



Full wwPDB NMR Structure Validation Report ⓘ

Feb 14, 2022 – 07:54 AM EST

PDB ID : 1JM4
Title : NMR Structure of P/CAF Bromodomain in Complex with HIV-1 Tat Peptide
Authors : Mujtaba, S.; He, Y.; Zeng, L.; Farooq, A.; Carlson, J.E.; Ott, M.; Verdin, E.; Zhou, M.-M.
Deposited on : 2001-07-17

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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

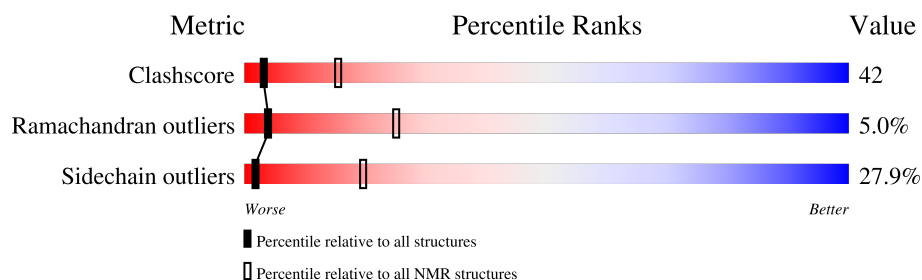
1 Overall quality at a glance

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	11	100%
2	B	118	19% 65% 5% 10%

2 Ensemble composition and analysis

This entry contains 25 models. Model 13 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	B:721-B:752, B:757-B:830 (106)	0.42	13

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

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

The models can be grouped into 6 clusters and 7 single-model clusters were found.

Cluster number	Models
1	2, 10, 11, 16, 19
2	3, 9, 12, 13, 18
3	5, 7
4	8, 14
5	4, 6
6	20, 23
Single-model clusters	1; 15; 17; 21; 22; 24; 25

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2188 atoms, of which 1098 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HIV-1 Tat Peptide.

Mol	Chain	Residues	Atoms						Trace
1	A	11	Total	C	H	N	O	S	0
			214	60	111	26	16	1	

- Molecule 2 is a protein called P300/CBP-associated Factor.

Mol	Chain	Residues	Atoms						Trace
2	B	118	Total	C	H	N	O	S	0
			1974	636	987	164	180	7	

There are 4 discrepancies between the modelled and reference sequences:

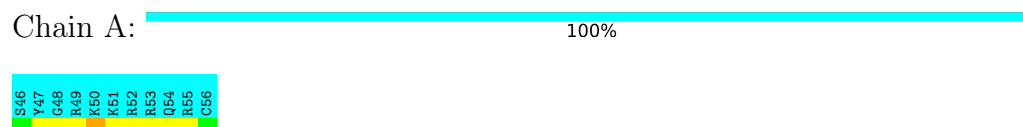
Chain	Residue	Modelled	Actual	Comment	Reference
B	715	GLY	-	cloning artifact	UNP Q92831
B	716	SER	-	cloning artifact	UNP Q92831
B	717	HIS	-	cloning artifact	UNP Q92831
B	718	MET	-	cloning artifact	UNP Q92831

4 Residue-property plots

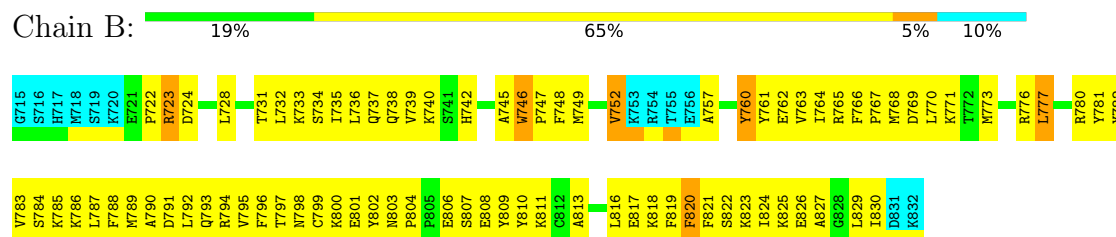
4.1 Average score per residue in the NMR ensemble

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: HIV-1 Tat Peptide



- Molecule 2: P300/CBP-associated Factor

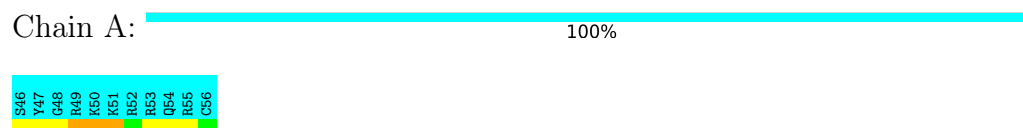


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

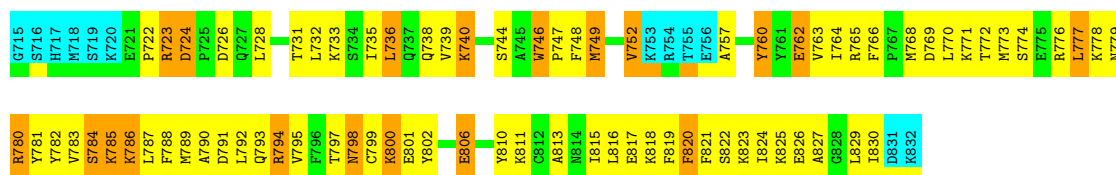
4.2.1 Score per residue for model 1

- Molecule 1: HIV-1 Tat Peptide



- Molecule 2: P300/CBP-associated Factor





4.2.2 Score per residue for model 2

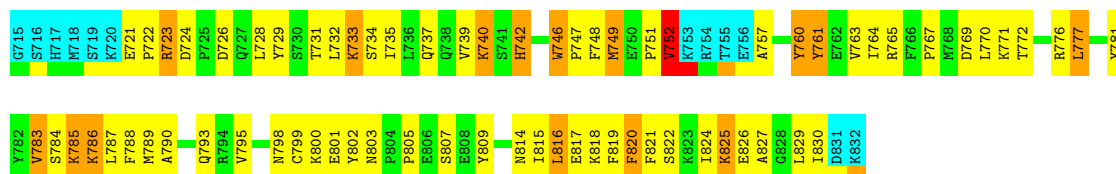
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  31% 46% 13% 10%



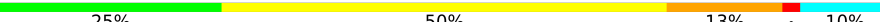
4.2.3 Score per residue for model 3

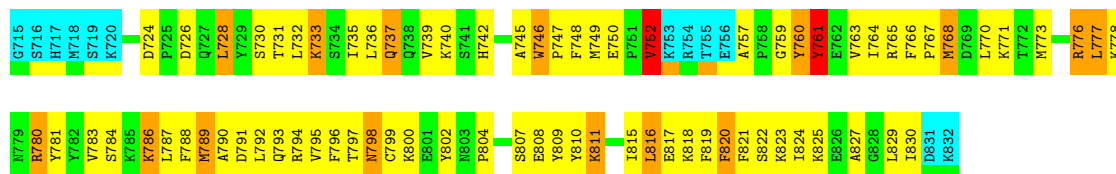
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  25% 50% 13% 10%



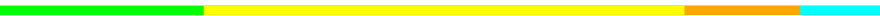
4.2.4 Score per residue for model 4

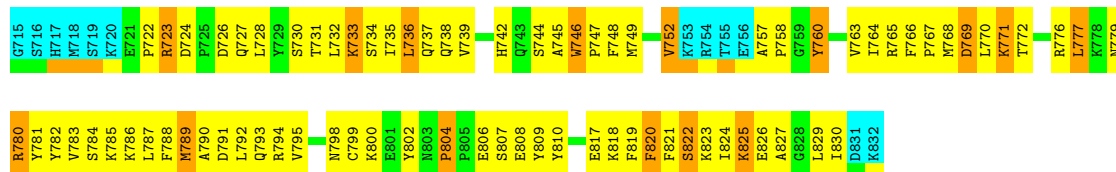
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  23% 54% 13% 10%



4.2.5 Score per residue for model 5

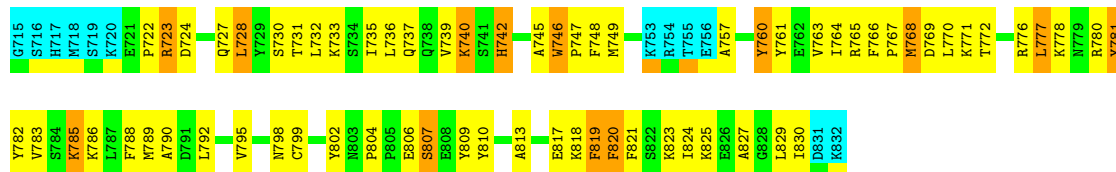
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  33% 46% 11% 10%



4.2.6 Score per residue for model 6

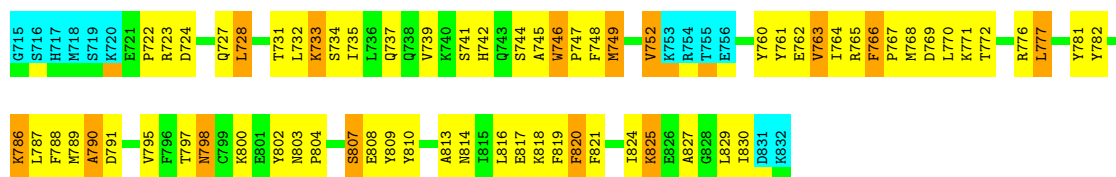
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  32% 46% 12% 10%



4.2.7 Score per residue for model 7

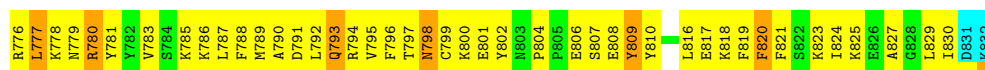
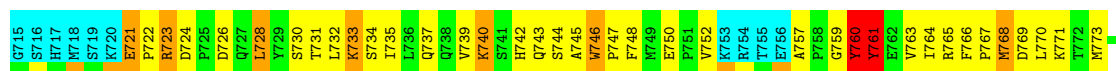
- Molecule 1: HIV-1 Tat Peptide

Chain A: 100%



- Molecule 2: P300/CBP-associated Factor

Chain B: 21% 56% 11% 10%



4.2.8 Score per residue for model 8

- Molecule 1: HIV-1 Tat Peptide

Chain A: 100%



- Molecule 2: P300/CBP-associated Factor

Chain B: 29% 48% 12% 10%



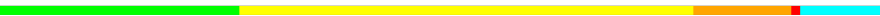
4.2.9 Score per residue for model 9

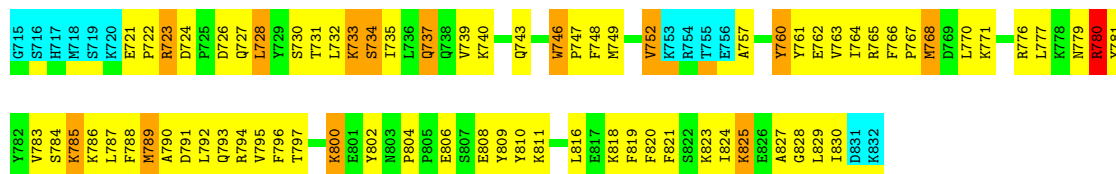
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  27% 51% 11% • 10%



4.2.10 Score per residue for model 10

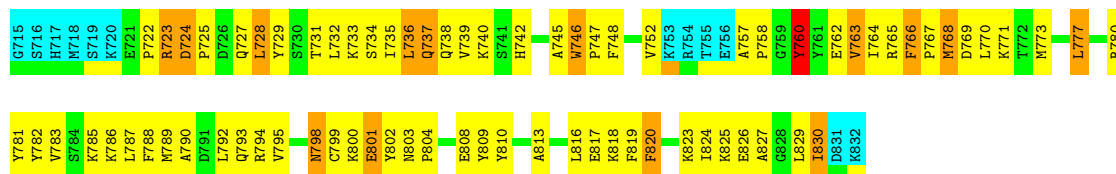
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  26% 51% 12% • 10%



4.2.11 Score per residue for model 11

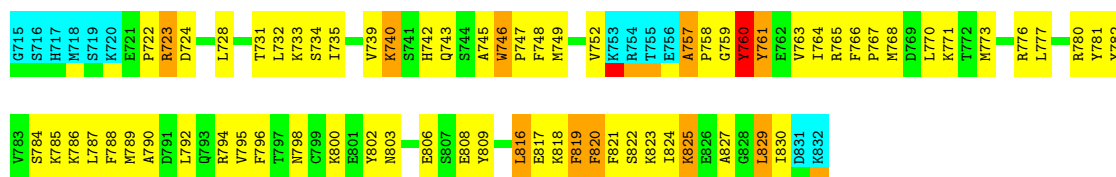
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  31% 49% 8% • 10%



4.2.12 Score per residue for model 12

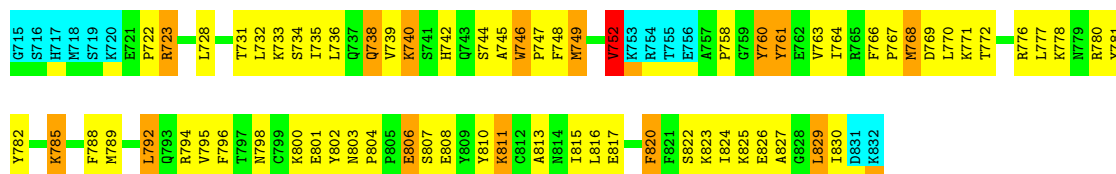
- Molecule 1: HIV-1 Tat Peptide

Chain A: 100%



- Molecule 2: P300/CBP-associated Factor

Chain B: 31% 46% 12% 10%



4.2.13 Score per residue for model 13 (medoid)

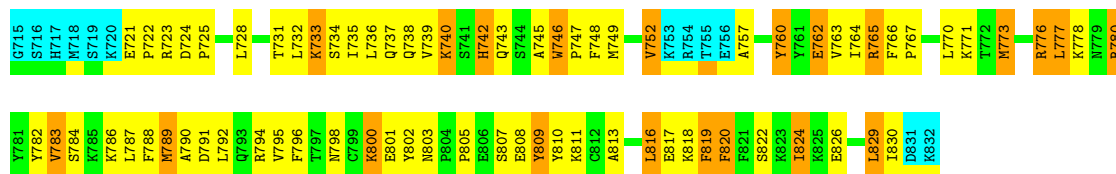
- Molecule 1: HIV-1 Tat Peptide

Chain A: 100%



- Molecule 2: P300/CBP-associated Factor

Chain B: 27% 45% 18% 10%




4.2.14 Score per residue for model 14

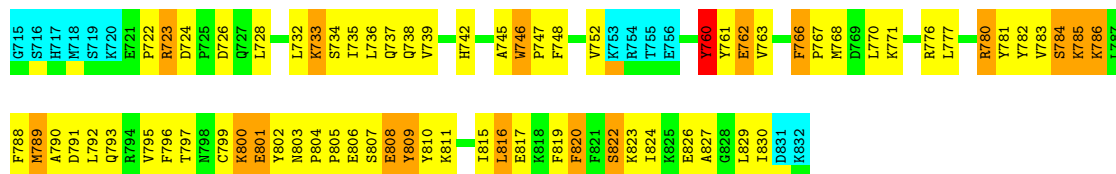
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  30% 45% 14% 10%



4.2.15 Score per residue for model 15

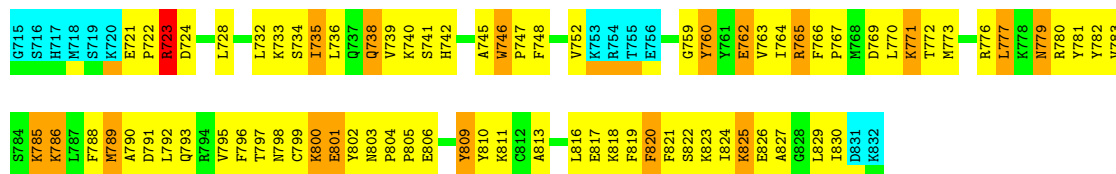
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

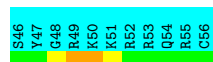
Chain B:  24% 51% 14% 10%



4.2.16 Score per residue for model 16

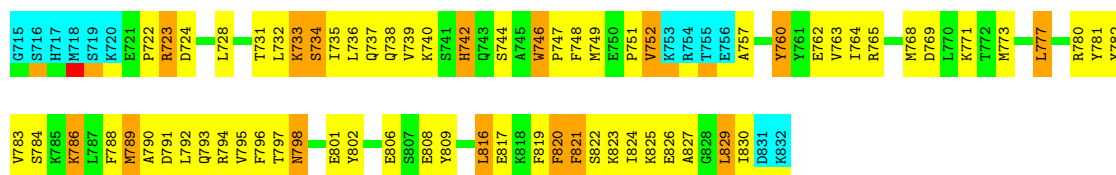
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

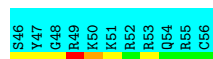
Chain B:  32% 45% 13% 10%



4.2.17 Score per residue for model 17

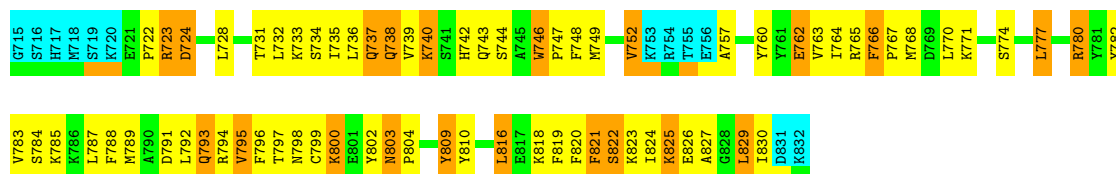
- Molecule 1: HIV-1 Tat Peptide

Chain A: 100%



- Molecule 2: P300/CBP-associated Factor

Chain B: 30% 42% 18% 10%



4.2.18 Score per residue for model 18

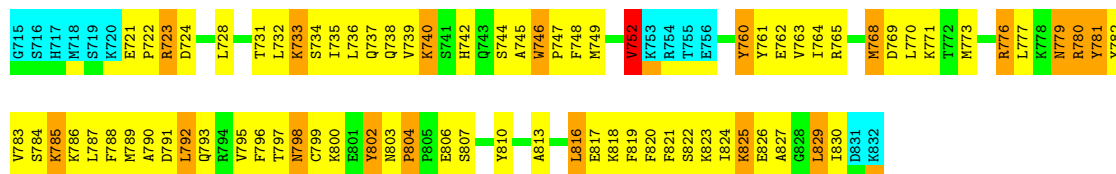
- Molecule 1: HIV-1 Tat Peptide

Chain A: 100%



- Molecule 2: P300/CBP-associated Factor

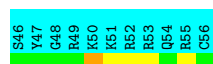
Chain B: 24% 50% 15% 10%



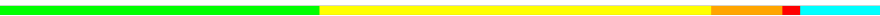
4.2.19 Score per residue for model 19

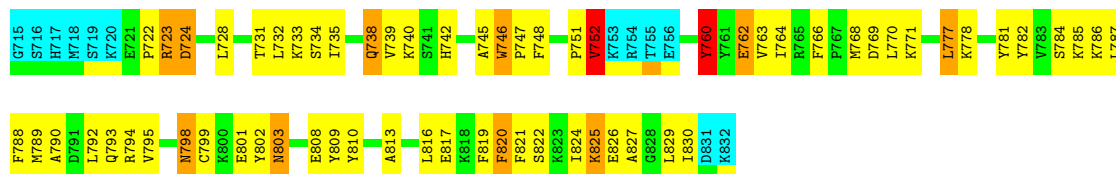
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  36% 44% 8% 10%



4.2.20 Score per residue for model 20

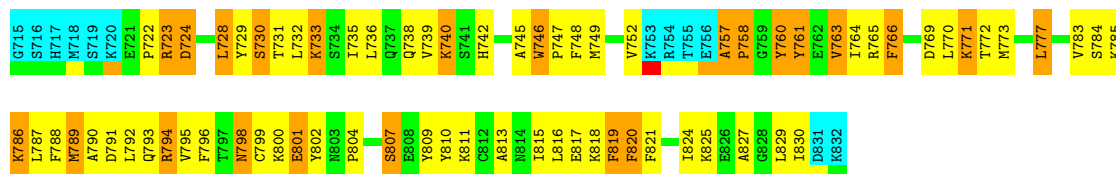
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

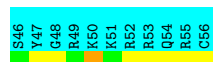
Chain B:  29% 42% 19% 10%



4.2.21 Score per residue for model 21

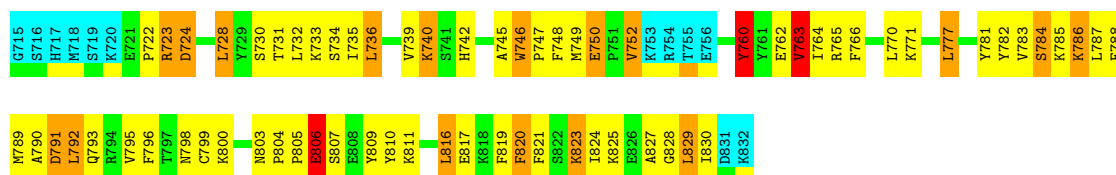
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  32% 41% 14% 10%



4.2.22 Score per residue for model 22

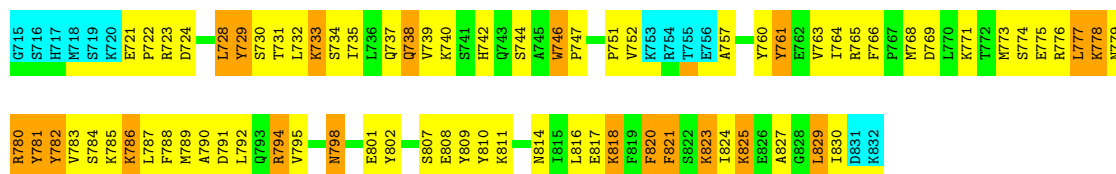
- Molecule 1: HIV-1 Tat Peptide

Chain A: 100%



- Molecule 2: P300/CBP-associated Factor

Chain B: 27% 46% 17% 10%



4.2.23 Score per residue for model 23

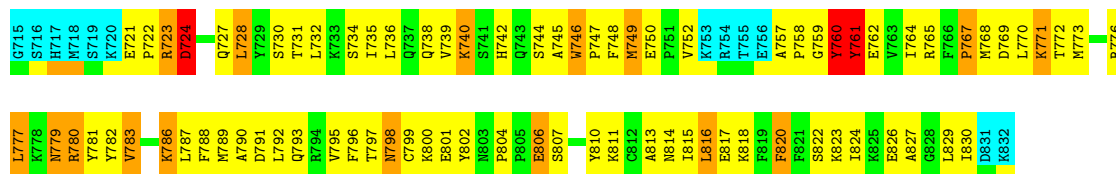
- Molecule 1: HIV-1 Tat Peptide

Chain A: 100%



- Molecule 2: P300/CBP-associated Factor

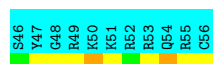
Chain B: 21% 53% 14% 10%



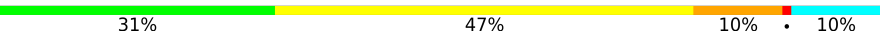
4.2.24 Score per residue for model 24

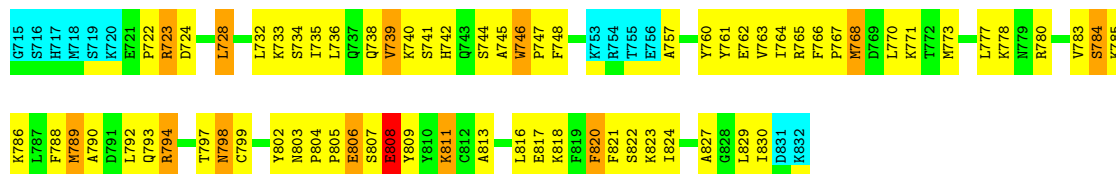
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  31% 47% 10% 10%



4.2.25 Score per residue for model 25

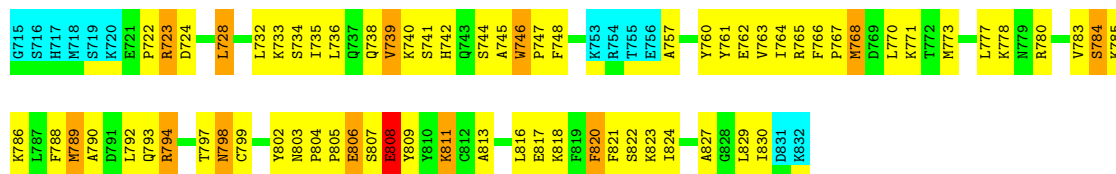
- Molecule 1: HIV-1 Tat Peptide

Chain A:  100%



- Molecule 2: P300/CBP-associated Factor

Chain B:  31% 47% 10% 10%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Distance Geometry/Simulated Annealing*.

Of the 100 calculated structures, 25 were deposited, based on the following criterion: *Back Calculated Data Agree with Experimental NOESY Spectrum, Structures with Acceptable Covalent Geometry, Structures with Favorable Non-bond Energy, Structures with the Least Restraint Violations, Structures with the Lowest Energy*.

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

Software name	Classification	Version
X-PLOR/ARIA	structure solution	2
X-PLOR 3.851	refinement	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ALY

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
2	B	1.01±0.00	0±0/916 (0.0± 0.0%)	1.27±0.01	0±0/1236 (0.0± 0.0%)
All	All	1.01	0/22900 (0.0%)	1.27	3/30900 (0.0%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	749	MET	N-CA-CB	-5.74	100.26	110.60	23	2
2	B	757	ALA	N-CA-CB	-5.12	102.94	110.10	20	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	0	0	0	0±0
2	B	890	887	887	75±10
All	All	22250	22175	22175	1863

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 42.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:824:ILE:HD12	2:B:830:ILE:HD13	1.06	1.24	10	2
2:B:796:PHE:CE1	2:B:816:LEU:HD13	0.94	1.97	17	5
2:B:760:TYR:CE2	2:B:764:ILE:HG21	0.92	1.98	7	11
2:B:732:LEU:HD22	2:B:788:PHE:CG	0.91	2.00	13	14
2:B:824:ILE:HG22	2:B:829:LEU:HD12	0.90	1.41	23	10
2:B:788:PHE:CE2	2:B:792:LEU:HD12	0.88	2.04	5	7
2:B:731:THR:HG21	2:B:827:ALA:HB1	0.88	1.47	21	7
2:B:752:VAL:HG11	2:B:760:TYR:CE2	0.87	2.04	13	11
2:B:752:VAL:HG21	2:B:760:TYR:CE2	0.86	2.06	11	4
2:B:731:THR:O	2:B:735:ILE:HD12	0.86	1.70	22	15
2:B:789:MET:CG	2:B:829:LEU:HD12	0.85	2.01	22	5
2:B:739:VAL:HB	2:B:816:LEU:HD21	0.85	1.47	18	6
2:B:733:LYS:CD	2:B:777:LEU:HD22	0.85	2.01	4	2
2:B:735:ILE:O	2:B:739:VAL:HG13	0.84	1.73	24	11
2:B:769:ASP:OD1	2:B:772:THR:HG22	0.83	1.74	2	6
2:B:748:PHE:CD2	2:B:816:LEU:HD12	0.82	2.08	11	6
2:B:789:MET:SD	2:B:829:LEU:HD13	0.82	2.14	19	3
2:B:763:VAL:HG12	2:B:801:GLU:OE2	0.82	1.73	20	2
2:B:768:MET:O	2:B:795:VAL:HG22	0.82	1.75	18	6
2:B:728:LEU:HD12	2:B:732:LEU:HD21	0.81	1.49	5	9
2:B:739:VAL:HB	2:B:816:LEU:HD11	0.81	1.51	10	5
2:B:792:LEU:HD22	2:B:796:PHE:CZ	0.81	2.11	17	5
2:B:789:MET:SD	2:B:830:ILE:HD11	0.81	2.16	23	9
2:B:763:VAL:O	2:B:764:ILE:HD13	0.80	1.76	3	11
2:B:792:LEU:HD23	2:B:820:PHE:CD2	0.80	2.11	23	7
2:B:732:LEU:HD13	2:B:788:PHE:HB2	0.80	1.51	22	20
2:B:799:CYS:SG	2:B:813:ALA:HB2	0.80	2.17	10	2
2:B:827:ALA:CB	2:B:829:LEU:HD23	0.79	2.06	24	8
2:B:824:ILE:CG2	2:B:829:LEU:HD12	0.79	2.06	23	6
2:B:732:LEU:HD22	2:B:788:PHE:CD2	0.79	2.13	8	14
2:B:731:THR:HG23	2:B:827:ALA:HB1	0.79	1.54	9	3
2:B:732:LEU:HB3	2:B:777:LEU:HD11	0.79	1.54	21	5
2:B:820:PHE:CE1	2:B:824:ILE:HG21	0.79	2.12	15	3
2:B:728:LEU:HD13	2:B:731:THR:HB	0.79	1.55	5	2
2:B:788:PHE:CE1	2:B:792:LEU:HD22	0.78	2.13	15	3
2:B:789:MET:SD	2:B:829:LEU:HD12	0.78	2.18	17	7
2:B:752:VAL:HG21	2:B:760:TYR:CZ	0.78	2.13	22	6
2:B:811:LYS:O	2:B:815:ILE:HD12	0.78	1.76	3	5
2:B:732:LEU:HB2	2:B:777:LEU:HD11	0.78	1.55	8	7
2:B:736:LEU:HA	2:B:739:VAL:HG22	0.78	1.56	18	11
2:B:791:ASP:O	2:B:795:VAL:HG23	0.77	1.78	3	12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:792:LEU:HD22	2:B:796:PHE:CE2	0.77	2.14	18	5
2:B:745:ALA:HB2	2:B:816:LEU:HD22	0.77	1.54	19	2
2:B:764:ILE:HG23	2:B:798:ASN:HB2	0.77	1.56	6	7
2:B:820:PHE:CE2	2:B:824:ILE:HD13	0.77	2.15	18	3
2:B:732:LEU:CB	2:B:777:LEU:HD11	0.76	2.10	16	8
2:B:752:VAL:HG21	2:B:760:TYR:CE1	0.76	2.16	6	3
2:B:722:PRO:CB	2:B:728:LEU:HD13	0.76	2.09	7	5
2:B:763:VAL:C	2:B:764:ILE:HD13	0.76	2.01	16	13
2:B:824:ILE:CD1	2:B:830:ILE:HD12	0.75	2.12	13	2
2:B:824:ILE:HD12	2:B:830:ILE:CD1	0.75	2.08	10	4
2:B:829:LEU:C	2:B:830:ILE:HD12	0.75	2.02	10	2
2:B:732:LEU:HD13	2:B:788:PHE:CB	0.74	2.12	1	11
2:B:788:PHE:CE2	2:B:792:LEU:HD22	0.74	2.17	19	6
2:B:763:VAL:HG23	2:B:764:ILE:HG12	0.74	1.58	12	14
2:B:793:GLN:O	2:B:797:THR:HG22	0.74	1.83	7	4
2:B:824:ILE:CB	2:B:829:LEU:HD12	0.74	2.13	3	6
2:B:728:LEU:HD12	2:B:732:LEU:CD2	0.73	2.13	5	3
2:B:752:VAL:HG11	2:B:760:TYR:OH	0.73	1.83	15	2
2:B:762:GLU:O	2:B:763:VAL:HG13	0.73	1.82	8	4
2:B:752:VAL:HG11	2:B:760:TYR:CZ	0.73	2.17	13	6
2:B:764:ILE:HG23	2:B:798:ASN:OD1	0.73	1.83	24	2
2:B:736:LEU:HD13	2:B:736:LEU:O	0.73	1.84	15	3
2:B:824:ILE:CD1	2:B:830:ILE:HD13	0.72	2.15	19	2
2:B:824:ILE:HG22	2:B:829:LEU:CD1	0.71	2.15	14	5
2:B:733:LYS:HD2	2:B:777:LEU:HD22	0.71	1.60	4	2
2:B:777:LEU:O	2:B:777:LEU:HD13	0.71	1.85	20	8
2:B:820:PHE:O	2:B:824:ILE:HG23	0.71	1.86	8	7
2:B:789:MET:CE	2:B:830:ILE:HD11	0.71	2.15	7	2
2:B:792:LEU:HD13	2:B:820:PHE:CD2	0.70	2.20	21	4
2:B:732:LEU:HD22	2:B:788:PHE:CD1	0.70	2.20	22	6
2:B:788:PHE:CZ	2:B:792:LEU:HD22	0.69	2.22	22	4
2:B:736:LEU:HD21	2:B:770:LEU:HD22	0.69	1.63	20	2
2:B:731:THR:CG2	2:B:827:ALA:HB1	0.68	2.18	19	8
2:B:764:ILE:HG22	2:B:767:PRO:HD3	0.68	1.65	11	2
2:B:784:SER:OG	2:B:787:LEU:HD12	0.68	1.89	9	2
2:B:824:ILE:HB	2:B:829:LEU:HD12	0.68	1.64	3	4
2:B:773:MET:CE	2:B:792:LEU:HD13	0.67	2.18	3	7
2:B:786:LYS:O	2:B:790:ALA:HB2	0.67	1.90	19	22
2:B:735:ILE:HG23	2:B:820:PHE:HB2	0.67	1.64	21	3
2:B:732:LEU:HD13	2:B:788:PHE:CG	0.67	2.25	1	4
2:B:739:VAL:HG22	2:B:816:LEU:CD2	0.67	2.20	21	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:745:ALA:CB	2:B:816:LEU:HD22	0.67	2.19	19	2
2:B:722:PRO:HB3	2:B:728:LEU:HD13	0.67	1.66	7	5
2:B:722:PRO:HA	2:B:728:LEU:HD13	0.67	1.65	23	5
2:B:829:LEU:HD23	2:B:829:LEU:N	0.67	2.04	13	3
2:B:792:LEU:HD23	2:B:820:PHE:CD1	0.67	2.25	15	3
2:B:722:PRO:CA	2:B:728:LEU:HD13	0.66	2.20	7	5
2:B:745:ALA:HB2	2:B:816:LEU:CD2	0.65	2.20	19	2
2:B:764:ILE:HD11	2:B:802:TYR:CD1	0.65	2.27	15	4
2:B:731:THR:HG22	2:B:735:ILE:HD11	0.65	1.68	16	4
2:B:739:VAL:HG22	2:B:816:LEU:HD11	0.65	1.67	12	1
2:B:783:VAL:HG13	2:B:783:VAL:O	0.65	1.91	21	12
2:B:784:SER:HB2	2:B:787:LEU:HD22	0.65	1.69	1	1
2:B:829:LEU:O	2:B:830:ILE:HD12	0.64	1.90	10	1
2:B:782:TYR:HA	2:B:787:LEU:HD23	0.64	1.70	23	1
2:B:739:VAL:HG12	2:B:770:LEU:CD1	0.63	2.22	6	5
2:B:764:ILE:HD11	2:B:802:TYR:CD2	0.63	2.29	17	1
2:B:748:PHE:CD2	2:B:816:LEU:HD23	0.62	2.28	12	8
2:B:764:ILE:HG23	2:B:798:ASN:HB3	0.61	1.70	4	2
2:B:735:ILE:HD11	2:B:829:LEU:CD1	0.61	2.25	9	2
2:B:824:ILE:HA	2:B:829:LEU:HD12	0.61	1.71	19	2
2:B:739:VAL:HG12	2:B:770:LEU:HD13	0.61	1.72	7	3
2:B:764:ILE:HD12	2:B:798:ASN:HB2	0.61	1.72	23	3
2:B:783:VAL:HG22	2:B:783:VAL:O	0.61	1.96	13	4
2:B:789:MET:HG2	2:B:829:LEU:HD12	0.61	1.72	22	1
2:B:783:VAL:O	2:B:783:VAL:HG12	0.61	1.95	2	3
2:B:827:ALA:HB3	2:B:829:LEU:HD23	0.61	1.71	24	8
2:B:784:SER:HB3	2:B:787:LEU:HD12	0.61	1.73	21	1
2:B:785:LYS:CB	2:B:829:LEU:HD13	0.61	2.26	5	2
2:B:739:VAL:HG12	2:B:770:LEU:HD11	0.61	1.71	6	3
2:B:821:PHE:CE2	2:B:830:ILE:HG21	0.61	2.31	6	3
2:B:728:LEU:HD11	2:B:732:LEU:HD21	0.61	1.72	22	3
2:B:733:LYS:CD	2:B:777:LEU:HD12	0.61	2.26	17	1
2:B:748:PHE:HB3	2:B:795:VAL:HG11	0.60	1.70	6	1
2:B:739:VAL:CB	2:B:816:LEU:HD11	0.60	2.26	15	4
2:B:803:ASN:N	2:B:804:PRO:CD	0.60	2.64	24	2
2:B:789:MET:HE3	2:B:830:ILE:HD11	0.60	1.73	7	1
2:B:789:MET:HE1	2:B:824:ILE:HD12	0.60	1.73	16	2
2:B:732:LEU:HD12	2:B:782:TYR:O	0.60	1.97	12	7
2:B:824:ILE:HD12	2:B:830:ILE:HG13	0.60	1.73	4	1
2:B:746:TRP:N	2:B:747:PRO:HD2	0.60	2.12	23	25
2:B:728:LEU:HD11	2:B:829:LEU:HD21	0.59	1.73	23	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:830:ILE:O	2:B:830:ILE:HG22	0.59	1.97	4	3
2:B:792:LEU:HD23	2:B:820:PHE:CE2	0.58	2.33	3	4
2:B:789:MET:HE1	2:B:824:ILE:HD13	0.58	1.75	10	4
2:B:824:ILE:HD12	2:B:830:ILE:CG1	0.58	2.29	20	14
2:B:739:VAL:CB	2:B:816:LEU:HD21	0.58	2.28	13	5
2:B:787:LEU:HD12	2:B:787:LEU:N	0.58	2.13	2	9
2:B:773:MET:HE1	2:B:792:LEU:HD13	0.58	1.75	15	3
2:B:728:LEU:O	2:B:728:LEU:HD13	0.58	1.99	10	2
2:B:789:MET:CE	2:B:824:ILE:HD12	0.58	2.29	16	2
2:B:785:LYS:HB3	2:B:829:LEU:HD13	0.58	1.75	12	2
2:B:731:THR:HG21	2:B:827:ALA:CB	0.58	2.29	6	2
2:B:742:HIS:CE1	2:B:819:PHE:CD2	0.58	2.92	11	2
2:B:829:LEU:N	2:B:829:LEU:CD2	0.57	2.68	17	9
2:B:733:LYS:HD2	2:B:777:LEU:HD21	0.57	1.76	8	1
2:B:827:ALA:HB1	2:B:829:LEU:HD23	0.56	1.76	24	4
2:B:792:LEU:HD23	2:B:820:PHE:CE1	0.56	2.34	15	3
2:B:722:PRO:HB3	2:B:728:LEU:HD22	0.56	1.74	7	5
2:B:764:ILE:HG23	2:B:798:ASN:CG	0.56	2.20	1	2
2:B:728:LEU:CD1	2:B:732:LEU:HD21	0.56	2.28	16	8
2:B:760:TYR:CE1	2:B:764:ILE:HG21	0.56	2.36	19	1
2:B:742:HIS:CE1	2:B:815:ILE:HG22	0.56	2.35	2	1
2:B:763:VAL:HG23	2:B:764:ILE:CD1	0.56	2.30	17	3
2:B:789:MET:HE1	2:B:824:ILE:HG21	0.56	1.76	21	2
2:B:763:VAL:HG23	2:B:764:ILE:CG1	0.55	2.31	12	7
2:B:748:PHE:CE2	2:B:816:LEU:HD23	0.55	2.36	15	4
2:B:764:ILE:HG22	2:B:767:PRO:CD	0.55	2.31	11	2
2:B:748:PHE:CD1	2:B:795:VAL:CG1	0.55	2.89	13	8
2:B:745:ALA:HB1	2:B:770:LEU:CD1	0.55	2.31	15	5
2:B:742:HIS:HB3	2:B:745:ALA:HB2	0.55	1.79	13	1
2:B:732:LEU:HB2	2:B:777:LEU:HD21	0.54	1.79	3	7
2:B:735:ILE:HD11	2:B:829:LEU:HD12	0.54	1.78	9	1
2:B:748:PHE:CG	2:B:795:VAL:CG1	0.54	2.90	23	4
2:B:789:MET:CE	2:B:824:ILE:HD13	0.54	2.31	23	1
2:B:789:MET:HE1	2:B:824:ILE:CD1	0.54	2.32	22	10
2:B:745:ALA:HB2	2:B:816:LEU:HD11	0.54	1.79	6	1
2:B:722:PRO:HB2	2:B:728:LEU:HD23	0.54	1.79	5	3
2:B:789:MET:CE	2:B:820:PHE:CE2	0.54	2.91	21	1
2:B:824:ILE:HD12	2:B:830:ILE:HD11	0.54	1.79	14	5
2:B:739:VAL:CG1	2:B:770:LEU:HD11	0.54	2.33	11	5
2:B:728:LEU:HD11	2:B:829:LEU:CD2	0.54	2.33	8	2
2:B:776:ARG:CD	2:B:782:TYR:CE2	0.54	2.91	15	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:731:THR:HG22	2:B:735:ILE:CD1	0.53	2.33	16	4
2:B:760:TYR:CE1	2:B:802:TYR:CZ	0.53	2.96	16	2
2:B:829:LEU:CB	2:B:830:ILE:HD12	0.53	2.33	19	1
2:B:786:LYS:CD	2:B:787:LEU:HD12	0.53	2.33	23	1
2:B:732:LEU:HD23	2:B:732:LEU:N	0.53	2.17	15	1
2:B:746:TRP:CE3	2:B:746:TRP:N	0.53	2.77	4	12
2:B:722:PRO:CB	2:B:728:LEU:HD23	0.53	2.34	10	5
2:B:820:PHE:CD1	2:B:821:PHE:N	0.53	2.77	6	5
2:B:748:PHE:N	2:B:748:PHE:CD1	0.53	2.76	20	8
2:B:746:TRP:N	2:B:746:TRP:CE3	0.53	2.77	2	9
2:B:739:VAL:HG12	2:B:740:LYS:N	0.53	2.19	11	2
2:B:796:PHE:CZ	2:B:816:LEU:HD22	0.53	2.39	17	1
2:B:736:LEU:HD11	2:B:770:LEU:CD2	0.52	2.34	23	1
2:B:798:ASN:OD1	2:B:799:CYS:N	0.52	2.43	15	9
2:B:769:ASP:CG	2:B:772:THR:HG22	0.52	2.24	2	3
2:B:747:PRO:CB	2:B:809:TYR:CE2	0.52	2.92	24	2
2:B:788:PHE:CE2	2:B:792:LEU:CD1	0.52	2.92	8	5
2:B:766:PHE:CE2	2:B:768:MET:CE	0.52	2.92	24	2
2:B:742:HIS:CE1	2:B:819:PHE:CG	0.52	2.97	11	1
2:B:742:HIS:CB	2:B:745:ALA:HB2	0.52	2.35	13	1
2:B:735:ILE:O	2:B:739:VAL:HG23	0.52	2.04	7	6
2:B:764:ILE:HD12	2:B:798:ASN:CB	0.52	2.34	23	3
2:B:748:PHE:CD1	2:B:748:PHE:N	0.52	2.78	21	3
2:B:752:VAL:O	2:B:757:ALA:HB2	0.52	2.05	23	1
2:B:820:PHE:CE2	2:B:824:ILE:CD1	0.52	2.92	18	1
2:B:764:ILE:O	2:B:766:PHE:N	0.51	2.43	21	7
2:B:742:HIS:NE2	2:B:819:PHE:CG	0.51	2.77	13	2
2:B:764:ILE:HD12	2:B:798:ASN:OD1	0.51	2.06	19	1
2:B:824:ILE:HA	2:B:827:ALA:HB3	0.51	1.82	2	2
2:B:800:LYS:CD	2:B:810:TYR:CE1	0.51	2.94	1	1
2:B:789:MET:CE	2:B:824:ILE:HG21	0.51	2.36	23	2
2:B:783:VAL:H	2:B:787:LEU:HD23	0.51	1.66	22	1
2:B:789:MET:HE2	2:B:830:ILE:HD11	0.51	1.82	19	3
2:B:800:LYS:CD	2:B:810:TYR:CZ	0.51	2.94	3	4
2:B:824:ILE:CD1	2:B:830:ILE:CG1	0.50	2.89	2	5
2:B:792:LEU:CD2	2:B:796:PHE:CZ	0.50	2.92	17	4
2:B:796:PHE:HE1	2:B:816:LEU:HD13	0.50	1.64	11	1
2:B:760:TYR:CD2	2:B:764:ILE:HG21	0.50	2.41	23	1
2:B:728:LEU:HD13	2:B:731:THR:CB	0.50	2.31	5	1
2:B:824:ILE:HB	2:B:829:LEU:HB2	0.50	1.84	1	5
2:B:742:HIS:O	2:B:746:TRP:CH2	0.50	2.65	18	22

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:722:PRO:CB	2:B:728:LEU:CD2	0.50	2.90	19	13
2:B:804:PRO:HB2	2:B:805:PRO:CA	0.50	2.37	24	2
2:B:820:PHE:CE1	2:B:824:ILE:CG2	0.50	2.92	15	1
2:B:784:SER:CB	2:B:787:LEU:HD12	0.50	2.36	21	2
2:B:786:LYS:O	2:B:790:ALA:CB	0.49	2.60	22	17
2:B:822:SER:O	2:B:826:GLU:CG	0.49	2.60	16	12
2:B:824:ILE:CA	2:B:829:LEU:HD12	0.49	2.37	19	1
2:B:738:GLN:OE1	2:B:739:VAL:HG23	0.49	2.07	12	4
2:B:784:SER:HB3	2:B:787:LEU:HD13	0.49	1.82	2	2
2:B:776:ARG:CD	2:B:782:TYR:CE1	0.49	2.95	4	1
2:B:792:LEU:HD23	2:B:820:PHE:HE2	0.49	1.66	19	1
2:B:792:LEU:HD13	2:B:820:PHE:CE2	0.49	2.43	20	2
2:B:780:ARG:O	2:B:783:VAL:HG23	0.49	2.07	9	1
2:B:776:ARG:NH1	2:B:782:TYR:CZ	0.49	2.81	12	1
2:B:804:PRO:HB2	2:B:805:PRO:HA	0.49	1.84	24	2
2:B:736:LEU:CD1	2:B:770:LEU:HD22	0.49	2.38	18	1
2:B:792:LEU:CD2	2:B:796:PHE:CE2	0.49	2.96	21	1
2:B:747:PRO:CB	2:B:809:TYR:CD2	0.49	2.95	24	2
2:B:768:MET:C	2:B:795:VAL:HG22	0.49	2.28	11	2
2:B:745:ALA:CB	2:B:816:LEU:HD11	0.49	2.38	6	1
2:B:740:LYS:HA	2:B:749:MET:HE2	0.49	1.85	13	1
2:B:735:ILE:CD1	2:B:829:LEU:HD11	0.49	2.38	14	2
2:B:810:TYR:CD1	2:B:810:TYR:O	0.48	2.66	10	5
2:B:739:VAL:O	2:B:745:ALA:HB2	0.48	2.09	24	8
2:B:782:TYR:CE2	2:B:787:LEU:O	0.48	2.67	6	2
2:B:739:VAL:CG1	2:B:770:LEU:CD1	0.48	2.92	7	2
2:B:798:ASN:O	2:B:802:TYR:CE1	0.48	2.66	8	3
2:B:802:TYR:CD2	2:B:803:ASN:N	0.48	2.81	10	1
2:B:766:PHE:CZ	2:B:768:MET:CE	0.48	2.97	19	2
2:B:742:HIS:O	2:B:746:TRP:CZ2	0.48	2.67	14	5
2:B:820:PHE:CE1	2:B:824:ILE:HD13	0.48	2.42	19	1
2:B:735:ILE:HG21	2:B:788:PHE:HE2	0.48	1.68	21	1
2:B:757:ALA:HB1	2:B:760:TYR:CD1	0.48	2.44	3	1
2:B:742:HIS:O	2:B:746:TRP:CZ3	0.48	2.67	19	5
2:B:817:GLU:O	2:B:820:PHE:CD1	0.48	2.67	10	4
2:B:739:VAL:CG1	2:B:770:LEU:HD13	0.48	2.38	7	1
2:B:745:ALA:CA	2:B:816:LEU:HD22	0.48	2.39	15	4
2:B:773:MET:CE	2:B:788:PHE:CE1	0.48	2.96	20	2
2:B:789:MET:HE3	2:B:824:ILE:HG21	0.48	1.85	16	3
2:B:777:LEU:O	2:B:781:TYR:CD1	0.48	2.67	22	1
2:B:817:GLU:OE1	2:B:820:PHE:CD1	0.48	2.67	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:817:GLU:O	2:B:820:PHE:CE1	0.48	2.67	12	5
2:B:789:MET:CG	2:B:829:LEU:HD22	0.48	2.38	15	1
2:B:751:PRO:O	2:B:752:VAL:HG13	0.48	2.09	19	1
2:B:789:MET:CE	2:B:824:ILE:CD1	0.48	2.92	16	5
2:B:782:TYR:CZ	2:B:791:ASP:OD2	0.48	2.67	16	3
2:B:728:LEU:HD12	2:B:784:SER:O	0.48	2.09	17	1
2:B:742:HIS:NE2	2:B:819:PHE:CB	0.48	2.77	19	1
2:B:748:PHE:CG	2:B:795:VAL:HG11	0.48	2.44	23	1
2:B:823:LYS:O	2:B:827:ALA:N	0.48	2.47	14	18
2:B:789:MET:HE2	2:B:824:ILE:HD12	0.48	1.84	12	1
2:B:798:ASN:O	2:B:802:TYR:CE2	0.48	2.67	20	2
2:B:787:LEU:N	2:B:787:LEU:CD1	0.47	2.77	10	3
2:B:792:LEU:O	2:B:796:PHE:CD2	0.47	2.67	3	4
2:B:796:PHE:CD2	2:B:817:GLU:OE1	0.47	2.67	23	3
2:B:776:ARG:HD2	2:B:782:TYR:CE1	0.47	2.44	4	1
2:B:830:ILE:O	2:B:830:ILE:CG2	0.47	2.62	10	3
2:B:736:LEU:HD13	2:B:736:LEU:C	0.47	2.30	15	2
2:B:820:PHE:CZ	2:B:824:ILE:HD13	0.47	2.44	19	1
2:B:781:TYR:O	2:B:782:TYR:CD1	0.47	2.67	5	1
2:B:752:VAL:CG2	2:B:757:ALA:CB	0.47	2.92	8	2
2:B:773:MET:CE	2:B:792:LEU:CD1	0.47	2.93	15	2
2:B:800:LYS:CD	2:B:810:TYR:CE2	0.47	2.97	12	4
2:B:802:TYR:CZ	2:B:803:ASN:OD1	0.47	2.67	19	2
2:B:768:MET:CB	2:B:795:VAL:CG2	0.47	2.92	17	1
2:B:780:ARG:NH2	2:B:787:LEU:CD2	0.47	2.77	22	1
2:B:797:THR:HG23	2:B:798:ASN:N	0.47	2.25	8	4
2:B:800:LYS:HD2	2:B:810:TYR:CZ	0.47	2.44	3	2
2:B:788:PHE:CZ	2:B:792:LEU:HD12	0.47	2.44	5	2
2:B:782:TYR:CE1	2:B:791:ASP:OD2	0.47	2.67	17	2
2:B:788:PHE:CE2	2:B:792:LEU:CD2	0.47	2.96	19	2
2:B:747:PRO:HB2	2:B:809:TYR:CD2	0.47	2.45	24	2
2:B:748:PHE:O	2:B:770:LEU:N	0.47	2.47	21	19
2:B:733:LYS:CE	2:B:777:LEU:CD1	0.47	2.93	2	1
2:B:798:ASN:O	2:B:802:TYR:CD1	0.47	2.67	10	2
2:B:829:LEU:N	2:B:829:LEU:HD23	0.47	2.24	11	3
2:B:736:LEU:HD11	2:B:770:LEU:HD22	0.47	1.86	23	2
2:B:782:TYR:CG	2:B:791:ASP:OD2	0.47	2.67	18	1
2:B:802:TYR:CE2	2:B:803:ASN:OD1	0.47	2.67	2	3
2:B:784:SER:HB2	2:B:787:LEU:HD13	0.47	1.84	20	2
2:B:799:CYS:O	2:B:803:ASN:ND2	0.47	2.47	24	5
2:B:760:TYR:CD1	2:B:802:TYR:CE1	0.47	3.03	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:781:TYR:O	2:B:782:TYR:C	0.47	2.53	22	1
2:B:785:LYS:CE	2:B:786:LYS:N	0.47	2.78	2	1
2:B:804:PRO:CD	2:B:809:TYR:CB	0.47	2.93	17	2
2:B:740:LYS:CD	2:B:749:MET:CE	0.47	2.93	17	1
2:B:823:LYS:O	2:B:827:ALA:CB	0.47	2.63	16	10
2:B:731:THR:CG2	2:B:827:ALA:CB	0.47	2.92	21	2
2:B:760:TYR:O	2:B:761:TYR:CB	0.47	2.63	22	2
2:B:760:TYR:CE1	2:B:764:ILE:HG13	0.46	2.44	16	5
2:B:796:PHE:N	2:B:796:PHE:CD1	0.46	2.79	17	2
2:B:746:TRP:N	2:B:747:PRO:CD	0.46	2.78	4	8
2:B:733:LYS:CE	2:B:777:LEU:CD2	0.46	2.93	16	2
2:B:731:THR:C	2:B:735:ILE:HD12	0.46	2.30	16	5
2:B:800:LYS:HD3	2:B:810:TYR:CE2	0.46	2.45	12	3
2:B:782:TYR:CE2	2:B:791:ASP:OD2	0.46	2.68	21	3
2:B:742:HIS:NE2	2:B:815:ILE:CG2	0.46	2.79	14	1
2:B:733:LYS:HD2	2:B:777:LEU:HD12	0.46	1.87	17	1
2:B:776:ARG:O	2:B:780:ARG:N	0.46	2.49	15	3
2:B:728:LEU:CD1	2:B:732:LEU:CD2	0.46	2.92	5	2
2:B:742:HIS:NE2	2:B:819:PHE:CD2	0.46	2.84	5	2
2:B:764:ILE:HD12	2:B:798:ASN:HB3	0.46	1.86	17	2
2:B:782:TYR:CE1	2:B:787:LEU:HD22	0.46	2.45	19	1
2:B:748:PHE:CD1	2:B:795:VAL:HG12	0.46	2.45	19	3
2:B:805:PRO:O	2:B:806:GLU:C	0.46	2.54	24	2
2:B:817:GLU:HA	2:B:820:PHE:CE1	0.46	2.46	2	13
2:B:764:ILE:HD13	2:B:764:ILE:N	0.46	2.26	17	6
2:B:760:TYR:CE1	2:B:802:TYR:CE1	0.46	3.04	16	2
2:B:817:GLU:OE1	2:B:820:PHE:CE1	0.46	2.69	19	1
2:B:792:LEU:HD13	2:B:820:PHE:HD2	0.46	1.69	21	1
2:B:817:GLU:HA	2:B:820:PHE:CD1	0.46	2.46	2	5
2:B:766:PHE:O	2:B:768:MET:CG	0.46	2.64	24	2
2:B:746:TRP:HB2	2:B:747:PRO:CD	0.46	2.41	12	12
2:B:800:LYS:HD3	2:B:810:TYR:CZ	0.46	2.46	8	4
2:B:820:PHE:CD2	2:B:824:ILE:HD13	0.46	2.44	18	1
2:B:735:ILE:HA	2:B:738:GLN:NE2	0.46	2.26	17	2
2:B:821:PHE:CD2	2:B:825:LYS:CE	0.46	2.99	17	1
2:B:722:PRO:CB	2:B:728:LEU:HD21	0.45	2.40	17	3
2:B:802:TYR:CD1	2:B:802:TYR:C	0.45	2.87	18	2
2:B:824:ILE:HD12	2:B:830:ILE:HG12	0.45	1.87	20	2
2:B:748:PHE:CE1	2:B:799:CYS:SG	0.45	3.10	5	3
2:B:735:ILE:CD1	2:B:829:LEU:CD1	0.45	2.94	14	3
2:B:821:PHE:CZ	2:B:825:LYS:CD	0.45	2.99	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:745:ALA:HA	2:B:816:LEU:HD11	0.45	1.89	7	1
2:B:728:LEU:HD21	2:B:829:LEU:CD2	0.45	2.42	23	1
2:B:824:ILE:HG13	2:B:825:LYS:N	0.45	2.27	8	17
2:B:730:SER:HA	2:B:733:LYS:CB	0.45	2.41	20	1
2:B:776:ARG:HB3	2:B:782:TYR:CE2	0.45	2.46	22	1
2:B:803:ASN:O	2:B:807:SER:CB	0.45	2.64	24	2
2:B:745:ALA:HB1	2:B:770:LEU:HD12	0.45	1.89	3	4
2:B:788:PHE:CZ	2:B:792:LEU:CD1	0.45	2.99	8	1
2:B:776:ARG:O	2:B:779:ASN:N	0.45	2.49	22	4
2:B:739:VAL:O	2:B:745:ALA:CB	0.45	2.65	11	9
2:B:733:LYS:O	2:B:737:GLN:CB	0.45	2.65	10	6
2:B:785:LYS:CD	2:B:829:LEU:HD23	0.45	2.41	15	1
2:B:733:LYS:CE	2:B:777:LEU:HD22	0.45	2.41	16	1
2:B:776:ARG:CB	2:B:782:TYR:CE2	0.45	3.00	22	1
2:B:763:VAL:HG11	2:B:801:GLU:OE1	0.45	2.11	14	1
2:B:813:ALA:O	2:B:817:GLU:CB	0.45	2.64	19	14
2:B:738:GLN:OE1	2:B:739:VAL:N	0.45	2.50	12	4
2:B:789:MET:CE	2:B:820:PHE:CZ	0.45	3.00	8	4
2:B:820:PHE:CD1	2:B:820:PHE:C	0.45	2.90	21	3
2:B:768:MET:HB2	2:B:795:VAL:HG23	0.45	1.88	17	1
2:B:796:PHE:CE2	2:B:820:PHE:CE1	0.45	3.05	18	1
2:B:740:LYS:O	2:B:749:MET:HE3	0.45	2.12	23	1
2:B:722:PRO:O	2:B:724:ASP:N	0.44	2.50	7	22
2:B:777:LEU:HD13	2:B:777:LEU:C	0.44	2.33	14	2
2:B:804:PRO:CB	2:B:807:SER:CB	0.44	2.94	23	3
2:B:789:MET:HE2	2:B:824:ILE:HG21	0.44	1.87	23	1
2:B:782:TYR:CD1	2:B:787:LEU:O	0.44	2.70	1	1
2:B:734:SER:O	2:B:738:GLN:CG	0.44	2.66	22	2
2:B:740:LYS:O	2:B:749:MET:CE	0.44	2.66	13	10
2:B:823:LYS:O	2:B:827:ALA:HB2	0.44	2.11	16	4
2:B:824:ILE:HD13	2:B:830:ILE:CD1	0.44	2.43	13	2
2:B:736:LEU:HA	2:B:739:VAL:CG2	0.44	2.41	15	1
2:B:830:ILE:HD12	2:B:830:ILE:N	0.44	2.27	19	1
2:B:764:ILE:CD1	2:B:802:TYR:CD1	0.44	3.00	24	2
2:B:784:SER:CB	2:B:787:LEU:HD13	0.44	2.42	13	2
2:B:795:VAL:HA	2:B:798:ASN:OD1	0.44	2.12	15	2
2:B:803:ASN:HB2	2:B:809:TYR:CB	0.44	2.42	13	1
2:B:787:LEU:CD1	2:B:787:LEU:N	0.44	2.80	22	1
2:B:804:PRO:O	2:B:810:TYR:CB	0.44	2.66	18	6
2:B:736:LEU:CD2	2:B:770:LEU:HD22	0.44	2.43	4	1
2:B:733:LYS:CD	2:B:777:LEU:CD2	0.44	2.93	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:748:PHE:CD2	2:B:816:LEU:CD1	0.44	3.01	7	2
2:B:800:LYS:HD2	2:B:810:TYR:CE2	0.44	2.47	23	3
2:B:734:SER:OG	2:B:735:ILE:N	0.44	2.51	12	1
2:B:776:ARG:HD2	2:B:782:TYR:CE2	0.44	2.46	15	2
2:B:735:ILE:O	2:B:738:GLN:CG	0.44	2.66	13	7
2:B:780:ARG:O	2:B:780:ARG:CG	0.44	2.65	23	5
2:B:733:LYS:O	2:B:737:GLN:CG	0.44	2.66	16	8
2:B:752:VAL:CG1	2:B:760:TYR:CE2	0.44	3.01	10	1
2:B:728:LEU:N	2:B:728:LEU:CD2	0.44	2.81	14	1
2:B:824:ILE:CG1	2:B:830:ILE:HD13	0.44	2.41	19	1
2:B:749:MET:O	2:B:749:MET:CG	0.44	2.65	2	2
2:B:764:ILE:HG23	2:B:798:ASN:HD22	0.44	1.73	5	3
2:B:810:TYR:C	2:B:810:TYR:CD1	0.44	2.91	23	8
2:B:794:ARG:O	2:B:798:ASN:ND2	0.44	2.51	8	7
2:B:783:VAL:O	2:B:783:VAL:HG22	0.44	2.13	14	3
2:B:763:VAL:HG12	2:B:801:GLU:HB3	0.44	1.88	19	1
2:B:799:CYS:HA	2:B:802:TYR:CE1	0.44	2.47	2	5
2:B:766:PHE:O	2:B:768:MET:N	0.44	2.50	12	7
2:B:735:ILE:O	2:B:738:GLN:HG3	0.44	2.13	14	2
2:B:817:GLU:O	2:B:821:PHE:CB	0.44	2.66	21	2
2:B:804:PRO:HD2	2:B:809:TYR:CB	0.44	2.43	17	3
2:B:752:VAL:CG2	2:B:757:ALA:HB1	0.44	2.42	9	1
2:B:760:TYR:O	2:B:762:GLU:N	0.44	2.51	14	1
2:B:768:MET:O	2:B:769:ASP:CB	0.44	2.66	22	1
2:B:780:ARG:HG2	2:B:783:VAL:HG11	0.43	1.90	4	1
2:B:722:PRO:HB3	2:B:728:LEU:CD2	0.43	2.43	6	4
2:B:776:ARG:NH1	2:B:782:TYR:CE1	0.43	2.86	12	1
2:B:803:ASN:ND2	2:B:809:TYR:O	0.43	2.51	17	1
2:B:782:TYR:CD2	2:B:791:ASP:OD2	0.43	2.71	18	1
2:B:784:SER:HB2	2:B:787:LEU:HD12	0.43	1.88	18	1
2:B:739:VAL:HG22	2:B:816:LEU:HD22	0.43	1.89	21	1
2:B:736:LEU:HD23	2:B:739:VAL:CG2	0.43	2.42	24	2
2:B:722:PRO:HB2	2:B:728:LEU:CD2	0.43	2.44	13	6
2:B:800:LYS:HD2	2:B:810:TYR:CE1	0.43	2.49	1	1
2:B:736:LEU:HD11	2:B:740:LYS:HE2	0.43	1.90	8	1
2:B:752:VAL:HG21	2:B:760:TYR:OH	0.43	2.12	21	1
2:B:789:MET:O	2:B:793:GLN:CB	0.43	2.66	3	8
2:B:783:VAL:O	2:B:783:VAL:CG1	0.43	2.66	22	4
2:B:768:MET:CB	2:B:795:VAL:HG23	0.43	2.43	17	1
2:B:729:TYR:CE1	2:B:733:LYS:HE2	0.43	2.48	20	1
2:B:729:TYR:CD1	2:B:729:TYR:C	0.43	2.92	22	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:735:ILE:O	2:B:739:VAL:CG2	0.43	2.67	6	7
2:B:733:LYS:HD3	2:B:777:LEU:HD22	0.43	1.85	4	1
2:B:762:GLU:O	2:B:763:VAL:CG1	0.43	2.65	6	2
2:B:804:PRO:CB	2:B:806:GLU:N	0.43	2.81	24	2
2:B:824:ILE:CD1	2:B:830:ILE:HG13	0.43	2.43	1	6
2:B:732:LEU:CD1	2:B:782:TYR:O	0.43	2.67	5	3
2:B:760:TYR:CZ	2:B:764:ILE:HG13	0.43	2.47	16	3
2:B:797:THR:CG2	2:B:798:ASN:N	0.43	2.81	15	1
2:B:779:ASN:O	2:B:780:ARG:HG3	0.43	2.14	7	2
2:B:795:VAL:O	2:B:799:CYS:CB	0.43	2.66	23	3
2:B:810:TYR:CD1	2:B:810:TYR:C	0.43	2.92	21	5
2:B:807:SER:OG	2:B:808:GLU:N	0.43	2.52	22	2
2:B:817:GLU:O	2:B:821:PHE:N	0.43	2.52	19	1
2:B:785:LYS:CE	2:B:828:GLY:O	0.43	2.67	21	1
2:B:814:ASN:O	2:B:818:LYS:CD	0.43	2.67	22	1
2:B:792:LEU:CD2	2:B:820:PHE:CD2	0.43	2.98	3	1
2:B:782:TYR:C	2:B:783:VAL:HG13	0.43	2.33	23	1
2:B:794:ARG:HA	2:B:797:THR:HG22	0.43	1.90	1	2
2:B:797:THR:O	2:B:801:GLU:N	0.43	2.52	15	1
2:B:751:PRO:C	2:B:752:VAL:CG1	0.43	2.86	19	1
2:B:784:SER:OG	2:B:787:LEU:HD13	0.43	2.14	22	1
2:B:764:ILE:HG23	2:B:798:ASN:CB	0.43	2.43	16	3
2:B:759:GLY:O	2:B:761:TYR:N	0.43	2.52	3	4
2:B:732:LEU:O	2:B:736:LEU:CB	0.43	2.66	5	1
2:B:771:LYS:O	2:B:771:LYS:CE	0.43	2.67	8	1
2:B:773:MET:HE1	2:B:792:LEU:CD1	0.43	2.43	10	1
2:B:808:GLU:O	2:B:811:LYS:CG	0.43	2.67	24	2
2:B:722:PRO:CB	2:B:728:LEU:HG	0.43	2.44	9	6
2:B:740:LYS:O	2:B:749:MET:HE1	0.43	2.14	2	1
2:B:798:ASN:N	2:B:798:ASN:OD1	0.43	2.52	12	1
2:B:804:PRO:CB	2:B:807:SER:OG	0.43	2.67	18	2
2:B:805:PRO:O	2:B:806:GLU:CB	0.43	2.66	21	2
2:B:738:GLN:OE1	2:B:739:VAL:HG12	0.43	2.14	15	1
2:B:764:ILE:CD1	2:B:798:ASN:O	0.43	2.67	15	1
2:B:764:ILE:HD12	2:B:798:ASN:CA	0.43	2.44	23	1
2:B:814:ASN:O	2:B:818:LYS:CG	0.42	2.66	2	2
2:B:762:GLU:C	2:B:763:VAL:HG13	0.42	2.34	10	1
2:B:742:HIS:ND1	2:B:744:SER:OG	0.42	2.52	12	1
2:B:820:PHE:O	2:B:824:ILE:CG1	0.42	2.67	13	1
2:B:769:ASP:OD1	2:B:771:LYS:CB	0.42	2.67	15	3
2:B:782:TYR:CE2	2:B:791:ASP:CG	0.42	2.92	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:785:LYS:CD	2:B:828:GLY:O	0.42	2.67	21	1
2:B:774:SER:O	2:B:778:LYS:CD	0.42	2.68	1	2
2:B:786:LYS:O	2:B:790:ALA:N	0.42	2.51	1	2
2:B:804:PRO:O	2:B:806:GLU:N	0.42	2.52	9	3
2:B:793:GLN:O	2:B:797:THR:CB	0.42	2.67	9	3
2:B:765:ARG:O	2:B:766:PHE:CB	0.42	2.66	13	1
2:B:776:ARG:CZ	2:B:781:TYR:CD2	0.42	3.02	18	1
2:B:722:PRO:CA	2:B:728:LEU:HD21	0.42	2.44	17	2
2:B:763:VAL:CG1	2:B:801:GLU:OE1	0.42	2.67	14	2
2:B:769:ASP:OD1	2:B:772:THR:N	0.42	2.52	6	3
2:B:766:PHE:CZ	2:B:768:MET:HE3	0.42	2.49	11	1
2:B:740:LYS:HD3	2:B:749:MET:CE	0.42	2.44	17	1
2:B:768:MET:HB2	2:B:795:VAL:CG2	0.42	2.44	17	1
2:B:800:LYS:HD3	2:B:810:TYR:CD1	0.42	2.49	1	1
2:B:800:LYS:HD3	2:B:810:TYR:CE1	0.42	2.49	1	1
2:B:821:PHE:CZ	2:B:825:LYS:HD2	0.42	2.50	4	1
2:B:796:PHE:O	2:B:800:LYS:CE	0.42	2.67	7	1
2:B:722:PRO:O	2:B:723:ARG:HG2	0.42	2.14	12	1
2:B:776:ARG:CB	2:B:782:TYR:CD2	0.42	3.03	13	1
2:B:731:THR:O	2:B:734:SER:N	0.42	2.53	16	1
2:B:779:ASN:N	2:B:779:ASN:OD1	0.42	2.52	1	1
2:B:795:VAL:HA	2:B:798:ASN:ND2	0.42	2.30	10	1
2:B:725:PRO:O	2:B:783:VAL:CG2	0.42	2.68	13	1
2:B:779:ASN:O	2:B:781:TYR:N	0.42	2.52	18	1
2:B:751:PRO:O	2:B:752:VAL:O	0.42	2.37	19	1
2:B:801:GLU:OE1	2:B:801:GLU:CA	0.42	2.67	20	1
2:B:789:MET:SD	2:B:830:ILE:CD1	0.42	3.08	9	7
2:B:749:MET:O	2:B:771:LYS:CB	0.42	2.67	4	1
2:B:722:PRO:HB3	2:B:728:LEU:CD1	0.42	2.40	7	2
2:B:780:ARG:CD	2:B:780:ARG:O	0.42	2.67	7	2
2:B:732:LEU:HB3	2:B:777:LEU:CD1	0.42	2.45	8	1
2:B:728:LEU:O	2:B:728:LEU:CD1	0.42	2.68	10	1
2:B:789:MET:SD	2:B:830:ILE:CG1	0.42	3.07	13	1
2:B:751:PRO:C	2:B:752:VAL:HG13	0.42	2.34	19	1
2:B:744:SER:O	2:B:747:PRO:CG	0.42	2.68	23	1
2:B:821:PHE:O	2:B:824:ILE:CG1	0.42	2.68	3	1
2:B:732:LEU:HD13	2:B:788:PHE:CD1	0.42	2.50	8	2
2:B:824:ILE:CA	2:B:829:LEU:HB2	0.42	2.45	8	3
2:B:738:GLN:OE1	2:B:739:VAL:CG1	0.42	2.67	15	1
2:B:785:LYS:HD3	2:B:829:LEU:HD13	0.42	1.90	18	1
2:B:789:MET:CG	2:B:829:LEU:HB3	0.42	2.44	21	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:723:ARG:O	2:B:724:ASP:CB	0.42	2.66	23	1
2:B:747:PRO:HB3	2:B:809:TYR:CE2	0.42	2.49	24	3
2:B:796:PHE:O	2:B:800:LYS:CG	0.42	2.68	11	1
2:B:732:LEU:HD11	2:B:784:SER:N	0.42	2.30	16	1
2:B:747:PRO:HB3	2:B:809:TYR:CZ	0.42	2.49	24	2
2:B:776:ARG:NH1	2:B:782:TYR:OH	0.42	2.52	12	1
2:B:796:PHE:CD1	2:B:796:PHE:N	0.42	2.87	16	1
2:B:799:CYS:HA	2:B:802:TYR:CE2	0.42	2.49	17	1
2:B:761:TYR:CD2	2:B:761:TYR:O	0.42	2.73	18	1
2:B:775:GLU:O	2:B:779:ASN:N	0.42	2.51	22	1
2:B:760:TYR:CD1	2:B:764:ILE:HG13	0.42	2.50	5	1
2:B:752:VAL:HG21	2:B:760:TYR:CD1	0.42	2.50	7	1
2:B:804:PRO:HB2	2:B:807:SER:CB	0.41	2.44	5	5
2:B:728:LEU:CD1	2:B:829:LEU:HD21	0.41	2.45	8	1
2:B:738:GLN:NE2	2:B:823:LYS:HG3	0.41	2.30	18	2
2:B:797:THR:O	2:B:800:LYS:CG	0.41	2.68	17	1
2:B:732:LEU:CB	2:B:777:LEU:HD21	0.41	2.45	23	1
2:B:804:PRO:CA	2:B:805:PRO:C	0.41	2.88	24	2
2:B:792:LEU:HD23	2:B:820:PHE:HD2	0.41	1.68	7	1
2:B:776:ARG:HG2	2:B:782:TYR:CE2	0.41	2.50	13	2
2:B:725:PRO:O	2:B:729:TYR:N	0.41	2.53	10	1
2:B:804:PRO:CD	2:B:809:TYR:HB2	0.41	2.45	17	1
2:B:789:MET:HE1	2:B:820:PHE:CZ	0.41	2.50	21	1
2:B:773:MET:CE	2:B:791:ASP:OD1	0.41	2.68	1	1
2:B:793:GLN:O	2:B:797:THR:N	0.41	2.47	16	2
2:B:804:PRO:CB	2:B:807:SER:HB2	0.41	2.45	12	2
2:B:804:PRO:HD3	2:B:809:TYR:CB	0.41	2.45	14	1
2:B:750:GLU:OE1	2:B:750:GLU:N	0.41	2.53	21	1
2:B:796:PHE:CB	2:B:817:GLU:OE1	0.41	2.69	3	1
2:B:724:ASP:HB3	2:B:727:GLN:NE2	0.41	2.31	6	1
2:B:789:MET:HE1	2:B:820:PHE:CE2	0.41	2.50	6	1
2:B:792:LEU:HD22	2:B:820:PHE:CD2	0.41	2.49	8	1
2:B:783:VAL:O	2:B:783:VAL:CG2	0.41	2.68	10	1
2:B:796:PHE:CZ	2:B:816:LEU:HD13	0.41	2.51	13	1
2:B:721:GLU:O	2:B:723:ARG:CD	0.41	2.69	15	1
2:B:723:ARG:O	2:B:727:GLN:CG	0.41	2.69	23	1
2:B:733:LYS:HD3	2:B:777:LEU:CD2	0.41	2.45	5	1
2:B:798:ASN:O	2:B:802:TYR:CD2	0.41	2.74	17	1
2:B:760:TYR:CG	2:B:764:ILE:HG13	0.41	2.50	20	1
2:B:736:LEU:HD13	2:B:788:PHE:CZ	0.41	2.50	12	1
2:B:802:TYR:CD2	2:B:803:ASN:OD1	0.41	2.74	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:760:TYR:CD2	2:B:767:PRO:HG3	0.41	2.49	13	1
2:B:824:ILE:HD13	2:B:830:ILE:HD12	0.41	1.92	23	2
2:B:760:TYR:CE1	2:B:764:ILE:CG1	0.41	3.03	16	1
2:B:731:THR:HG23	2:B:827:ALA:CB	0.41	2.44	20	1
2:B:728:LEU:HA	2:B:731:THR:CB	0.41	2.46	23	1
2:B:802:TYR:CG	2:B:803:ASN:N	0.41	2.88	10	1
2:B:733:LYS:O	2:B:737:GLN:HB2	0.41	2.16	14	1
2:B:734:SER:O	2:B:738:GLN:HG2	0.41	2.16	17	1
2:B:722:PRO:HD3	2:B:785:LYS:CE	0.41	2.46	24	2
2:B:813:ALA:O	2:B:817:GLU:HB3	0.41	2.16	6	1
2:B:824:ILE:CD1	2:B:830:ILE:CD1	0.41	2.92	13	1
2:B:736:LEU:O	2:B:740:LYS:N	0.41	2.51	18	1
2:B:777:LEU:CD2	2:B:782:TYR:O	0.41	2.69	19	1
2:B:736:LEU:O	2:B:739:VAL:N	0.41	2.53	1	1
2:B:821:PHE:HA	2:B:824:ILE:HG12	0.41	1.93	1	1
2:B:748:PHE:CB	2:B:795:VAL:HG11	0.41	2.45	6	1
2:B:821:PHE:CE1	2:B:825:LYS:HB2	0.41	2.51	6	1
2:B:780:ARG:O	2:B:780:ARG:HD3	0.41	2.16	7	1
2:B:742:HIS:HB3	2:B:745:ALA:CB	0.41	2.46	13	1
2:B:785:LYS:HD2	2:B:829:LEU:HD23	0.41	1.93	15	1
2:B:728:LEU:O	2:B:731:THR:N	0.41	2.54	17	1
2:B:821:PHE:CZ	2:B:825:LYS:HG3	0.41	2.51	18	1
2:B:820:PHE:CE2	2:B:824:ILE:HG21	0.41	2.51	19	1
2:B:732:LEU:HD21	2:B:829:LEU:HD11	0.41	1.92	21	1
2:B:740:LYS:HG2	2:B:749:MET:CE	0.41	2.46	5	1
2:B:747:PRO:HB3	2:B:809:TYR:CE1	0.41	2.51	13	1
2:B:742:HIS:NE2	2:B:815:ILE:HG22	0.41	2.31	14	1
2:B:740:LYS:HA	2:B:749:MET:CE	0.41	2.46	18	1
2:B:821:PHE:CZ	2:B:830:ILE:HG21	0.41	2.51	20	1
2:B:728:LEU:HD22	2:B:784:SER:HA	0.41	1.93	21	3
2:B:732:LEU:HD13	2:B:788:PHE:CD2	0.40	2.50	1	1
2:B:799:CYS:SG	2:B:803:ASN:ND2	0.40	2.95	2	2
2:B:733:LYS:O	2:B:737:GLN:N	0.40	2.53	7	1
2:B:803:ASN:ND2	2:B:810:TYR:CA	0.40	2.84	13	1
2:B:777:LEU:O	2:B:777:LEU:CD1	0.40	2.68	17	1
2:B:780:ARG:NH2	2:B:787:LEU:HD21	0.40	2.31	22	1
2:B:791:ASP:O	2:B:795:VAL:CG2	0.40	2.67	7	1
2:B:821:PHE:CD2	2:B:825:LYS:HD2	0.40	2.51	16	1
2:B:733:LYS:HD2	2:B:777:LEU:CD1	0.40	2.45	17	1
2:B:745:ALA:CB	2:B:816:LEU:CD2	0.40	2.91	19	1
2:B:803:ASN:N	2:B:803:ASN:OD1	0.40	2.52	21	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:747:PRO:C	2:B:748:PHE:CD1	0.40	2.94	23	1
2:B:773:MET:SD	2:B:791:ASP:CB	0.40	3.09	18	2
2:B:824:ILE:HB	2:B:829:LEU:CB	0.40	2.47	9	1
2:B:821:PHE:CD1	2:B:824:ILE:HD11	0.40	2.51	17	1
2:B:789:MET:CE	2:B:820:PHE:CE1	0.40	3.04	24	2
2:B:749:MET:O	2:B:749:MET:HG3	0.40	2.17	6	1
2:B:782:TYR:CD1	2:B:791:ASP:OD2	0.40	2.74	18	1
2:B:769:ASP:O	2:B:773:MET:N	0.40	2.52	20	1
2:B:722:PRO:HB3	2:B:728:LEU:CB	0.40	2.46	21	1
2:B:787:LEU:N	2:B:787:LEU:HD12	0.40	2.31	1	1
2:B:760:TYR:CD2	2:B:764:ILE:HG13	0.40	2.51	8	1
2:B:824:ILE:CG1	2:B:825:LYS:N	0.40	2.85	8	1
2:B:730:SER:O	2:B:734:SER:N	0.40	2.52	9	1
2:B:722:PRO:O	2:B:723:ARG:C	0.40	2.59	12	1
2:B:784:SER:OG	2:B:785:LYS:N	0.40	2.52	14	1
2:B:736:LEU:CA	2:B:739:VAL:HG22	0.40	2.44	15	1
2:B:797:THR:O	2:B:800:LYS:HG3	0.40	2.17	17	1
2:B:748:PHE:CD2	2:B:816:LEU:HD13	0.40	2.51	18	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	0	-	-	-	-	
2	B	106/118 (90%)	84±3 (79±2%)	17±3 (16±3%)	5±1 (5±1%)	4	25
All	All	2650/3225 (82%)	2105 (79%)	413 (16%)	132 (5%)	4	25

All 28 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	723	ARG	22
2	B	767	PRO	16
2	B	752	VAL	13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	B	760	TYR	13
2	B	761	TYR	10
2	B	806	GLU	7
2	B	765	ARG	6
2	B	762	GLU	5
2	B	763	VAL	4
2	B	803	ASN	4
2	B	780	ARG	4
2	B	785	LYS	3
2	B	751	PRO	3
2	B	783	VAL	3
2	B	805	PRO	3
2	B	757	ALA	2
2	B	758	PRO	2
2	B	808	GLU	2
2	B	768	MET	1
2	B	804	PRO	1
2	B	790	ALA	1
2	B	721	GLU	1
2	B	784	SER	1
2	B	735	ILE	1
2	B	795	VAL	1
2	B	815	ILE	1
2	B	782	TYR	1
2	B	724	ASP	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	0	-	-	-
2	B	99/110 (90%)	71±3 (72±3%)	28±3 (28±3%)	2 19
All	All	2475/2975 (83%)	1784 (72%)	691 (28%)	2 19

All 75 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)
2	B	746	TRP	25
2	B	771	LYS	25
2	B	820	PHE	24
2	B	777	LEU	23
2	B	733	LYS	21
2	B	740	LYS	21
2	B	723	ARG	20
2	B	781	TYR	19
2	B	809	TYR	19
2	B	734	SER	18
2	B	765	ARG	17
2	B	780	ARG	17
2	B	818	LYS	17
2	B	819	PHE	16
2	B	785	LYS	15
2	B	798	ASN	15
2	B	808	GLU	15
2	B	794	ARG	13
2	B	825	LYS	13
2	B	728	LEU	13
2	B	760	TYR	13
2	B	762	GLU	11
2	B	786	LYS	11
2	B	776	ARG	11
2	B	801	GLU	11
2	B	768	MET	11
2	B	789	MET	11
2	B	811	LYS	11
2	B	744	SER	10
2	B	761	TYR	10
2	B	816	LEU	10
2	B	821	PHE	10
2	B	766	PHE	9
2	B	806	GLU	9
2	B	778	LYS	9
2	B	793	GLN	9
2	B	724	ASP	8
2	B	800	LYS	8
2	B	730	SER	8
2	B	822	SER	8
2	B	738	GLN	8
2	B	829	LEU	8
2	B	726	ASP	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	B	807	SER	7
2	B	784	SER	6
2	B	721	GLU	6
2	B	743	GLN	6
2	B	736	LEU	5
2	B	749	MET	5
2	B	737	GLN	5
2	B	742	HIS	5
2	B	752	VAL	5
2	B	741	SER	5
2	B	797	THR	5
2	B	750	GLU	4
2	B	727	GLN	4
2	B	779	ASN	4
2	B	792	LEU	4
2	B	773	MET	4
2	B	769	ASP	3
2	B	763	VAL	3
2	B	772	THR	2
2	B	729	TYR	2
2	B	823	LYS	2
2	B	739	VAL	2
2	B	826	GLU	1
2	B	830	ILE	1
2	B	787	LEU	1
2	B	824	ILE	1
2	B	803	ASN	1
2	B	774	SER	1
2	B	802	TYR	1
2	B	804	PRO	1
2	B	791	ASP	1
2	B	814	ASN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics

could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	ALY	A	50	1	10,11,12	0.80±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	ALY	A	50	1	7,12,14	1.34±0.03	1±0 (14±2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	A	50	1	-	0±0,9,10,12	-

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	50	ALY	CD-CE-NZ	2.78	104.27	112.21	14	25
1	A	50	ALY	CE-NZ-CH	2.20	119.18	122.56	12	1

There are no chirality outliers.

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	50	ALY	CH3-CH-NZ-CE	2

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided