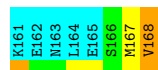
4.2.16 Score per residue for model 16

- Molecule 1: Tax1-binding protein 3



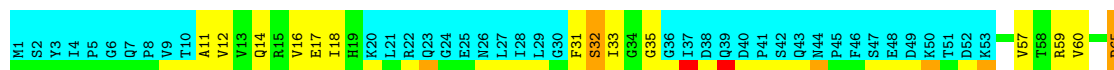


- Molecule 2: Glutaminase L peptide



4.2.17 Score per residue for model 17

- Molecule 1: Tax1-binding protein 3

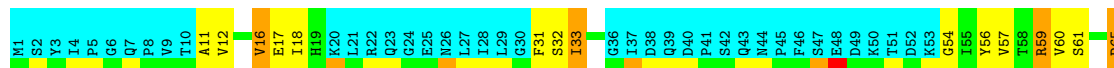


- Molecule 2: Glutaminase L peptide

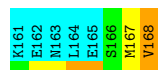


4.2.18 Score per residue for model 18

- Molecule 1: Tax1-binding protein 3

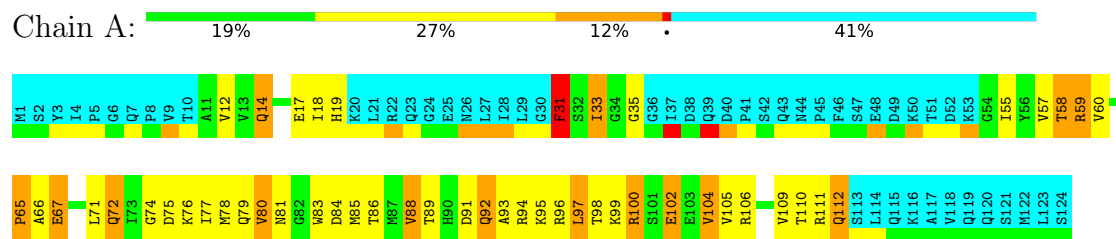


- Molecule 2: Glutaminase L peptide

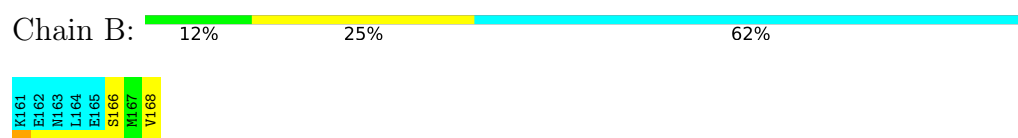


4.2.19 Score per residue for model 19

- Molecule 1: Tax1-binding protein 3

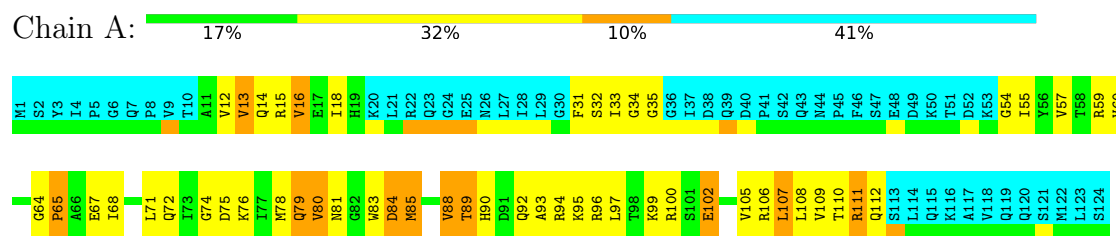


- Molecule 2: Glutaminase L peptide

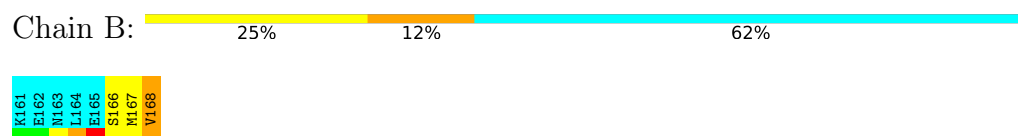


4.2.20 Score per residue for model 20

- Molecule 1: Tax1-binding protein 3



- Molecule 2: Glutaminase L peptide



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 200 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
ARIA	refinement	1.1

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	0.95±0.03	0±0/576 (0.0± 0.1%)	0.97±0.03	0±1/776 (0.1± 0.1%)
2	B	0.52±0.14	0±0/21 (0.0± 0.0%)	0.76±0.27	0±0/25 (0.0± 0.0%)
All	All	0.94	2/11940 (0.0%)	0.96	9/16020 (0.1%)

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	0.1±0.4
2	B	0.0±0.0	0.1±0.2
All	All	0	4

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	105	VAL	N-CA	-7.96	1.37	1.46	11	1
1	A	62	GLU	N-CA	-6.09	1.38	1.45	15	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	64	GLY	CA-C-N	8.47	130.43	119.84	6	3
1	A	64	GLY	C-N-CA	8.47	130.43	119.84	6	3
1	A	105	VAL	N-CA-CB	-7.61	101.95	111.31	11	1
1	A	12	VAL	CB-CA-C	-6.33	103.20	110.41	20	1
1	A	103	GLU	N-CA-C	-5.22	106.86	114.12	15	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	56	TYR	Sidechain	1
2	B	166	SER	Peptide	1
1	A	103	GLU	Peptide	1
1	A	31	PHE	Sidechain	1

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	569	590	588	54±8
2	B	22	23	23	2±2
All	All	11820	12260	12220	1076

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 45.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:VAL:HG13	1:A:92:GLN:HG3	1.08	1.16	13	2
1:A:31:PHE:HB2	1:A:60:VAL:HA	0.97	1.32	13	19
1:A:79:GLN:HG2	1:A:84:ASP:HA	0.96	1.34	18	3
1:A:15:ARG:HD2	1:A:108:LEU:HD22	0.95	1.34	3	1
1:A:18:ILE:HG13	1:A:66:ALA:HA	0.94	1.36	16	1
1:A:11:ALA:HB1	1:A:110:THR:HB	0.90	1.43	14	4
1:A:89:THR:HB	1:A:92:GLN:HG2	0.89	1.43	19	11
1:A:79:GLN:HA	1:A:85:MET:HG3	0.88	1.43	15	6
1:A:79:GLN:HG3	1:A:108:LEU:HB2	0.86	1.44	5	12
1:A:79:GLN:HB2	1:A:108:LEU:HB2	0.85	1.47	8	2
1:A:13:VAL:HB	1:A:111:ARG:H	0.85	1.29	20	1
1:A:79:GLN:HB3	1:A:84:ASP:HA	0.85	1.47	20	9
1:A:13:VAL:HB	1:A:111:ARG:N	0.84	1.87	20	1
1:A:12:VAL:HB	1:A:111:ARG:HB2	0.83	1.50	1	2
1:A:35:GLY:HA3	1:A:55:ILE:HD13	0.81	1.50	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:ALA:HB1	1:A:71:LEU:HG	0.80	1.53	14	1
1:A:89:THR:HG22	1:A:92:GLN:HB2	0.80	1.53	10	2
1:A:18:ILE:HG12	1:A:107:LEU:HD21	0.78	1.55	5	4
1:A:76:LYS:HB3	1:A:78:MET:HE3	0.78	1.54	7	2
1:A:79:GLN:HB3	1:A:84:ASP:N	0.78	1.94	3	12
1:A:88:VAL:HG13	1:A:92:GLN:CG	0.77	2.08	10	2
1:A:92:GLN:HA	1:A:95:LYS:CD	0.76	2.09	6	1
1:A:89:THR:HB	1:A:92:GLN:CG	0.76	2.11	2	12
1:A:32:SER:HB3	1:A:59:ARG:HG3	0.76	1.56	9	2
1:A:33:ILE:HG22	1:A:57:VAL:HG23	0.75	1.57	7	6
1:A:79:GLN:HG2	1:A:80:VAL:N	0.75	1.95	7	1
1:A:35:GLY:HA2	1:A:55:ILE:HD13	0.75	1.59	19	3
1:A:81:ASN:HA	1:A:106:ARG:HB2	0.74	1.59	8	5
1:A:17:GLU:HG2	1:A:106:ARG:HG3	0.74	1.59	15	4
1:A:18:ILE:HG23	1:A:66:ALA:HA	0.74	1.58	12	10
1:A:13:VAL:CG1	1:A:109:VAL:HG13	0.74	2.13	20	1
1:A:85:MET:HE2	1:A:93:ALA:HB1	0.73	1.59	11	5
1:A:79:GLN:HB3	1:A:84:ASP:CA	0.73	2.13	11	11
1:A:88:VAL:HG12	1:A:92:GLN:HG2	0.73	1.61	18	1
1:A:56:TYR:CE2	1:A:74:GLY:HA2	0.72	2.18	6	1
1:A:92:GLN:NE2	1:A:93:ALA:H	0.72	1.81	18	1
1:A:18:ILE:HG21	1:A:31:PHE:CE1	0.72	2.20	10	2
1:A:31:PHE:CB	1:A:60:VAL:HA	0.72	2.14	8	19
1:A:17:GLU:HB3	1:A:105:VAL:HG23	0.72	1.60	11	1
1:A:12:VAL:O	1:A:110:THR:HA	0.71	1.84	18	15
1:A:79:GLN:HB2	1:A:84:ASP:HA	0.71	1.63	7	3
1:A:18:ILE:HD13	1:A:107:LEU:HD22	0.71	1.62	9	1
1:A:57:VAL:HG12	1:A:75:ASP:H	0.70	1.46	1	16
1:A:89:THR:HG22	1:A:90:HIS:H	0.70	1.47	18	1
1:A:32:SER:HB2	2:B:167:MET:HG3	0.70	1.62	20	1
1:A:94:ARG:NH2	2:B:166:SER:HB3	0.70	2.01	20	1
1:A:18:ILE:HG12	1:A:107:LEU:CD2	0.70	2.17	5	3
1:A:92:GLN:HA	1:A:95:LYS:HD3	0.69	1.62	6	1
1:A:16:VAL:HG13	1:A:107:LEU:HD12	0.69	1.63	13	1
1:A:88:VAL:HG12	1:A:92:GLN:HB2	0.69	1.65	15	2
1:A:62:GLU:HA	1:A:67:GLU:OE1	0.69	1.88	10	2
1:A:19:HIS:HA	1:A:104:VAL:HA	0.69	1.63	14	4
1:A:79:GLN:HB3	1:A:108:LEU:HB2	0.69	1.62	7	1
1:A:76:LYS:HB2	1:A:110:THR:OG1	0.68	1.88	16	17
1:A:65:PRO:HA	1:A:68:ILE:HG12	0.68	1.65	14	2
1:A:18:ILE:O	1:A:104:VAL:HG22	0.68	1.89	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ILE:HD12	1:A:107:LEU:HD22	0.68	1.63	4	2
1:A:88:VAL:HG13	1:A:92:GLN:NE2	0.68	2.03	6	4
1:A:81:ASN:HA	1:A:106:ARG:HB3	0.67	1.66	11	8
1:A:93:ALA:HA	1:A:96:ARG:HE	0.67	1.48	15	1
1:A:88:VAL:HG12	1:A:92:GLN:CB	0.67	2.19	15	7
1:A:93:ALA:O	1:A:97:LEU:HG	0.67	1.89	17	9
1:A:92:GLN:O	1:A:96:ARG:HG2	0.67	1.88	17	4
1:A:97:LEU:HD12	1:A:98:THR:HG23	0.66	1.68	8	7
1:A:80:VAL:HG12	1:A:85:MET:SD	0.66	2.31	19	1
1:A:67:GLU:HA	1:A:71:LEU:O	0.66	1.91	12	12
1:A:71:LEU:HG	1:A:72:GLN:H	0.66	1.50	10	4
1:A:104:VAL:HG22	1:A:105:VAL:H	0.66	1.49	11	1
1:A:80:VAL:HA	1:A:106:ARG:O	0.66	1.90	8	8
1:A:99:LYS:HG2	1:A:102:GLU:OE2	0.65	1.90	10	5
1:A:66:ALA:HB1	1:A:71:LEU:HD23	0.65	1.68	5	4
1:A:79:GLN:HG3	1:A:108:LEU:CB	0.65	2.21	5	4
1:A:66:ALA:HB1	1:A:71:LEU:CG	0.65	2.21	14	1
1:A:91:ASP:O	1:A:94:ARG:HG2	0.65	1.92	16	3
1:A:15:ARG:HG2	1:A:108:LEU:CD2	0.65	2.22	9	1
1:A:67:GLU:HA	1:A:71:LEU:HD12	0.64	1.68	14	1
1:A:76:LYS:HG2	1:A:110:THR:OG1	0.64	1.91	3	1
1:A:99:LYS:HG2	1:A:102:GLU:OE1	0.64	1.92	9	1
1:A:64:GLY:O	1:A:67:GLU:HG3	0.64	1.92	15	1
1:A:18:ILE:HG21	1:A:31:PHE:HE2	0.64	1.52	14	1
1:A:78:MET:HA	1:A:78:MET:HE2	0.64	1.70	15	19
1:A:17:GLU:HG2	1:A:106:ARG:HG2	0.64	1.69	5	1
1:A:65:PRO:HA	1:A:68:ILE:CG1	0.64	2.22	14	2
1:A:79:GLN:CG	1:A:108:LEU:HB2	0.63	2.22	1	5
1:A:31:PHE:O	2:B:167:MET:HA	0.63	1.93	8	8
1:A:18:ILE:HB	1:A:105:VAL:HG13	0.63	1.69	3	1
1:A:18:ILE:HB	1:A:105:VAL:HG23	0.63	1.69	13	2
1:A:18:ILE:CA	1:A:105:VAL:HB	0.63	2.23	11	1
1:A:59:ARG:HG3	1:A:60:VAL:N	0.63	2.08	4	9
1:A:94:ARG:HH21	2:B:166:SER:HB2	0.63	1.53	19	1
1:A:79:GLN:HG3	1:A:83:TRP:C	0.63	2.19	7	1
1:A:88:VAL:HB	1:A:96:ARG:NH2	0.62	2.08	15	1
1:A:66:ALA:CB	1:A:71:LEU:HG	0.62	2.25	14	1
1:A:80:VAL:HG12	1:A:85:MET:HB3	0.62	1.72	4	2
1:A:35:GLY:CA	1:A:55:ILE:HD13	0.62	2.23	20	4
1:A:89:THR:HG22	1:A:92:GLN:CB	0.62	2.23	13	2
1:A:92:GLN:HE21	1:A:93:ALA:N	0.62	1.93	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:GLN:HG2	1:A:84:ASP:CA	0.62	2.20	18	2
1:A:15:ARG:HA	1:A:107:LEU:O	0.62	1.93	5	2
1:A:32:SER:HB3	1:A:59:ARG:HG2	0.62	1.69	20	4
1:A:77:ILE:HA	1:A:109:VAL:HG12	0.61	1.72	10	3
1:A:97:LEU:HB2	1:A:105:VAL:HG21	0.61	1.71	12	1
1:A:92:GLN:HA	1:A:95:LYS:CG	0.61	2.25	17	1
1:A:79:GLN:HB3	1:A:83:TRP:C	0.61	2.21	3	6
1:A:17:GLU:HB3	1:A:106:ARG:HG3	0.61	1.71	14	1
1:A:57:VAL:HG12	1:A:75:ASP:N	0.61	2.09	14	11
1:A:79:GLN:OE1	1:A:108:LEU:HD23	0.61	1.95	7	1
1:A:13:VAL:HG12	1:A:109:VAL:C	0.61	2.20	20	1
1:A:75:ASP:OD1	1:A:111:ARG:HB3	0.61	1.95	13	4
1:A:71:LEU:HD13	1:A:72:GLN:N	0.61	2.11	8	10
1:A:56:TYR:HA	1:A:76:LYS:HA	0.61	1.72	18	9
1:A:88:VAL:CG1	1:A:93:ALA:HB2	0.61	2.26	17	3
1:A:94:ARG:NH2	2:B:166:SER:HB2	0.60	2.10	19	1
1:A:89:THR:CB	1:A:92:GLN:HG2	0.60	2.26	2	9
1:A:18:ILE:O	1:A:105:VAL:HG22	0.60	1.96	5	4
1:A:18:ILE:N	1:A:105:VAL:HB	0.60	2.11	11	1
1:A:80:VAL:HG21	1:A:97:LEU:HB3	0.60	1.74	15	4
1:A:88:VAL:HG22	1:A:92:GLN:HE22	0.60	1.55	17	2
1:A:16:VAL:HG13	1:A:107:LEU:HD23	0.60	1.74	15	5
1:A:13:VAL:CG2	1:A:111:ARG:HB2	0.60	2.26	20	1
1:A:104:VAL:HG22	1:A:105:VAL:N	0.60	2.11	11	1
1:A:19:HIS:HB2	1:A:105:VAL:HA	0.60	1.72	11	1
1:A:85:MET:HA	1:A:88:VAL:HG23	0.60	1.74	11	1
1:A:16:VAL:HG13	1:A:107:LEU:CD2	0.60	2.26	15	4
1:A:18:ILE:HG12	1:A:66:ALA:HA	0.60	1.73	18	2
1:A:35:GLY:HA3	1:A:55:ILE:CD1	0.60	2.26	20	2
1:A:89:THR:H	1:A:92:GLN:HG3	0.60	1.56	19	3
1:A:32:SER:HB2	2:B:167:MET:HB3	0.60	1.73	18	1
1:A:76:LYS:C	1:A:109:VAL:HG23	0.60	2.22	5	1
1:A:31:PHE:HB3	1:A:60:VAL:HA	0.59	1.73	15	4
1:A:33:ILE:HG23	1:A:94:ARG:HH22	0.59	1.55	19	1
1:A:35:GLY:HA2	1:A:54:GLY:O	0.59	1.98	5	2
1:A:16:VAL:HB	1:A:107:LEU:CD1	0.59	2.26	6	1
1:A:33:ILE:HG12	2:B:167:MET:HE2	0.59	1.74	10	1
1:A:15:ARG:N	1:A:15:ARG:HD3	0.59	2.12	4	1
1:A:57:VAL:HG13	1:A:74:GLY:H	0.59	1.58	10	7
1:A:57:VAL:HG21	1:A:71:LEU:HD11	0.58	1.75	2	4
1:A:99:LYS:HE2	1:A:102:GLU:HB3	0.58	1.75	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:VAL:HG13	1:A:66:ALA:HB3	0.58	1.76	17	4
1:A:11:ALA:HA	1:A:111:ARG:O	0.58	1.97	14	1
1:A:77:ILE:HG23	1:A:107:LEU:HG	0.58	1.74	9	1
1:A:62:GLU:OE1	1:A:65:PRO:HD2	0.58	1.98	15	1
1:A:12:VAL:CG2	1:A:111:ARG:HB3	0.58	2.28	10	1
1:A:92:GLN:O	1:A:95:LYS:HG2	0.58	1.98	12	2
1:A:76:LYS:O	1:A:109:VAL:HA	0.58	1.98	7	7
1:A:83:TRP:N	1:A:83:TRP:CD1	0.58	2.70	8	6
1:A:58:THR:HG23	1:A:59:ARG:HG2	0.58	1.75	9	1
1:A:90:HIS:O	1:A:94:ARG:HB3	0.57	1.99	5	4
1:A:88:VAL:HG13	1:A:92:GLN:HG2	0.57	1.74	10	1
1:A:93:ALA:HA	1:A:96:ARG:NE	0.57	2.14	15	1
1:A:19:HIS:HB2	1:A:104:VAL:HG23	0.57	1.76	13	2
1:A:94:ARG:HA	1:A:97:LEU:CD2	0.57	2.29	12	2
1:A:76:LYS:HB2	1:A:110:THR:HG1	0.57	1.59	16	3
1:A:85:MET:CE	1:A:93:ALA:HB1	0.57	2.29	19	4
1:A:97:LEU:HD12	1:A:98:THR:HG22	0.57	1.76	19	2
1:A:91:ASP:O	1:A:94:ARG:HB2	0.57	2.00	11	5
1:A:80:VAL:HG21	1:A:97:LEU:HD23	0.57	1.76	1	2
1:A:89:THR:HG22	1:A:92:GLN:HG2	0.57	1.75	5	2
1:A:17:GLU:HG3	1:A:106:ARG:HG3	0.57	1.76	19	1
1:A:106:ARG:C	1:A:107:LEU:HD13	0.57	2.25	15	4
1:A:64:GLY:O	1:A:66:ALA:N	0.56	2.37	14	2
1:A:18:ILE:HB	1:A:105:VAL:CG2	0.56	2.30	17	3
1:A:31:PHE:O	2:B:167:MET:HB2	0.56	1.99	10	1
1:A:71:LEU:C	1:A:71:LEU:CD1	0.56	2.78	14	1
1:A:80:VAL:O	1:A:83:TRP:CD1	0.56	2.59	12	19
1:A:19:HIS:HB2	1:A:104:VAL:HG22	0.56	1.76	16	1
1:A:19:HIS:HA	1:A:104:VAL:HG23	0.56	1.78	9	1
1:A:112:GLN:CA	1:A:112:GLN:HE21	0.56	2.14	19	3
1:A:19:HIS:CA	1:A:104:VAL:HG23	0.56	2.31	9	1
1:A:75:ASP:OD1	1:A:109:VAL:HB	0.56	2.00	6	2
1:A:79:GLN:HG3	1:A:84:ASP:N	0.56	2.16	7	1
1:A:111:ARG:O	1:A:112:GLN:HB2	0.55	2.01	14	1
1:A:64:GLY:O	1:A:68:ILE:HG12	0.55	2.02	5	7
1:A:75:ASP:OD1	1:A:111:ARG:HA	0.55	2.02	19	2
1:A:92:GLN:CD	1:A:93:ALA:N	0.55	2.65	18	1
1:A:81:ASN:CA	1:A:106:ARG:HB2	0.55	2.31	7	5
1:A:32:SER:HB3	1:A:59:ARG:HB2	0.55	1.77	16	4
1:A:107:LEU:HD22	1:A:107:LEU:N	0.55	2.17	8	5
1:A:101:SER:O	1:A:102:GLU:HG2	0.55	2.01	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:LYS:O	1:A:99:LYS:HB3	0.55	2.01	19	5
1:A:19:HIS:HB2	1:A:105:VAL:CA	0.55	2.32	11	1
1:A:89:THR:C	1:A:92:GLN:NE2	0.55	2.65	18	1
1:A:92:GLN:CD	1:A:93:ALA:H	0.55	2.09	18	1
1:A:76:LYS:HB3	1:A:76:LYS:NZ	0.55	2.17	3	1
1:A:35:GLY:HA3	1:A:90:HIS:HD2	0.54	1.62	5	1
1:A:31:PHE:CZ	2:B:167:MET:HG3	0.54	2.36	10	1
1:A:80:VAL:O	1:A:83:TRP:HD1	0.54	1.84	18	7
1:A:16:VAL:O	1:A:107:LEU:HD22	0.54	2.02	18	4
1:A:112:GLN:HG2	1:A:112:GLN:O	0.54	2.02	18	1
1:A:99:LYS:HE2	1:A:101:SER:HB2	0.54	1.79	13	1
1:A:109:VAL:HG22	1:A:110:THR:H	0.54	1.63	15	2
1:A:57:VAL:HG11	1:A:72:GLN:O	0.54	2.02	11	3
1:A:15:ARG:O	1:A:15:ARG:HD2	0.54	2.03	5	1
1:A:56:TYR:HA	1:A:75:ASP:O	0.54	2.02	5	2
1:A:79:GLN:CB	1:A:84:ASP:HA	0.54	2.33	7	2
1:A:71:LEU:C	1:A:71:LEU:HD13	0.53	2.29	14	1
1:A:18:ILE:HD12	1:A:66:ALA:HA	0.53	1.80	10	4
1:A:99:LYS:HE2	1:A:101:SER:HB3	0.53	1.80	6	1
1:A:79:GLN:HB3	1:A:108:LEU:CB	0.53	2.33	7	1
1:A:79:GLN:NE2	1:A:108:LEU:HD12	0.53	2.18	3	2
1:A:18:ILE:HD13	1:A:107:LEU:CD2	0.53	2.34	16	1
1:A:13:VAL:HG13	1:A:14:GLN:H	0.53	1.64	20	1
1:A:80:VAL:HG12	1:A:85:MET:CG	0.53	2.34	16	1
1:A:85:MET:HA	1:A:96:ARG:NH2	0.53	2.19	1	1
1:A:33:ILE:HG13	2:B:166:SER:O	0.53	2.04	10	1
1:A:17:GLU:CB	1:A:105:VAL:HG23	0.53	2.33	11	1
1:A:32:SER:HB2	1:A:59:ARG:HB2	0.53	1.81	17	1
1:A:16:VAL:HB	1:A:107:LEU:HD12	0.53	1.80	6	1
1:A:62:GLU:HA	1:A:67:GLU:OE2	0.52	2.03	8	1
1:A:13:VAL:HG12	1:A:109:VAL:HG13	0.52	1.80	20	1
1:A:91:ASP:HA	1:A:94:ARG:HD2	0.52	1.79	9	1
1:A:18:ILE:C	1:A:105:VAL:HB	0.52	2.30	11	1
1:A:80:VAL:HG22	1:A:81:ASN:OD1	0.52	2.05	7	2
1:A:12:VAL:HB	1:A:111:ARG:HG3	0.52	1.81	14	2
1:A:12:VAL:HG12	1:A:111:ARG:O	0.52	2.05	15	1
1:A:15:ARG:HE	1:A:108:LEU:HD21	0.52	1.64	15	1
1:A:91:ASP:O	1:A:95:LYS:HG3	0.52	2.04	4	3
1:A:18:ILE:HD11	1:A:71:LEU:HG	0.52	1.80	2	1
1:A:83:TRP:CD1	1:A:83:TRP:N	0.52	2.77	2	5
1:A:15:ARG:NE	1:A:108:LEU:HD21	0.52	2.19	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ILE:HB	1:A:57:VAL:HG23	0.52	1.82	19	1
1:A:18:ILE:O	1:A:105:VAL:HG23	0.51	2.05	14	2
1:A:88:VAL:HG21	1:A:96:ARG:HH22	0.51	1.66	16	1
1:A:91:ASP:O	1:A:95:LYS:HG2	0.51	2.05	19	2
1:A:16:VAL:O	1:A:107:LEU:HB2	0.51	2.04	2	1
2:B:167:MET:O	2:B:168:VAL:HB	0.51	2.05	10	1
1:A:62:GLU:CB	1:A:67:GLU:HG2	0.51	2.35	15	1
1:A:83:TRP:HB3	1:A:96:ARG:HH11	0.51	1.65	15	1
1:A:88:VAL:HG12	1:A:92:GLN:HG3	0.51	1.83	19	1
1:A:14:GLN:NE2	1:A:111:ARG:HE	0.51	2.04	5	1
1:A:60:VAL:HG23	1:A:73:ILE:CD1	0.51	2.36	4	2
1:A:12:VAL:HB	1:A:111:ARG:O	0.51	2.06	7	1
1:A:83:TRP:HZ2	1:A:96:ARG:NE	0.51	2.03	10	1
1:A:89:THR:H	1:A:92:GLN:CG	0.51	2.19	20	7
1:A:99:LYS:HE3	1:A:101:SER:HB3	0.51	1.82	3	1
1:A:56:TYR:CE2	1:A:74:GLY:CA	0.51	2.93	6	1
1:A:15:ARG:N	1:A:15:ARG:HD2	0.50	2.21	7	2
1:A:96:ARG:HH21	1:A:97:LEU:HA	0.50	1.65	8	1
1:A:12:VAL:HG23	1:A:112:GLN:NE2	0.50	2.20	14	1
1:A:13:VAL:HB	1:A:110:THR:HA	0.50	1.81	20	1
1:A:76:LYS:HB3	1:A:110:THR:OG1	0.50	2.06	14	1
1:A:90:HIS:O	1:A:94:ARG:HG3	0.50	2.07	8	1
1:A:18:ILE:CG2	1:A:66:ALA:HA	0.50	2.35	1	1
1:A:94:ARG:O	1:A:97:LEU:HG	0.50	2.06	14	3
1:A:56:TYR:CZ	1:A:74:GLY:HA2	0.50	2.42	1	1
1:A:88:VAL:HB	1:A:92:GLN:CD	0.50	2.31	7	1
1:A:80:VAL:HG11	1:A:85:MET:HE3	0.50	1.84	7	1
1:A:90:HIS:CE1	2:B:166:SER:HB2	0.50	2.42	12	2
1:A:19:HIS:HB2	1:A:105:VAL:HG12	0.50	1.82	11	1
1:A:89:THR:HG22	1:A:92:GLN:H	0.50	1.67	13	1
1:A:83:TRP:CB	1:A:96:ARG:HH11	0.50	2.20	15	1
1:A:94:ARG:HA	1:A:97:LEU:CD1	0.50	2.37	2	1
1:A:71:LEU:HG	1:A:72:GLN:N	0.49	2.22	15	3
1:A:67:GLU:HG2	1:A:68:ILE:N	0.49	2.22	8	1
1:A:83:TRP:CE3	1:A:96:ARG:HD2	0.49	2.43	11	1
1:A:33:ILE:HG23	1:A:94:ARG:NH2	0.49	2.22	19	1
1:A:103:GLU:O	1:A:104:VAL:HB	0.49	2.06	5	2
1:A:80:VAL:HG12	1:A:85:MET:HG2	0.49	1.84	16	3
1:A:88:VAL:HB	1:A:92:GLN:OE1	0.49	2.06	18	1
1:A:32:SER:HB2	1:A:59:ARG:HG2	0.49	1.83	12	2
1:A:96:ARG:NE	1:A:96:ARG:HA	0.49	2.23	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ASN:N	1:A:106:ARG:O	0.49	2.43	1	1
1:A:13:VAL:CB	1:A:110:THR:HA	0.49	2.38	20	1
1:A:65:PRO:O	1:A:68:ILE:HG13	0.49	2.07	16	7
1:A:18:ILE:O	1:A:105:VAL:HG12	0.49	2.08	16	2
1:A:77:ILE:CG2	1:A:107:LEU:HG	0.49	2.37	9	1
1:A:17:GLU:HA	1:A:105:VAL:O	0.49	2.08	7	4
1:A:19:HIS:CB	1:A:105:VAL:HG12	0.49	2.38	11	1
1:A:83:TRP:N	1:A:83:TRP:HD1	0.48	2.06	8	1
1:A:31:PHE:HB2	1:A:59:ARG:O	0.48	2.09	15	3
1:A:99:LYS:HE2	1:A:101:SER:OG	0.48	2.08	7	2
1:A:88:VAL:HG23	1:A:89:THR:N	0.48	2.23	7	1
1:A:89:THR:O	1:A:92:GLN:HB3	0.48	2.08	10	1
1:A:18:ILE:HD12	1:A:107:LEU:HD11	0.48	1.83	1	1
1:A:15:ARG:HB3	1:A:108:LEU:HG	0.48	1.85	5	1
1:A:97:LEU:HD11	2:B:168:VAL:HG21	0.48	1.84	16	1
1:A:33:ILE:HG13	1:A:77:ILE:HG13	0.48	1.86	19	1
1:A:112:GLN:HE21	1:A:112:GLN:HA	0.48	1.69	2	3
1:A:97:LEU:CD1	1:A:98:THR:HG23	0.48	2.38	4	4
1:A:31:PHE:HB2	1:A:60:VAL:CA	0.48	2.23	13	1
1:A:57:VAL:CG1	1:A:74:GLY:H	0.48	2.22	3	8
1:A:97:LEU:HD13	2:B:168:VAL:HG21	0.48	1.86	18	2
1:A:59:ARG:HA	1:A:73:ILE:HD12	0.48	1.86	4	1
1:A:19:HIS:HB3	1:A:104:VAL:HG23	0.48	1.84	19	4
1:A:11:ALA:HA	1:A:112:GLN:HE22	0.48	1.69	5	2
1:A:31:PHE:CE2	2:B:167:MET:HG3	0.48	2.43	10	1
1:A:111:ARG:HD3	1:A:112:GLN:HG3	0.48	1.85	10	1
1:A:94:ARG:HA	1:A:97:LEU:HG	0.48	1.86	12	1
1:A:18:ILE:HD12	1:A:69:ALA:CB	0.47	2.38	16	1
1:A:13:VAL:HG13	1:A:14:GLN:N	0.47	2.25	20	1
1:A:66:ALA:O	1:A:69:ALA:HB3	0.47	2.09	9	2
1:A:97:LEU:HD13	2:B:168:VAL:HG11	0.47	1.86	4	1
1:A:80:VAL:HG21	1:A:97:LEU:CB	0.47	2.39	16	1
1:A:100:ARG:O	1:A:101:SER:HB2	0.47	2.09	17	1
1:A:66:ALA:C	1:A:71:LEU:HB3	0.47	2.35	8	3
1:A:12:VAL:HG13	1:A:111:ARG:HB2	0.47	1.86	15	1
1:A:14:GLN:NE2	1:A:111:ARG:HG2	0.47	2.25	19	1
1:A:73:ILE:N	1:A:73:ILE:HD13	0.47	2.25	12	5
1:A:94:ARG:CD	1:A:97:LEU:HD11	0.47	2.39	19	1
1:A:96:ARG:O	1:A:99:LYS:HD2	0.47	2.09	16	1
1:A:101:SER:C	1:A:103:GLU:H	0.47	2.18	17	1
1:A:32:SER:CB	1:A:59:ARG:HG2	0.47	2.40	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:VAL:CG1	1:A:92:GLN:NE2	0.47	2.78	12	1
1:A:67:GLU:CA	1:A:71:LEU:HD12	0.47	2.39	14	1
1:A:76:LYS:HB2	1:A:110:THR:O	0.47	2.09	14	1
1:A:75:ASP:CG	1:A:111:ARG:HB3	0.46	2.35	3	1
1:A:66:ALA:C	1:A:71:LEU:HG	0.46	2.34	14	1
1:A:80:VAL:CG2	1:A:97:LEU:HB3	0.46	2.40	4	1
1:A:97:LEU:HD12	1:A:98:THR:N	0.46	2.25	16	3
1:A:19:HIS:HB3	1:A:104:VAL:CB	0.46	2.41	6	1
1:A:79:GLN:O	1:A:107:LEU:HA	0.46	2.08	12	1
1:A:100:ARG:NH1	1:A:101:SER:HB3	0.46	2.25	17	1
1:A:92:GLN:NE2	1:A:92:GLN:N	0.46	2.63	18	1
1:A:105:VAL:HG23	1:A:105:VAL:O	0.46	2.11	11	1
1:A:96:ARG:HA	1:A:96:ARG:HE	0.46	1.70	18	4
1:A:19:HIS:N	1:A:105:VAL:CB	0.46	2.78	11	1
1:A:57:VAL:HG21	1:A:71:LEU:HD21	0.46	1.87	8	1
1:A:60:VAL:HG11	1:A:71:LEU:HD11	0.46	1.86	14	1
1:A:11:ALA:HB1	1:A:110:THR:HG22	0.46	1.86	17	1
1:A:13:VAL:HG23	1:A:111:ARG:HB2	0.46	1.85	20	1
1:A:33:ILE:HD11	1:A:90:HIS:HE1	0.46	1.71	3	1
1:A:32:SER:HB3	1:A:59:ARG:CG	0.46	2.35	9	1
1:A:79:GLN:HA	1:A:85:MET:HG2	0.46	1.88	19	2
1:A:13:VAL:CG1	1:A:14:GLN:N	0.46	2.79	20	1
1:A:92:GLN:HA	1:A:95:LYS:HE3	0.46	1.88	5	1
1:A:18:ILE:HD12	1:A:107:LEU:HD21	0.46	1.88	6	1
1:A:112:GLN:CA	1:A:112:GLN:NE2	0.46	2.79	19	1
1:A:13:VAL:HA	1:A:14:GLN:NE2	0.46	2.26	20	1
1:A:97:LEU:HA	1:A:105:VAL:CG1	0.46	2.40	2	1
1:A:79:GLN:HB2	1:A:83:TRP:C	0.46	2.36	10	1
1:A:89:THR:H	1:A:92:GLN:NE2	0.46	2.09	17	1
1:A:97:LEU:O	1:A:105:VAL:HG11	0.46	2.10	5	1
1:A:79:GLN:HA	1:A:83:TRP:O	0.45	2.10	8	1
1:A:109:VAL:HG22	1:A:110:THR:N	0.45	2.27	9	3
1:A:19:HIS:HB3	1:A:104:VAL:CG2	0.45	2.41	14	2
1:A:80:VAL:HG13	1:A:83:TRP:CD1	0.45	2.46	9	1
1:A:94:ARG:HA	1:A:97:LEU:CG	0.45	2.41	12	1
1:A:55:ILE:HG22	1:A:77:ILE:HB	0.45	1.88	5	1
1:A:85:MET:HA	1:A:88:VAL:CG2	0.45	2.42	18	3
1:A:76:LYS:HB2	1:A:110:THR:CB	0.45	2.42	17	1
1:A:106:ARG:O	1:A:107:LEU:HD12	0.45	2.12	2	2
1:A:79:GLN:HB2	1:A:84:ASP:N	0.45	2.27	10	1
1:A:94:ARG:HA	1:A:97:LEU:HD21	0.45	1.86	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ILE:HD13	1:A:31:PHE:CE2	0.45	2.45	18	1
1:A:80:VAL:HG23	1:A:105:VAL:HG23	0.45	1.88	19	1
1:A:111:ARG:C	1:A:112:GLN:HE21	0.45	2.19	19	1
1:A:96:ARG:HE	1:A:96:ARG:CA	0.45	2.24	20	1
1:A:15:ARG:HG3	1:A:108:LEU:HD22	0.45	1.87	8	1
1:A:60:VAL:HG11	1:A:67:GLU:HB3	0.45	1.89	8	2
1:A:81:ASN:CA	1:A:106:ARG:HB3	0.45	2.41	11	1
1:A:88:VAL:CG1	1:A:92:GLN:HB2	0.45	2.41	19	2
1:A:17:GLU:HB3	1:A:104:VAL:CG2	0.45	2.41	17	1
1:A:89:THR:HG23	1:A:92:GLN:H	0.45	1.71	5	1
1:A:56:TYR:CE1	1:A:74:GLY:HA2	0.45	2.47	1	1
1:A:18:ILE:CD1	1:A:71:LEU:HG	0.45	2.42	2	1
1:A:81:ASN:HB2	1:A:83:TRP:NE1	0.45	2.27	7	1
1:A:16:VAL:HG13	1:A:107:LEU:CD1	0.45	2.37	13	1
1:A:106:ARG:C	1:A:107:LEU:HD12	0.45	2.37	2	1
1:A:55:ILE:HG21	1:A:85:MET:SD	0.45	2.52	3	2
1:A:19:HIS:CB	1:A:105:VAL:HA	0.45	2.42	11	1
1:A:85:MET:O	1:A:88:VAL:HB	0.45	2.12	17	1
1:A:81:ASN:HA	1:A:106:ARG:CB	0.45	2.41	11	2
1:A:12:VAL:HG23	1:A:112:GLN:HE22	0.45	1.71	14	1
1:A:78:MET:O	1:A:84:ASP:HA	0.45	2.12	4	1
1:A:64:GLY:C	1:A:66:ALA:H	0.45	2.20	6	1
1:A:19:HIS:N	1:A:105:VAL:HG12	0.45	2.26	11	1
1:A:60:VAL:CG1	1:A:71:LEU:HD11	0.45	2.42	14	1
1:A:18:ILE:CG1	1:A:107:LEU:HD22	0.45	2.42	17	1
1:A:79:GLN:CA	1:A:85:MET:HG3	0.44	2.39	9	1
1:A:88:VAL:HG12	1:A:92:GLN:CG	0.44	2.38	18	1
1:A:33:ILE:C	1:A:33:ILE:HD13	0.44	2.37	19	1
1:A:112:GLN:HE21	1:A:112:GLN:N	0.44	2.09	19	1
1:A:92:GLN:NE2	1:A:92:GLN:C	0.44	2.75	16	3
1:A:68:ILE:HG13	1:A:69:ALA:N	0.44	2.27	1	1
1:A:18:ILE:HD11	1:A:71:LEU:HB2	0.44	1.88	11	1
1:A:104:VAL:CG2	1:A:105:VAL:N	0.44	2.79	11	1
1:A:79:GLN:HA	1:A:85:MET:CG	0.44	2.31	15	1
1:A:71:LEU:HD22	1:A:111:ARG:HH12	0.44	1.71	19	1
1:A:85:MET:SD	1:A:93:ALA:HB1	0.44	2.52	19	1
1:A:35:GLY:HA3	1:A:90:HIS:CD2	0.44	2.47	5	1
1:A:31:PHE:CD1	1:A:66:ALA:HB2	0.44	2.47	8	1
1:A:32:SER:HA	2:B:166:SER:O	0.44	2.13	13	1
1:A:19:HIS:N	1:A:105:VAL:HB	0.44	2.27	11	1
1:A:66:ALA:HB1	1:A:71:LEU:CD2	0.44	2.42	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:THR:HB	1:A:92:GLN:HG3	0.44	1.88	6	2
1:A:79:GLN:HG2	1:A:108:LEU:HB2	0.44	1.90	16	2
1:A:18:ILE:CD1	1:A:69:ALA:HB3	0.43	2.43	5	1
1:A:18:ILE:HB	1:A:105:VAL:HG22	0.43	1.90	17	1
1:A:19:HIS:HB2	1:A:103:GLU:O	0.43	2.13	1	1
1:A:63:GLY:H	1:A:67:GLU:CD	0.43	2.20	1	2
1:A:32:SER:CB	1:A:59:ARG:HB2	0.43	2.42	5	1
1:A:92:GLN:HA	1:A:95:LYS:HG2	0.43	1.90	7	4
1:A:94:ARG:NH1	2:B:166:SER:HB2	0.43	2.27	1	1
1:A:94:ARG:NH1	2:B:168:VAL:HG13	0.43	2.27	1	1
1:A:80:VAL:C	1:A:82:GLY:H	0.43	2.20	15	3
1:A:19:HIS:HB3	1:A:104:VAL:HB	0.43	1.90	6	1
1:A:79:GLN:CB	1:A:108:LEU:HB2	0.43	2.33	8	1
1:A:80:VAL:HG23	1:A:105:VAL:CG2	0.43	2.43	19	1
1:A:58:THR:O	1:A:59:ARG:HG2	0.43	2.13	5	1
1:A:32:SER:OG	2:B:167:MET:HG2	0.43	2.13	12	1
1:A:79:GLN:CD	1:A:108:LEU:HD12	0.43	2.39	18	1
1:A:75:ASP:OD1	1:A:109:VAL:HG22	0.43	2.13	20	1
1:A:94:ARG:HH11	1:A:94:ARG:HG2	0.43	1.74	20	1
1:A:18:ILE:HD12	1:A:107:LEU:CD1	0.43	2.44	1	1
1:A:13:VAL:HG12	1:A:109:VAL:O	0.43	2.13	20	1
1:A:72:GLN:N	1:A:72:GLN:CD	0.43	2.77	2	1
1:A:15:ARG:HG2	1:A:108:LEU:HD22	0.43	1.91	9	1
1:A:90:HIS:C	1:A:92:GLN:NE2	0.43	2.77	18	1
1:A:55:ILE:O	1:A:76:LYS:HA	0.43	2.14	5	1
1:A:59:ARG:HA	1:A:73:ILE:HG23	0.43	1.91	6	1
1:A:85:MET:HA	1:A:88:VAL:HB	0.42	1.91	16	2
1:A:92:GLN:HE21	1:A:92:GLN:C	0.42	2.22	16	2
1:A:72:GLN:HE22	1:A:75:ASP:HB2	0.42	1.74	7	1
1:A:97:LEU:HD12	1:A:97:LEU:C	0.42	2.39	10	1
1:A:59:ARG:CG	1:A:60:VAL:N	0.42	2.82	14	3
1:A:15:ARG:N	1:A:15:ARG:CD	0.42	2.81	8	2
1:A:31:PHE:CE1	1:A:66:ALA:HB2	0.42	2.50	8	1
1:A:104:VAL:CG2	1:A:105:VAL:H	0.42	2.21	11	1
1:A:83:TRP:HB2	1:A:96:ARG:HD2	0.42	1.90	15	1
1:A:75:ASP:HB3	1:A:109:VAL:HG21	0.42	1.91	5	1
1:A:15:ARG:HD3	1:A:108:LEU:HD21	0.42	1.92	14	1
1:A:31:PHE:CE1	2:B:168:VAL:HG23	0.42	2.50	8	2
1:A:12:VAL:HG23	1:A:111:ARG:O	0.42	2.15	18	1
1:A:75:ASP:HB3	1:A:111:ARG:HE	0.42	1.75	9	1
1:A:18:ILE:HG21	1:A:31:PHE:HE1	0.42	1.70	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ARG:NE	1:A:96:ARG:CA	0.42	2.83	20	1
1:A:14:GLN:O	1:A:109:VAL:HG12	0.41	2.15	5	1
1:A:14:GLN:N	1:A:14:GLN:NE2	0.41	2.67	20	1
1:A:99:LYS:HG2	1:A:102:GLU:CD	0.41	2.39	2	1
1:A:17:GLU:HA	1:A:106:ARG:HA	0.41	1.91	3	1
1:A:76:LYS:HB3	1:A:78:MET:CE	0.41	2.38	7	1
1:A:88:VAL:HG13	1:A:92:GLN:OE1	0.41	2.16	8	1
1:A:80:VAL:C	1:A:82:GLY:N	0.41	2.79	5	2
1:A:88:VAL:CG2	1:A:92:GLN:HE22	0.41	2.24	17	1
1:A:13:VAL:HB	1:A:110:THR:CA	0.41	2.45	20	1
1:A:94:ARG:HA	1:A:97:LEU:HD12	0.41	1.92	2	1
1:A:17:GLU:HB3	1:A:106:ARG:HG2	0.41	1.92	3	1
1:A:32:SER:HA	2:B:167:MET:HA	0.41	1.91	7	1
1:A:72:GLN:HB2	1:A:75:ASP:OD2	0.41	2.16	10	1
1:A:90:HIS:HE1	2:B:166:SER:HB2	0.41	1.76	10	1
1:A:16:VAL:HG12	1:A:69:ALA:HB1	0.41	1.92	11	1
1:A:60:VAL:HB	1:A:73:ILE:CD1	0.41	2.46	17	1
1:A:89:THR:HG22	1:A:90:HIS:N	0.41	2.24	18	1
1:A:18:ILE:CG1	1:A:107:LEU:HD11	0.41	2.46	3	1
1:A:85:MET:HB2	1:A:93:ALA:HB1	0.41	1.92	4	1
1:A:97:LEU:HB3	1:A:105:VAL:HG21	0.41	1.91	19	1
1:A:94:ARG:NH1	2:B:168:VAL:HA	0.41	2.29	6	1
1:A:18:ILE:H	1:A:105:VAL:C	0.41	2.24	11	1
1:A:97:LEU:HA	1:A:105:VAL:HG11	0.41	1.93	1	1
1:A:77:ILE:HG23	1:A:107:LEU:HB3	0.41	1.91	12	1
1:A:81:ASN:ND2	1:A:106:ARG:H	0.41	2.13	12	1
1:A:88:VAL:HG13	1:A:92:GLN:HE22	0.41	1.75	17	1
1:A:88:VAL:CG1	1:A:92:GLN:OE1	0.41	2.69	18	1
1:A:80:VAL:HG13	1:A:83:TRP:HB2	0.41	1.93	19	1
1:A:94:ARG:HD3	2:B:166:SER:OG	0.41	2.16	8	1
1:A:16:VAL:HG22	1:A:18:ILE:CD1	0.41	2.45	17	1
1:A:107:LEU:HD13	1:A:107:LEU:N	0.40	2.31	12	1
1:A:80:VAL:CG1	1:A:85:MET:SD	0.40	3.07	19	1
1:A:59:ARG:CA	1:A:73:ILE:HD12	0.40	2.47	5	2
1:A:81:ASN:HB2	1:A:83:TRP:CE2	0.40	2.51	7	1
1:A:97:LEU:HD13	2:B:168:VAL:CG1	0.40	2.46	11	1
1:A:94:ARG:NH2	1:A:97:LEU:HD21	0.40	2.31	15	1
1:A:14:GLN:HE21	1:A:14:GLN:N	0.40	2.13	19	1
1:A:100:ARG:HA	1:A:100:ARG:HE	0.40	1.75	19	1
1:A:15:ARG:HB3	1:A:108:LEU:CD2	0.40	2.46	20	1
1:A:15:ARG:HG3	1:A:108:LEU:CD1	0.40	2.47	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ILE:HG12	1:A:107:LEU:HD22	0.40	1.92	17	1
1:A:76:LYS:HB2	1:A:110:THR:HB	0.40	1.94	17	1
1:A:92:GLN:O	1:A:95:LYS:HG3	0.40	2.17	17	1
1:A:79:GLN:CD	1:A:108:LEU:HB2	0.40	2.41	10	1
1:A:19:HIS:HB2	1:A:105:VAL:CG1	0.40	2.47	11	1
1:A:18:ILE:HD13	1:A:107:LEU:HD23	0.40	1.92	16	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	73/124 (59%)	62±2 (85±3%)	9±2 (12±3%)	2±1 (3±1%)	6	40
2	B	2/8 (25%)	2±0 (90±20%)	0±0 (10±20%)	0±0 (0±0%)	100	100
All	All	1500/2640 (57%)	1277 (85%)	182 (12%)	41 (3%)	6	41

All 9 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	65	PRO	18
1	A	84	ASP	7
1	A	104	VAL	7
1	A	85	MET	4
1	A	112	GLN	1
1	A	64	GLY	1
1	A	99	LYS	1
1	A	101	SER	1
1	A	102	GLU	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	61/107 (57%)	49±2 (80±4%)	12±2 (20±4%)	3	33
2	B	3/8 (38%)	3±0 (88±16%)	0±0 (12±16%)	7	50
All	All	1280/2300 (56%)	1029 (80%)	251 (20%)	3	33

All 50 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	67	GLU	19
1	A	79	GLN	17
1	A	72	GLN	16
1	A	89	THR	13
1	A	102	GLU	12
1	A	88	VAL	12
1	A	80	VAL	11
1	A	107	LEU	11
1	A	14	GLN	10
1	A	92	GLN	9
1	A	96	ARG	8
1	A	57	VAL	7
1	A	61	SER	7
1	A	59	ARG	6
1	A	73	ILE	6
1	A	112	GLN	6
1	A	85	MET	6
1	A	75	ASP	6
1	A	16	VAL	5
2	B	168	VAL	5
1	A	100	ARG	5
1	A	108	LEU	5
1	A	76	LYS	4
1	A	33	ILE	4
1	A	105	VAL	3
1	A	110	THR	3
1	A	83	TRP	3
1	A	111	ARG	3
1	A	104	VAL	2
1	A	65	PRO	2
1	A	97	LEU	2
1	A	17	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	15	ARG	2
1	A	19	HIS	2
1	A	84	ASP	2
1	A	106	ARG	1
1	A	56	TYR	1
2	B	167	MET	1
2	B	166	SER	1
1	A	81	ASN	1
1	A	60	VAL	1
1	A	71	LEU	1
1	A	78	MET	1
1	A	95	LYS	1
1	A	18	ILE	1
1	A	98	THR	1
1	A	32	SER	1
1	A	31	PHE	1
1	A	58	THR	1
1	A	13	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no 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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided