



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 06:37 AM UTC

PDB ID : 2RNX / pdb_00002rnx
Title : The Structural Basis for Site-Specific Lysine-Acetylated Histone Recognition by the Bromodomains of the HUMAN Transcriptional Co-Activators PCAF and CBP
Authors : Zeng, L.; Zhang, Q.; Gerona-Navarro, G.; Zhou, M.M.
Deposited on : 2008-02-03

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

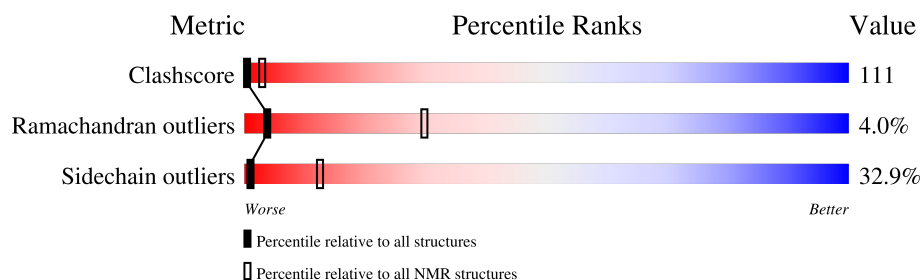
1 Overall quality at a glance

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	118	
2	B	13	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:724-A:830 (107)	0.23	2

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

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

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

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2192 atoms, of which 1100 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone acetyltransferase PCAF.

Mol	Chain	Residues	Atoms						Trace
1	A	118	Total	C	H	N	O	S	0
			1976	636	989	164	180	7	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	715	GLY	-	expression tag	UNP Q92831
A	716	SER	-	expression tag	UNP Q92831
A	717	HIS	-	expression tag	UNP Q92831
A	718	MET	-	expression tag	UNP Q92831

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms						Trace
2	B	13	Total	C	H	N	O	S	0
			216	65	111	21	18	1	

There is a discrepancy between the modelled and reference sequences:

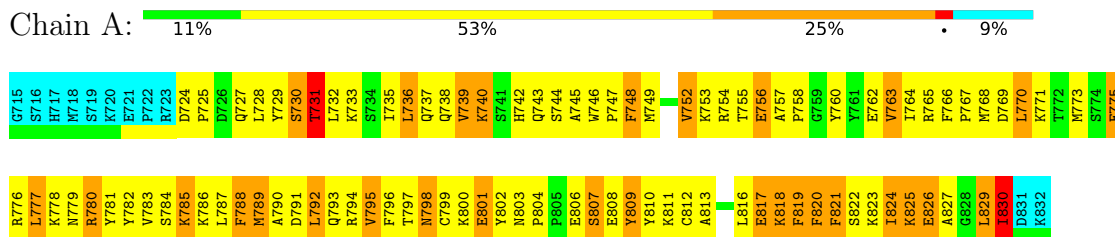
Chain	Residue	Modelled	Actual	Comment	Reference
B	43	CYS	-	insertion	UNP P61830

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Histone acetyltransferase PCAF



- Molecule 2: Histone H3

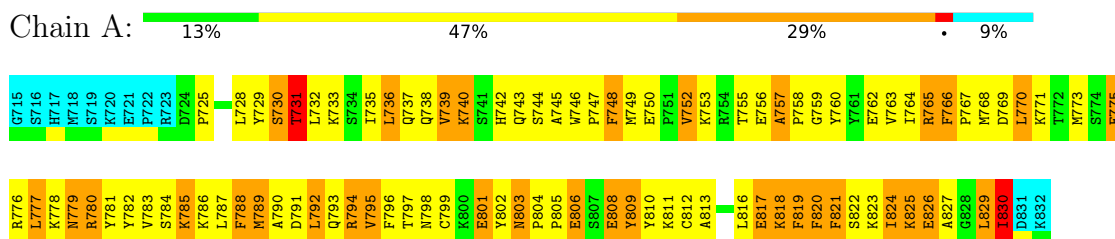


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

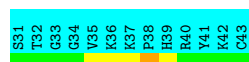
4.2.1 Score per residue for model 1

- Molecule 1: Histone acetyltransferase PCAF



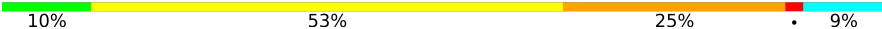
- Molecule 2: Histone H3

Chain B:  100%



4.2.2 Score per residue for model 2 (medoid)

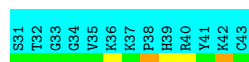
- Molecule 1: Histone acetyltransferase PCAF

Chain A:  10% 53% 25% 9%



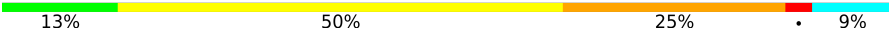
- Molecule 2: Histone H3

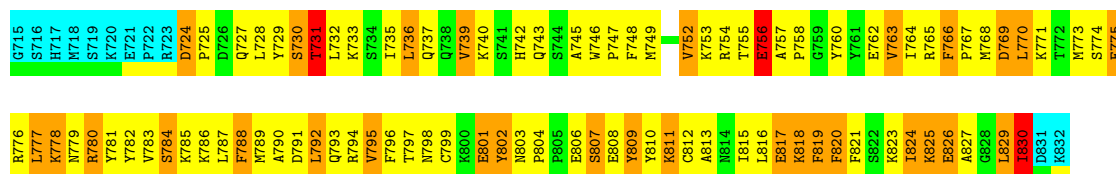
Chain B:  100%



4.2.3 Score per residue for model 3

- Molecule 1: Histone acetyltransferase PCAF

Chain A:  13% 50% 25% 9%



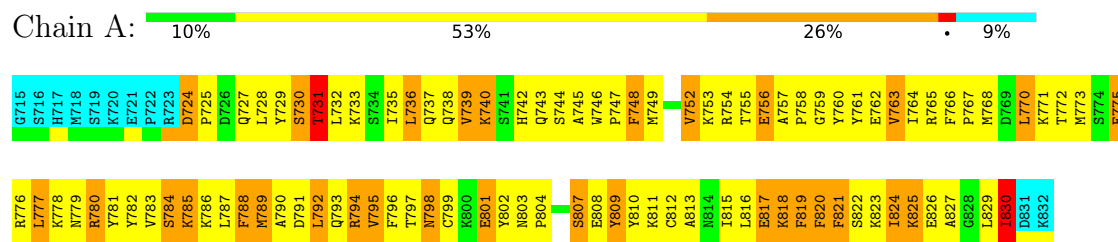
- Molecule 2: Histone H3

Chain B:  100%

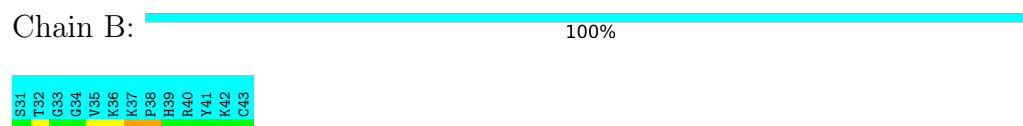


4.2.4 Score per residue for model 4

- Molecule 1: Histone acetyltransferase PCAF

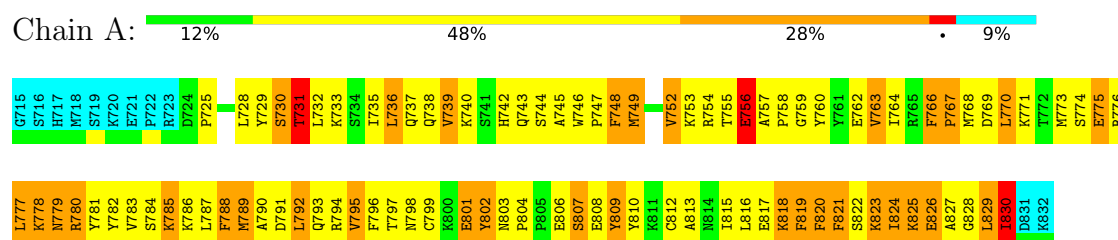


- Molecule 2: Histone H3

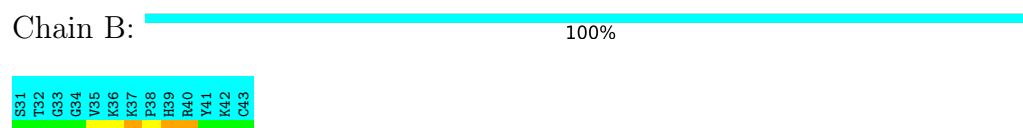


4.2.5 Score per residue for model 5

- Molecule 1: Histone acetyltransferase PCAF

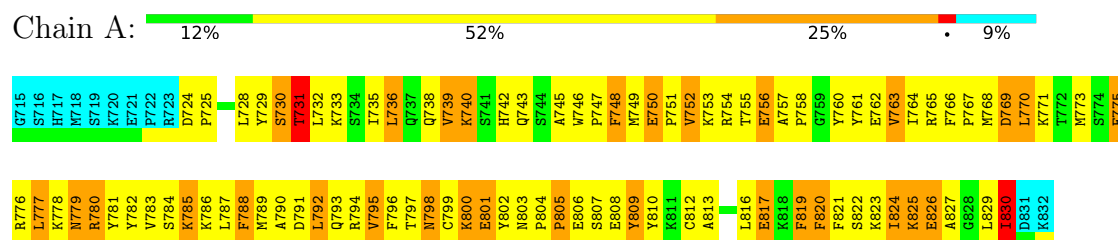


- Molecule 2: Histone H3



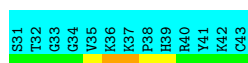
4.2.6 Score per residue for model 6

- Molecule 1: Histone acetyltransferase PCAF



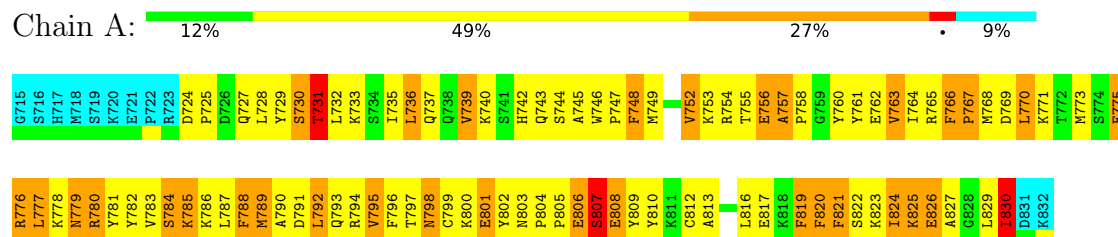
- Molecule 2: Histone H3



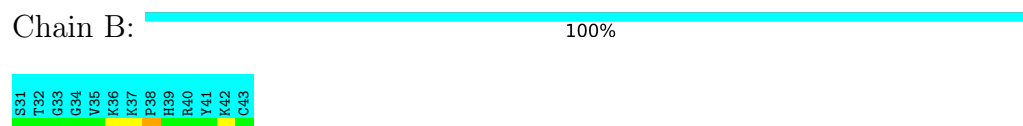


4.2.7 Score per residue for model 7

- Molecule 1: Histone acetyltransferase PCAF

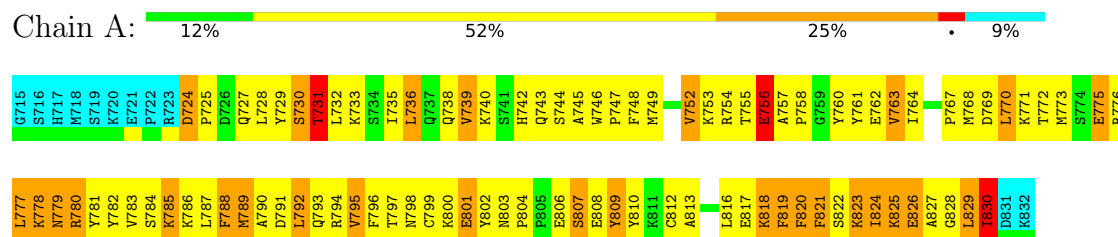


- Molecule 2: Histone H3

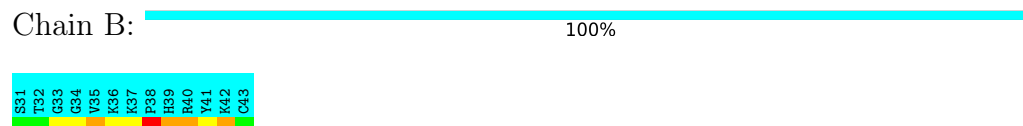


4.2.8 Score per residue for model 8

- Molecule 1: Histone acetyltransferase PCAF



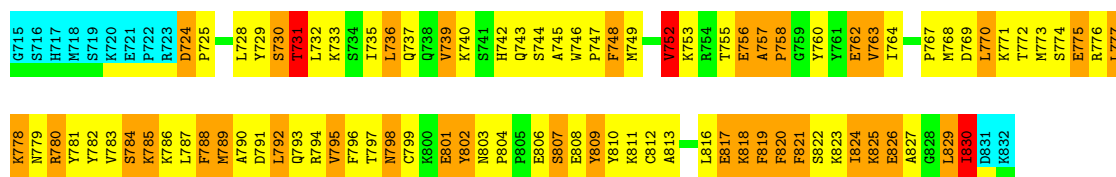
- Molecule 2: Histone H3



4.2.9 Score per residue for model 9

- Molecule 1: Histone acetyltransferase PCAF





- Molecule 2: Histone H3

Chain B: 100%



4.2.10 Score per residue for model 10

- Molecule 1: Histone acetyltransferase PCAF

Chain A: 9% 52% 28% 9%



- Molecule 2: Histone H3

Chain B: 100%



4.2.11 Score per residue for model 11

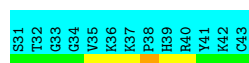
- Molecule 1: Histone acetyltransferase PCAF

Chain A: 16% 49% 23% 9%



- Molecule 2: Histone H3

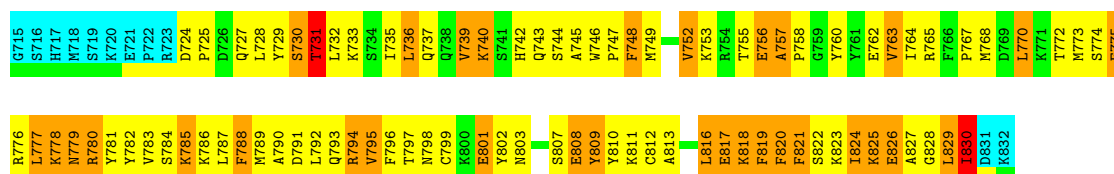
Chain B: 100%



4.2.12 Score per residue for model 12

- Molecule 1: Histone acetyltransferase PCAF

Chain A: 15% 47% 27% 9%



- Molecule 2: Histone H3

Chain B: 100%



4.2.13 Score per residue for model 13

- Molecule 1: Histone acetyltransferase PCAF

Chain A: 13% 49% 25% 9%



- Molecule 2: Histone H3

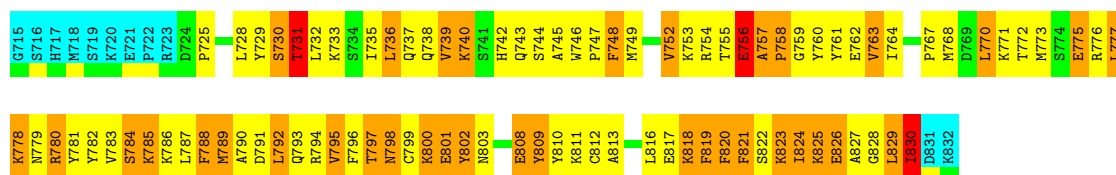
Chain B: 100%



4.2.14 Score per residue for model 14

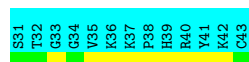
- Molecule 1: Histone acetyltransferase PCAF

Chain A: 14% 43% 31% 9%



- Molecule 2: Histone H3

Chain B: 100%



4.2.15 Score per residue for model 15

- Molecule 1: Histone acetyltransferase PCAF

Chain A: 10% 53% 25% 9%



- Molecule 2: Histone H3

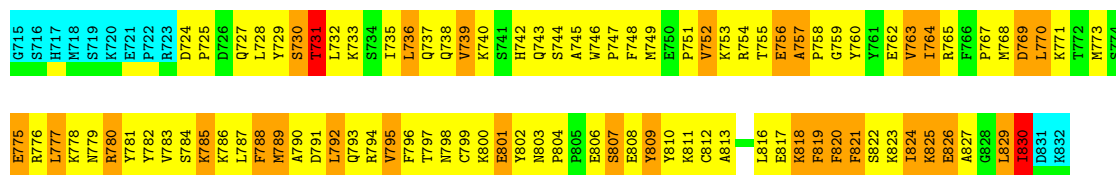
Chain B: 100%



4.2.16 Score per residue for model 16

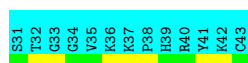
- Molecule 1: Histone acetyltransferase PCAF

Chain A: 10% 54% 25% 9%



- Molecule 2: Histone H3

Chain B: 100%



4.2.17 Score per residue for model 17

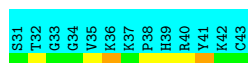
- Molecule 1: Histone acetyltransferase PCAF

Chain A: 10% 51% 27% 9%



- Molecule 2: Histone H3

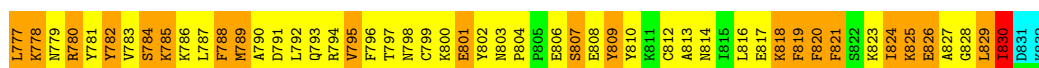
Chain B: 100%



4.2.18 Score per residue for model 18

- Molecule 1: Histone acetyltransferase PCAF

Chain A: 12% 49% 27% 9%



- Molecule 2: Histone H3

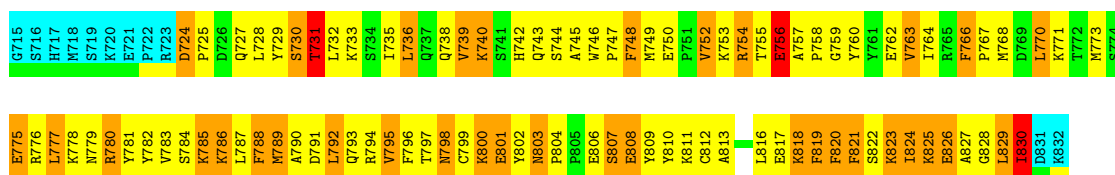
Chain B: 100%



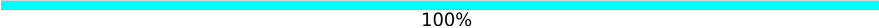
4.2.19 Score per residue for model 19

- Molecule 1: Histone acetyltransferase PCAF

Chain A: 11% 47% 30% 9%



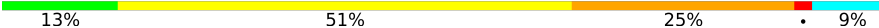
- Molecule 2: Histone H3

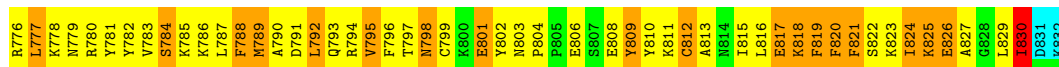
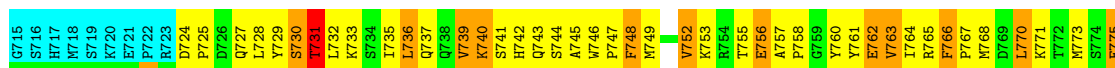
Chain B:  100%



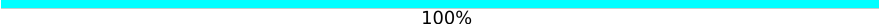
4.2.20 Score per residue for model 20

- Molecule 1: Histone acetyltransferase PCAF

Chain A:  13% 51% 25% 9%



- Molecule 2: Histone H3

Chain B:  100%



5 Refinement protocol and experimental data overview

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

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
CNS	structure solution	1.0
CNS	refinement	1.0

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
1	A	0.83±0.02	0±1/924 (0.1± 0.1%)	1.11±0.02	3±0/1245 (0.2± 0.0%)
All	All	0.83	10/18480 (0.1%)	1.11	62/24900 (0.2%)

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	757	ALA	CA-CB	-7.09	1.44	1.53	16	2
1	A	757	ALA	N-CA	-6.61	1.39	1.46	14	8

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	756	GLU	N-CA-C	-9.16	101.18	111.71	14	20
1	A	788	PHE	CA-CB-CG	-6.57	107.23	113.80	11	20
1	A	731	THR	N-CA-C	-6.13	104.28	110.97	20	20
1	A	756	GLU	O-C-N	5.69	128.15	122.12	12	1
1	A	764	ILE	N-CA-C	5.68	112.28	106.21	16	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	899	901	900	199±5
2	B	0	0	0	0±0
All	All	17980	18020	18000	3980

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 111.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:789:MET:HE1	1:A:830:ILE:HG23	1.07	1.26	11	20
1:A:757:ALA:HB3	1:A:760:TYR:HB2	1.00	1.26	10	11
1:A:763:VAL:HG21	1:A:802:TYR:HB2	0.96	1.36	5	17
1:A:824:ILE:HG22	1:A:829:LEU:HD12	0.95	1.37	20	19
1:A:732:LEU:HD23	1:A:829:LEU:HD11	0.90	1.43	11	2
1:A:757:ALA:CB	1:A:760:TYR:HB2	0.90	1.96	17	20
1:A:763:VAL:HG13	1:A:764:ILE:HG12	0.88	1.43	1	1
1:A:757:ALA:HB1	1:A:760:TYR:HB2	0.86	1.46	14	6
1:A:732:LEU:CD2	1:A:829:LEU:HD11	0.83	2.04	11	1
1:A:824:ILE:HG22	1:A:829:LEU:CD1	0.82	2.05	6	19
1:A:740:LYS:O	1:A:749:MET:HE2	0.82	1.74	8	18
1:A:770:LEU:HD23	1:A:792:LEU:HD21	0.82	1.50	18	20
1:A:821:PHE:HA	1:A:824:ILE:HD11	0.81	1.51	7	20
1:A:768:MET:HG3	1:A:795:VAL:HG12	0.79	1.55	10	20
1:A:820:PHE:O	1:A:824:ILE:HG12	0.76	1.80	11	18
1:A:789:MET:CE	1:A:824:ILE:HD12	0.75	2.11	5	18
1:A:824:ILE:CG2	1:A:829:LEU:HD12	0.75	2.11	15	19
1:A:728:LEU:HD21	1:A:785:LYS:HD2	0.75	1.55	1	4
1:A:735:ILE:HG23	1:A:823:LYS:HB3	0.75	1.58	5	4
1:A:789:MET:SD	1:A:830:ILE:HA	0.75	2.21	18	20
1:A:757:ALA:HB1	1:A:760:TYR:CB	0.75	2.11	16	3
1:A:731:THR:HG23	1:A:827:ALA:HB1	0.74	1.59	11	20
1:A:732:LEU:HB3	1:A:788:PHE:CD2	0.73	2.18	11	20
1:A:757:ALA:HB1	1:A:760:TYR:CD1	0.73	2.19	3	2
1:A:824:ILE:HG13	1:A:830:ILE:HD11	0.73	1.60	5	20
1:A:825:LYS:HG2	1:A:830:ILE:HD12	0.73	1.61	5	6
1:A:795:VAL:O	1:A:799:CYS:SG	0.71	2.49	17	10
1:A:760:TYR:CZ	1:A:767:PRO:HB3	0.71	2.21	4	14
1:A:732:LEU:HD23	1:A:829:LEU:HD13	0.71	1.63	2	19
1:A:752:VAL:HG13	1:A:756:GLU:HG3	0.70	1.63	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:749:MET:N	1:A:770:LEU:HD12	0.70	2.01	12	20
1:A:757:ALA:HB1	1:A:802:TYR:HE2	0.70	1.46	19	8
1:A:789:MET:HE3	1:A:824:ILE:HD12	0.70	1.63	12	17
1:A:732:LEU:HD23	1:A:829:LEU:CD1	0.70	2.17	8	19
1:A:746:TRP:HA	1:A:749:MET:HG3	0.70	1.63	5	6
1:A:752:VAL:HB	1:A:760:TYR:CE2	0.69	2.22	19	4
1:A:732:LEU:HB3	1:A:788:PHE:CE2	0.69	2.22	6	20
1:A:789:MET:HE2	1:A:793:GLN:NE2	0.69	2.01	6	15
1:A:825:LYS:HG3	1:A:830:ILE:HD12	0.69	1.64	1	14
1:A:736:LEU:HD12	1:A:777:LEU:HD23	0.69	1.65	16	20
1:A:799:CYS:SG	1:A:813:ALA:HB2	0.68	2.27	8	10
1:A:768:MET:HE1	1:A:772:THR:HG21	0.68	1.66	18	1
1:A:728:LEU:HD21	1:A:785:LYS:HE3	0.68	1.65	11	8
1:A:748:PHE:CE1	1:A:799:CYS:SG	0.68	2.87	5	10
1:A:824:ILE:HG22	1:A:829:LEU:HG	0.67	1.64	11	1
1:A:731:THR:O	1:A:735:ILE:HD12	0.67	1.89	11	20
1:A:763:VAL:CG2	1:A:802:TYR:HB2	0.67	2.18	5	17
1:A:733:LYS:HB2	1:A:777:LEU:HD11	0.67	1.67	15	20
1:A:789:MET:CE	1:A:830:ILE:HG23	0.67	2.19	14	14
1:A:793:GLN:HA	1:A:796:PHE:CD2	0.67	2.25	8	20
1:A:740:LYS:HA	1:A:770:LEU:HD13	0.66	1.65	5	19
1:A:799:CYS:O	1:A:803:ASN:HB2	0.66	1.90	13	16
1:A:735:ILE:HD13	1:A:829:LEU:HD11	0.66	1.67	9	19
1:A:740:LYS:O	1:A:745:ALA:HB3	0.66	1.91	19	6
1:A:771:LYS:C	1:A:771:LYS:HD3	0.66	2.15	10	1
1:A:764:ILE:HG23	1:A:798:ASN:HB2	0.66	1.68	2	17
1:A:728:LEU:HB3	1:A:732:LEU:HD11	0.65	1.67	2	20
1:A:824:ILE:HB	1:A:830:ILE:HG12	0.65	1.69	10	20
1:A:768:MET:HE1	1:A:776:ARG:NE	0.65	2.06	1	12
1:A:824:ILE:HG13	1:A:830:ILE:CD1	0.65	2.22	2	19
1:A:728:LEU:HD21	1:A:785:LYS:HE2	0.65	1.68	20	2
1:A:756:GLU:O	1:A:758:PRO:HD3	0.64	1.92	16	4
1:A:824:ILE:HB	1:A:829:LEU:HB2	0.64	1.69	9	20
1:A:768:MET:HE1	1:A:772:THR:CG2	0.64	2.22	18	1
1:A:764:ILE:HG23	1:A:798:ASN:OD1	0.64	1.93	8	1
1:A:809:TYR:CD1	1:A:809:TYR:N	0.64	2.65	14	15
1:A:730:SER:HA	1:A:733:LYS:CB	0.64	2.23	19	20
1:A:740:LYS:HB2	1:A:770:LEU:HB3	0.64	1.70	10	8
1:A:752:VAL:HG23	1:A:756:GLU:HG3	0.63	1.70	15	4
1:A:803:ASN:ND2	1:A:809:TYR:CZ	0.63	2.66	19	1
1:A:736:LEU:HD11	1:A:773:MET:HB3	0.63	1.68	5	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:752:VAL:HG22	1:A:754:ARG:H	0.63	1.52	16	6
1:A:735:ILE:HD11	1:A:827:ALA:CB	0.63	2.24	11	20
1:A:764:ILE:HD12	1:A:798:ASN:HB2	0.63	1.71	5	14
1:A:770:LEU:HD23	1:A:792:LEU:CD2	0.63	2.23	18	20
1:A:735:ILE:O	1:A:739:VAL:HG13	0.63	1.93	7	20
1:A:773:MET:HA	1:A:782:TYR:OH	0.63	1.94	16	20
1:A:749:MET:HA	1:A:770:LEU:HD12	0.63	1.71	10	20
1:A:772:THR:O	1:A:776:ARG:HG3	0.63	1.94	9	2
1:A:731:THR:CG2	1:A:827:ALA:HB1	0.62	2.23	18	20
1:A:792:LEU:HD13	1:A:820:PHE:CD1	0.62	2.29	10	8
1:A:752:VAL:HG13	1:A:756:GLU:HG2	0.62	1.70	19	1
1:A:792:LEU:HD13	1:A:820:PHE:CD2	0.62	2.29	1	12
1:A:735:ILE:HG23	1:A:823:LYS:HB2	0.62	1.71	6	16
1:A:763:VAL:HG22	1:A:764:ILE:HG12	0.62	1.70	20	19
1:A:745:ALA:O	1:A:749:MET:N	0.62	2.32	5	20
1:A:789:MET:HE2	1:A:793:GLN:HE21	0.62	1.54	19	14
1:A:749:MET:CA	1:A:770:LEU:HD12	0.62	2.24	20	20
1:A:763:VAL:HG22	1:A:764:ILE:N	0.62	2.08	5	9
1:A:739:VAL:HB	1:A:820:PHE:HB2	0.62	1.72	17	20
1:A:753:LYS:C	1:A:755:THR:H	0.62	2.01	9	20
1:A:803:ASN:HB3	1:A:809:TYR:CE1	0.61	2.30	13	5
1:A:785:LYS:CB	1:A:829:LEU:HD13	0.61	2.25	11	1
1:A:770:LEU:CD2	1:A:792:LEU:HD21	0.61	2.25	2	20
1:A:736:LEU:O	1:A:740:LYS:HB3	0.61	1.96	10	2
1:A:785:LYS:O	1:A:789:MET:HG3	0.61	1.96	6	9
1:A:752:VAL:HG13	1:A:760:TYR:CZ	0.61	2.30	4	11
1:A:752:VAL:HG21	1:A:757:ALA:HB3	0.60	1.72	7	10
1:A:777:LEU:HD23	1:A:788:PHE:HE2	0.60	1.55	3	20
1:A:821:PHE:O	1:A:830:ILE:HD11	0.60	1.96	3	11
1:A:740:LYS:HB2	1:A:749:MET:HE3	0.60	1.73	5	1
1:A:763:VAL:HG11	1:A:802:TYR:CD1	0.60	2.31	17	1
1:A:745:ALA:HB1	1:A:770:LEU:CD1	0.60	2.26	10	20
1:A:757:ALA:HB3	1:A:760:TYR:CB	0.60	2.20	19	4
1:A:728:LEU:HD22	1:A:785:LYS:HB3	0.60	1.72	19	4
1:A:757:ALA:HB1	1:A:760:TYR:CD2	0.60	2.31	18	2
1:A:792:LEU:HD22	1:A:796:PHE:CZ	0.60	2.31	5	20
1:A:824:ILE:CB	1:A:829:LEU:HB2	0.60	2.27	9	20
1:A:740:LYS:HB3	1:A:770:LEU:HB3	0.60	1.73	14	7
1:A:765:ARG:HG3	1:A:766:PHE:CE1	0.60	2.32	7	2
1:A:776:ARG:HA	1:A:779:ASN:ND2	0.59	2.12	12	19
1:A:730:SER:HB2	1:A:733:LYS:HE2	0.59	1.74	10	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:785:LYS:HD3	1:A:829:LEU:HA	0.59	1.74	3	14
1:A:821:PHE:HA	1:A:824:ILE:CD1	0.59	2.28	5	20
1:A:822:SER:O	1:A:826:GLU:HB3	0.59	1.97	11	17
1:A:748:PHE:C	1:A:770:LEU:HD12	0.58	2.22	13	20
1:A:799:CYS:O	1:A:803:ASN:CG	0.58	2.46	17	1
1:A:728:LEU:CD2	1:A:785:LYS:HB3	0.58	2.28	16	8
1:A:824:ILE:C	1:A:829:LEU:HB2	0.58	2.23	11	1
1:A:740:LYS:HB2	1:A:770:LEU:CB	0.58	2.28	20	3
1:A:759:GLY:O	1:A:763:VAL:HG12	0.58	1.99	1	5
1:A:748:PHE:N	1:A:748:PHE:CD1	0.58	2.69	9	8
1:A:730:SER:HA	1:A:733:LYS:HB3	0.58	1.74	16	20
1:A:739:VAL:CB	1:A:816:LEU:HD21	0.58	2.29	7	19
1:A:735:ILE:HG21	1:A:824:ILE:HG23	0.58	1.76	11	9
1:A:824:ILE:HG22	1:A:829:LEU:CG	0.57	2.29	11	1
1:A:752:VAL:HG21	1:A:757:ALA:CB	0.57	2.30	18	10
1:A:791:ASP:O	1:A:794:ARG:HB3	0.57	1.98	19	20
1:A:725:PRO:HB3	1:A:783:VAL:HG12	0.57	1.76	5	19
1:A:739:VAL:O	1:A:745:ALA:HB2	0.57	2.00	5	20
1:A:764:ILE:HG22	1:A:767:PRO:HG3	0.57	1.77	8	2
1:A:768:MET:HG2	1:A:791:ASP:O	0.57	2.00	13	13
1:A:755:THR:C	1:A:757:ALA:N	0.57	2.61	15	18
1:A:732:LEU:CD2	1:A:829:LEU:HD13	0.57	2.30	2	19
1:A:742:HIS:ND1	1:A:743:GLN:N	0.57	2.53	13	20
1:A:752:VAL:HG23	1:A:756:GLU:HG2	0.57	1.75	4	4
1:A:752:VAL:HG11	1:A:757:ALA:HB3	0.57	1.76	13	3
1:A:752:VAL:HG13	1:A:760:TYR:CE2	0.57	2.34	8	10
1:A:779:ASN:HD21	1:A:781:TYR:HB2	0.57	1.58	18	12
1:A:730:SER:HB2	1:A:733:LYS:HE3	0.56	1.77	17	9
1:A:738:GLN:NE2	1:A:823:LYS:HG3	0.56	2.15	5	4
1:A:728:LEU:O	1:A:729:TYR:C	0.56	2.49	5	20
1:A:735:ILE:HG23	1:A:823:LYS:CB	0.56	2.30	12	16
1:A:739:VAL:HB	1:A:816:LEU:HD21	0.56	1.77	8	19
1:A:781:TYR:CE2	1:A:787:LEU:HD22	0.56	2.36	18	2
1:A:802:TYR:CD1	1:A:802:TYR:C	0.56	2.80	3	8
1:A:768:MET:SD	1:A:772:THR:HB	0.56	2.41	18	8
1:A:760:TYR:CD2	1:A:802:TYR:CD2	0.56	2.94	16	2
1:A:736:LEU:HD22	1:A:740:LYS:HE2	0.56	1.77	5	1
1:A:746:TRP:HA	1:A:749:MET:CG	0.56	2.31	5	1
1:A:829:LEU:O	1:A:830:ILE:C	0.56	2.49	3	19
1:A:781:TYR:CE1	1:A:787:LEU:HD22	0.56	2.36	5	18
1:A:774:SER:O	1:A:778:LYS:HD3	0.56	2.01	11	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:807:SER:CB	1:A:809:TYR:CE1	0.56	2.89	10	5
1:A:757:ALA:CB	1:A:760:TYR:CB	0.56	2.82	16	4
1:A:818:LYS:HG2	1:A:819:PHE:N	0.55	2.15	12	16
1:A:820:PHE:CZ	1:A:824:ILE:HD13	0.55	2.36	3	18
1:A:744:SER:CB	1:A:812:CYS:HB3	0.55	2.32	20	1
1:A:728:LEU:HD13	1:A:785:LYS:N	0.55	2.16	17	4
1:A:789:MET:HE3	1:A:824:ILE:CD1	0.55	2.31	12	7
1:A:803:ASN:HD22	1:A:809:TYR:HB2	0.55	1.59	1	1
1:A:789:MET:HE1	1:A:830:ILE:CG2	0.55	2.25	3	4
1:A:764:ILE:HG22	1:A:767:PRO:CG	0.55	2.31	8	1
1:A:773:MET:SD	1:A:791:ASP:HB2	0.55	2.42	15	20
1:A:782:TYR:CE1	1:A:788:PHE:HA	0.55	2.36	13	20
1:A:753:LYS:C	1:A:755:THR:N	0.55	2.64	4	20
1:A:821:PHE:O	1:A:825:LYS:HB2	0.55	2.02	9	20
1:A:748:PHE:CZ	1:A:799:CYS:SG	0.55	3.00	17	2
1:A:753:LYS:HB2	1:A:756:GLU:HB3	0.55	1.76	10	1
1:A:785:LYS:HE3	1:A:829:LEU:HA	0.55	1.77	10	1
1:A:803:ASN:ND2	1:A:809:TYR:CD1	0.55	2.75	7	1
1:A:785:LYS:O	1:A:789:MET:N	0.55	2.39	15	11
1:A:812:CYS:O	1:A:816:LEU:HB2	0.55	2.02	15	19
1:A:740:LYS:HB2	1:A:770:LEU:HD13	0.55	1.76	18	6
1:A:752:VAL:HG22	1:A:760:TYR:CD2	0.54	2.37	17	9
1:A:764:ILE:HD11	1:A:802:TYR:HB2	0.54	1.78	10	13
1:A:760:TYR:CD1	1:A:764:ILE:HG13	0.54	2.37	14	12
1:A:773:MET:SD	1:A:791:ASP:CB	0.54	2.96	8	20
1:A:827:ALA:HB3	1:A:829:LEU:HG	0.54	1.79	12	14
1:A:824:ILE:HA	1:A:829:LEU:HG	0.54	1.79	11	1
1:A:757:ALA:O	1:A:760:TYR:HB2	0.54	2.02	13	8
1:A:803:ASN:CG	1:A:809:TYR:CZ	0.54	2.85	19	2
1:A:790:ALA:O	1:A:794:ARG:N	0.54	2.41	5	20
1:A:752:VAL:HG12	1:A:754:ARG:H	0.54	1.63	19	3
1:A:785:LYS:HG2	1:A:829:LEU:HD22	0.54	1.79	5	1
1:A:739:VAL:CA	1:A:816:LEU:HD11	0.54	2.32	12	1
1:A:813:ALA:O	1:A:817:GLU:HB2	0.54	2.03	2	20
1:A:752:VAL:HG23	1:A:753:LYS:N	0.54	2.18	12	12
1:A:763:VAL:HG21	1:A:802:TYR:CB	0.54	2.33	15	17
1:A:748:PHE:O	1:A:769:ASP:HB2	0.54	2.02	3	4
1:A:735:ILE:HD12	1:A:735:ILE:H	0.53	1.63	8	20
1:A:739:VAL:HG21	1:A:792:LEU:HD11	0.53	1.79	7	19
1:A:752:VAL:CG2	1:A:754:ARG:H	0.53	2.17	7	5
1:A:809:TYR:HA	1:A:812:CYS:SG	0.53	2.43	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:773:MET:HE2	1:A:792:LEU:HG	0.53	1.79	13	19
1:A:729:TYR:CG	1:A:780:ARG:HG3	0.53	2.39	13	19
1:A:732:LEU:HA	1:A:735:ILE:HD13	0.53	1.80	8	20
1:A:739:VAL:HG21	1:A:792:LEU:CD1	0.53	2.34	10	20
1:A:776:ARG:HA	1:A:779:ASN:HD22	0.53	1.63	10	7
1:A:776:ARG:O	1:A:781:TYR:HB3	0.53	2.03	9	5
1:A:776:ARG:HB3	1:A:781:TYR:HB3	0.53	1.81	18	10
1:A:724:ASP:HB3	1:A:727:GLN:HB2	0.53	1.81	10	7
1:A:785:LYS:HD2	1:A:829:LEU:HA	0.53	1.81	5	1
1:A:757:ALA:HB1	1:A:760:TYR:CG	0.53	2.38	16	2
1:A:759:GLY:O	1:A:762:GLU:CG	0.53	2.56	19	1
1:A:804:PRO:HD2	1:A:809:TYR:HE1	0.53	1.63	11	4
1:A:827:ALA:HB3	1:A:829:LEU:HD23	0.53	1.80	11	1
1:A:777:LEU:N	1:A:782:TYR:CE2	0.53	2.77	13	20
1:A:804:PRO:C	1:A:806:GLU:H	0.52	2.12	1	15
1:A:764:ILE:HD12	1:A:798:ASN:HB3	0.52	1.81	8	1
1:A:748:PHE:CD1	1:A:748:PHE:N	0.52	2.74	20	12
1:A:799:CYS:SG	1:A:809:TYR:C	0.52	2.92	12	10
1:A:795:VAL:HA	1:A:798:ASN:OD1	0.52	2.04	2	9
1:A:775:GLU:O	1:A:779:ASN:ND2	0.52	2.42	8	8
1:A:824:ILE:HB	1:A:829:LEU:CB	0.52	2.34	11	1
1:A:753:LYS:HG3	1:A:756:GLU:HG2	0.52	1.82	12	3
1:A:803:ASN:ND2	1:A:809:TYR:CE2	0.52	2.78	19	1
1:A:776:ARG:HB2	1:A:782:TYR:CZ	0.52	2.40	2	5
1:A:746:TRP:N	1:A:747:PRO:CD	0.52	2.72	19	20
1:A:732:LEU:HD22	1:A:788:PHE:CG	0.52	2.40	15	20
1:A:795:VAL:CG2	1:A:796:PHE:N	0.52	2.72	17	10
1:A:736:LEU:HG	1:A:788:PHE:CZ	0.52	2.40	18	20
1:A:730:SER:HA	1:A:733:LYS:HB2	0.51	1.81	2	19
1:A:797:THR:CG2	1:A:798:ASN:N	0.51	2.73	8	12
1:A:809:TYR:HD1	1:A:810:TYR:H	0.51	1.47	8	3
1:A:816:LEU:O	1:A:820:PHE:HB3	0.51	2.06	2	20
1:A:747:PRO:C	1:A:748:PHE:CD1	0.51	2.89	20	10
1:A:752:VAL:HG11	1:A:757:ALA:CB	0.51	2.35	13	3
1:A:776:ARG:HA	1:A:779:ASN:OD1	0.51	2.06	5	1
1:A:768:MET:HG3	1:A:795:VAL:CG1	0.51	2.34	12	11
1:A:825:LYS:HG2	1:A:830:ILE:CD1	0.51	2.32	5	6
1:A:733:LYS:N	1:A:777:LEU:HD21	0.51	2.21	15	20
1:A:724:ASP:HB2	1:A:727:GLN:HB2	0.51	1.81	17	4
1:A:773:MET:SD	1:A:792:LEU:N	0.51	2.84	8	19
1:A:744:SER:CA	1:A:812:CYS:HB3	0.51	2.35	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:759:GLY:O	1:A:762:GLU:HG2	0.51	2.06	19	1
1:A:795:VAL:HA	1:A:798:ASN:ND2	0.51	2.21	18	7
1:A:819:PHE:CD1	1:A:819:PHE:C	0.51	2.88	11	20
1:A:742:HIS:CD2	1:A:816:LEU:HA	0.51	2.41	10	12
1:A:752:VAL:HG13	1:A:756:GLU:CG	0.51	2.35	19	1
1:A:739:VAL:HB	1:A:816:LEU:CD2	0.51	2.36	8	19
1:A:745:ALA:HB1	1:A:770:LEU:HD13	0.51	1.82	11	12
1:A:760:TYR:CD2	1:A:802:TYR:HD2	0.51	2.23	16	2
1:A:740:LYS:HA	1:A:745:ALA:HB1	0.50	1.84	19	10
1:A:794:ARG:O	1:A:798:ASN:HB3	0.50	2.06	13	9
1:A:789:MET:HB3	1:A:793:GLN:NE2	0.50	2.22	12	11
1:A:764:ILE:HD12	1:A:798:ASN:HD22	0.50	1.64	10	8
1:A:815:ILE:O	1:A:818:LYS:HB2	0.50	2.06	15	1
1:A:736:LEU:O	1:A:740:LYS:HG2	0.50	2.07	5	1
1:A:778:LYS:HB2	1:A:778:LYS:HZ2	0.50	1.66	5	3
1:A:771:LYS:O	1:A:775:GLU:N	0.50	2.44	11	15
1:A:810:TYR:O	1:A:813:ALA:HB3	0.50	2.06	20	12
1:A:760:TYR:CD1	1:A:802:TYR:CD2	0.50	3.00	3	2
1:A:737:GLN:HA	1:A:740:LYS:HD3	0.50	1.82	4	6
1:A:804:PRO:HD2	1:A:807:SER:HB2	0.50	1.84	7	3
1:A:746:TRP:HA	1:A:749:MET:SD	0.50	2.47	7	14
1:A:798:ASN:C	1:A:798:ASN:OD1	0.50	2.54	18	4
1:A:740:LYS:C	1:A:742:HIS:N	0.50	2.69	19	5
1:A:822:SER:HB2	1:A:823:LYS:NZ	0.50	2.22	7	1
1:A:773:MET:SD	1:A:782:TYR:OH	0.50	2.68	9	2
1:A:753:LYS:HB2	1:A:756:GLU:CB	0.50	2.37	10	2
1:A:789:MET:HE2	1:A:793:GLN:HE22	0.50	1.67	13	3
1:A:776:ARG:HB3	1:A:781:TYR:CD1	0.49	2.41	1	8
1:A:736:LEU:HD22	1:A:740:LYS:CE	0.49	2.38	5	1
1:A:797:THR:O	1:A:801:GLU:N	0.49	2.45	3	18
1:A:742:HIS:CD2	1:A:816:LEU:HD13	0.49	2.42	12	1
1:A:757:ALA:HB1	1:A:802:TYR:CE2	0.49	2.39	20	3
1:A:740:LYS:HB3	1:A:740:LYS:HZ2	0.49	1.67	11	1
1:A:730:SER:HB3	1:A:733:LYS:HE3	0.49	1.82	13	1
1:A:735:ILE:CD1	1:A:829:LEU:HD11	0.49	2.38	9	19
1:A:799:CYS:SG	1:A:810:TYR:HA	0.49	2.48	13	6
1:A:798:ASN:HA	1:A:801:GLU:HB2	0.49	1.84	2	5
1:A:732:LEU:HD13	1:A:782:TYR:HB3	0.49	1.84	11	15
1:A:790:ALA:O	1:A:794:ARG:HB2	0.49	2.08	18	6
1:A:732:LEU:HD21	1:A:785:LYS:HB3	0.49	1.83	5	1
1:A:724:ASP:HB3	1:A:727:GLN:HE21	0.49	1.68	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:751:PRO:HD3	1:A:771:LYS:HB3	0.49	1.83	15	1
1:A:803:ASN:O	1:A:810:TYR:CD2	0.48	2.66	17	12
1:A:753:LYS:HG3	1:A:753:LYS:O	0.48	2.08	7	1
1:A:785:LYS:HE2	1:A:829:LEU:HA	0.48	1.84	15	3
1:A:785:LYS:HB3	1:A:829:LEU:HD13	0.48	1.84	11	1
1:A:745:ALA:C	1:A:749:MET:HE3	0.48	2.33	15	10
1:A:747:PRO:HB2	1:A:748:PHE:CE1	0.48	2.43	20	10
1:A:785:LYS:HB2	1:A:829:LEU:HD13	0.48	1.85	11	1
1:A:731:THR:HG21	1:A:829:LEU:HD21	0.48	1.84	15	18
1:A:740:LYS:CB	1:A:770:LEU:HB3	0.48	2.38	20	4
1:A:728:LEU:HD22	1:A:785:LYS:CG	0.48	2.39	5	1
1:A:795:VAL:HG22	1:A:796:PHE:CD1	0.48	2.43	2	20
1:A:746:TRP:N	1:A:749:MET:HE3	0.48	2.23	20	8
1:A:732:LEU:CD2	1:A:829:LEU:CD1	0.48	2.88	11	1
1:A:791:ASP:HA	1:A:794:ARG:HB2	0.48	1.85	13	8
1:A:819:PHE:CZ	1:A:823:LYS:HE3	0.48	2.44	18	11
1:A:760:TYR:OH	1:A:767:PRO:HB3	0.48	2.09	14	4
1:A:768:MET:H	1:A:798:ASN:HD22	0.48	1.51	15	2
1:A:808:GLU:N	1:A:808:GLU:CD	0.48	2.71	12	3
1:A:799:CYS:HB2	1:A:813:ALA:HB2	0.48	1.85	17	3
1:A:781:TYR:CZ	1:A:787:LEU:HD22	0.47	2.44	10	19
1:A:748:PHE:HB2	1:A:770:LEU:HD11	0.47	1.85	12	13
1:A:779:ASN:C	1:A:780:ARG:HD3	0.47	2.35	7	16
1:A:740:LYS:CA	1:A:770:LEU:HD13	0.47	2.39	4	4
1:A:740:LYS:CB	1:A:770:LEU:HD13	0.47	2.39	14	7
1:A:804:PRO:C	1:A:810:TYR:CD2	0.47	2.92	19	9
1:A:800:LYS:HZ3	1:A:817:GLU:CD	0.47	2.17	14	1
1:A:804:PRO:HD2	1:A:807:SER:CB	0.47	2.39	18	1
1:A:766:PHE:HB2	1:A:794:ARG:HD3	0.47	1.86	19	6
1:A:768:MET:HE1	1:A:772:THR:HG22	0.47	1.85	15	5
1:A:757:ALA:O	1:A:760:TYR:HB3	0.47	2.09	14	2
1:A:803:ASN:ND2	1:A:809:TYR:HB2	0.47	2.24	1	1
1:A:754:ARG:HG2	1:A:761:TYR:CD1	0.47	2.44	18	1
1:A:740:LYS:NZ	1:A:774:SER:HB3	0.47	2.25	5	1
1:A:764:ILE:HD11	1:A:802:TYR:HB3	0.47	1.87	5	1
1:A:724:ASP:CG	1:A:725:PRO:CD	0.47	2.87	10	3
1:A:782:TYR:C	1:A:784:SER:H	0.47	2.18	8	11
1:A:824:ILE:HG22	1:A:829:LEU:CB	0.47	2.39	13	8
1:A:797:THR:O	1:A:801:GLU:HB2	0.47	2.10	17	1
1:A:777:LEU:CD1	1:A:777:LEU:C	0.47	2.88	9	20
1:A:728:LEU:HD13	1:A:785:LYS:H	0.47	1.70	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:803:ASN:HB3	1:A:809:TYR:CD1	0.47	2.44	11	3
1:A:792:LEU:HD22	1:A:796:PHE:CE1	0.47	2.44	6	18
1:A:775:GLU:HA	1:A:778:LYS:HZ2	0.47	1.70	18	4
1:A:786:LYS:HA	1:A:789:MET:HB2	0.47	1.87	20	11
1:A:764:ILE:HD11	1:A:802:TYR:CB	0.47	2.40	11	16
1:A:760:TYR:O	1:A:763:VAL:HG13	0.47	2.10	12	3
1:A:823:LYS:O	1:A:826:GLU:HG3	0.47	2.10	18	14
1:A:736:LEU:HD11	1:A:773:MET:C	0.47	2.35	2	13
1:A:748:PHE:HB2	1:A:770:LEU:CD1	0.46	2.40	12	10
1:A:728:LEU:HD22	1:A:732:LEU:HD21	0.46	1.86	1	2
1:A:739:VAL:HG21	1:A:792:LEU:CD2	0.46	2.41	13	16
1:A:748:PHE:CD1	1:A:799:CYS:SG	0.46	3.07	5	2
1:A:826:GLU:HG3	1:A:827:ALA:N	0.46	2.25	6	13
1:A:803:ASN:O	1:A:810:TYR:HD2	0.46	1.92	20	6
1:A:824:ILE:O	1:A:829:LEU:HB2	0.46	2.11	11	1
1:A:738:GLN:NE2	1:A:823:LYS:HD2	0.46	2.26	1	9
1:A:752:VAL:C	1:A:754:ARG:H	0.46	2.16	16	10
1:A:823:LYS:O	1:A:826:GLU:HG2	0.46	2.11	11	3
1:A:750:GLU:HA	1:A:771:LYS:HB2	0.46	1.87	17	2
1:A:789:MET:O	1:A:793:GLN:CG	0.46	2.64	18	1
1:A:744:SER:O	1:A:812:CYS:HB3	0.46	2.10	9	11
1:A:791:ASP:O	1:A:794:ARG:N	0.46	2.48	7	18
1:A:809:TYR:O	1:A:812:CYS:HB2	0.46	2.11	4	9
1:A:799:CYS:SG	1:A:809:TYR:HB2	0.46	2.50	10	1
1:A:731:THR:CG2	1:A:829:LEU:HD21	0.46	2.41	15	17
1:A:725:PRO:HB3	1:A:783:VAL:HA	0.46	1.86	6	1
1:A:800:LYS:HG2	1:A:810:TYR:CE1	0.46	2.46	16	2
1:A:740:LYS:C	1:A:742:HIS:H	0.46	2.19	19	3
1:A:736:LEU:HD21	1:A:773:MET:CB	0.46	2.40	5	18
1:A:751:PRO:HG3	1:A:769:ASP:OD1	0.46	2.11	6	1
1:A:795:VAL:C	1:A:799:CYS:SG	0.46	2.99	17	1
1:A:768:MET:SD	1:A:769:ASP:N	0.46	2.88	18	1
1:A:744:SER:HB3	1:A:812:CYS:O	0.45	2.11	20	8
1:A:764:ILE:HB	1:A:767:PRO:HG3	0.45	1.89	1	1
1:A:739:VAL:CG2	1:A:770:LEU:HD22	0.45	2.42	2	5
1:A:773:MET:HE1	1:A:788:PHE:HA	0.45	1.88	2	16
1:A:779:ASN:O	1:A:780:ARG:HB2	0.45	2.10	2	18
1:A:810:TYR:CD1	1:A:810:TYR:C	0.45	2.94	20	12
1:A:760:TYR:O	1:A:764:ILE:HB	0.45	2.11	8	1
1:A:765:ARG:O	1:A:765:ARG:HD3	0.45	2.11	13	1
1:A:760:TYR:HE1	1:A:767:PRO:HB3	0.45	1.71	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:821:PHE:HA	1:A:824:ILE:CG1	0.45	2.41	11	12
1:A:821:PHE:CD1	1:A:824:ILE:HD11	0.45	2.47	11	10
1:A:754:ARG:HA	1:A:760:TYR:HD2	0.45	1.71	8	5
1:A:798:ASN:C	1:A:798:ASN:ND2	0.45	2.74	2	1
1:A:740:LYS:O	1:A:745:ALA:CB	0.45	2.62	19	3
1:A:752:VAL:HG22	1:A:760:TYR:CE2	0.45	2.47	12	2
1:A:819:PHE:CZ	1:A:823:LYS:HE2	0.45	2.47	13	2
1:A:752:VAL:HG12	1:A:754:ARG:N	0.45	2.26	19	1
1:A:784:SER:C	1:A:786:LYS:N	0.45	2.75	1	15
1:A:753:LYS:CG	1:A:756:GLU:HG2	0.45	2.42	14	5
1:A:803:ASN:ND2	1:A:809:TYR:CG	0.45	2.85	7	1
1:A:739:VAL:O	1:A:816:LEU:HD11	0.45	2.11	12	1
1:A:799:CYS:O	1:A:803:ASN:OD1	0.45	2.35	17	1
1:A:728:LEU:HB3	1:A:732:LEU:CD1	0.45	2.41	2	4
1:A:729:TYR:CD1	1:A:780:ARG:HG3	0.45	2.47	16	14
1:A:735:ILE:HA	1:A:738:GLN:HE21	0.45	1.71	1	8
1:A:764:ILE:CG2	1:A:767:PRO:HG3	0.45	2.41	8	3
1:A:749:MET:O	1:A:771:LYS:HB2	0.45	2.12	10	1
1:A:800:LYS:HG3	1:A:813:ALA:HB3	0.45	1.89	19	1
1:A:748:PHE:CE1	1:A:799:CYS:HB2	0.45	2.47	10	6
1:A:822:SER:HB3	1:A:823:LYS:NZ	0.45	2.27	9	2
1:A:798:ASN:OD1	1:A:799:CYS:N	0.45	2.50	16	5
1:A:756:GLU:C	1:A:758:PRO:HD3	0.45	2.36	16	1
1:A:733:LYS:O	1:A:737:GLN:HG3	0.45	2.12	10	9
1:A:739:VAL:HG21	1:A:792:LEU:HD21	0.45	1.89	11	9
1:A:804:PRO:C	1:A:806:GLU:N	0.45	2.74	1	4
1:A:820:PHE:CE2	1:A:824:ILE:HD13	0.45	2.47	5	4
1:A:776:ARG:O	1:A:781:TYR:N	0.45	2.50	9	2
1:A:804:PRO:HD2	1:A:807:SER:HB3	0.45	1.89	19	3
1:A:760:TYR:CE1	1:A:764:ILE:HG13	0.45	2.47	16	2
1:A:763:VAL:HG13	1:A:764:ILE:N	0.45	2.27	1	1
1:A:772:THR:HA	1:A:775:GLU:CD	0.44	2.37	2	1
1:A:820:PHE:O	1:A:824:ILE:CD1	0.44	2.65	2	2
1:A:763:VAL:CG2	1:A:764:ILE:N	0.44	2.80	7	2
1:A:793:GLN:O	1:A:797:THR:HB	0.44	2.12	13	3
1:A:803:ASN:OD1	1:A:810:TYR:CD2	0.44	2.70	17	1
1:A:824:ILE:CA	1:A:829:LEU:HB2	0.44	2.43	11	5
1:A:744:SER:HA	1:A:812:CYS:SG	0.44	2.53	4	4
1:A:728:LEU:CD2	1:A:785:LYS:CG	0.44	2.96	5	1
1:A:779:ASN:ND2	1:A:779:ASN:C	0.44	2.75	5	1
1:A:752:VAL:HG22	1:A:754:ARG:N	0.44	2.25	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:760:TYR:CD1	1:A:802:TYR:HD2	0.44	2.30	3	2
1:A:807:SER:O	1:A:808:GLU:HB3	0.44	2.12	6	1
1:A:745:ALA:HB2	1:A:816:LEU:CD2	0.44	2.42	12	1
1:A:785:LYS:HG2	1:A:786:LYS:HD3	0.44	1.89	20	1
1:A:728:LEU:O	1:A:732:LEU:HG	0.44	2.12	10	20
1:A:789:MET:HE3	1:A:824:ILE:HG21	0.44	1.89	2	2
1:A:770:LEU:HA	1:A:773:MET:HB2	0.44	1.89	12	5
1:A:736:LEU:HD22	1:A:740:LYS:HZ2	0.44	1.72	6	1
1:A:732:LEU:HD13	1:A:782:TYR:CB	0.44	2.42	11	2
1:A:824:ILE:HG13	1:A:830:ILE:HG12	0.44	1.90	9	1
1:A:765:ARG:HA	1:A:765:ARG:NE	0.44	2.27	11	4
1:A:768:MET:CG	1:A:791:ASP:O	0.44	2.65	11	12
1:A:797:THR:HG23	1:A:798:ASN:N	0.44	2.28	2	3
1:A:775:GLU:HA	1:A:778:LYS:NZ	0.44	2.28	8	3
1:A:765:ARG:HB3	1:A:766:PHE:CE1	0.44	2.48	1	2
1:A:777:LEU:N	1:A:782:TYR:HE2	0.44	2.11	6	14
1:A:725:PRO:CB	1:A:783:VAL:HG12	0.43	2.43	15	2
1:A:753:LYS:H	1:A:756:GLU:CG	0.43	2.26	8	1
1:A:758:PRO:C	1:A:760:TYR:H	0.43	2.21	9	2
1:A:768:MET:HE1	1:A:776:ARG:HD2	0.43	1.90	17	1
1:A:764:ILE:CG2	1:A:798:ASN:HB2	0.43	2.43	2	2
1:A:728:LEU:HD21	1:A:785:LYS:HB3	0.43	1.89	16	1
1:A:752:VAL:CG1	1:A:760:TYR:CZ	0.43	3.00	4	3
1:A:739:VAL:O	1:A:742:HIS:HB3	0.43	2.13	9	5
1:A:724:ASP:OD2	1:A:726:ASP:HB3	0.43	2.13	15	1
1:A:796:PHE:HA	1:A:799:CYS:SG	0.43	2.53	17	1
1:A:766:PHE:CB	1:A:794:ARG:HD3	0.43	2.43	6	2
1:A:745:ALA:O	1:A:749:MET:HG3	0.43	2.13	11	2
1:A:752:VAL:HG21	1:A:760:TYR:CZ	0.43	2.48	14	1
1:A:791:ASP:O	1:A:794:ARG:CB	0.43	2.67	9	13
1:A:809:TYR:O	1:A:810:TYR:C	0.43	2.62	6	3
1:A:819:PHE:HD1	1:A:820:PHE:N	0.43	2.11	20	12
1:A:758:PRO:HD2	1:A:802:TYR:OH	0.43	2.13	5	1
1:A:746:TRP:CD2	1:A:747:PRO:HD3	0.43	2.49	6	1
1:A:768:MET:H	1:A:798:ASN:ND2	0.43	2.09	15	2
1:A:804:PRO:O	1:A:806:GLU:N	0.43	2.52	7	2
1:A:737:GLN:O	1:A:741:SER:HB2	0.43	2.14	20	3
1:A:764:ILE:HG21	1:A:798:ASN:HD22	0.43	1.74	17	1
1:A:757:ALA:CB	1:A:760:TYR:CD1	0.43	2.98	3	1
1:A:829:LEU:N	1:A:829:LEU:HD23	0.43	2.29	5	4
1:A:777:LEU:HA	1:A:782:TYR:CD2	0.43	2.49	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:764:ILE:O	1:A:767:PRO:HD3	0.43	2.12	5	5
1:A:735:ILE:O	1:A:736:LEU:C	0.43	2.62	10	7
1:A:789:MET:O	1:A:793:GLN:CB	0.43	2.67	13	6
1:A:796:PHE:O	1:A:800:LYS:HG3	0.43	2.14	6	1
1:A:800:LYS:O	1:A:810:TYR:CE2	0.43	2.72	7	1
1:A:824:ILE:HG13	1:A:830:ILE:CG1	0.43	2.44	9	1
1:A:800:LYS:NZ	1:A:817:GLU:CD	0.43	2.77	14	1
1:A:800:LYS:HZ2	1:A:800:LYS:CB	0.43	2.26	17	1
1:A:827:ALA:O	1:A:829:LEU:HD23	0.43	2.12	19	1
1:A:803:ASN:OD1	1:A:803:ASN:N	0.43	2.52	1	1
1:A:736:LEU:C	1:A:740:LYS:HE3	0.43	2.38	5	1
1:A:765:ARG:CG	1:A:766:PHE:CE1	0.43	3.01	7	1
1:A:748:PHE:O	1:A:769:ASP:HB3	0.43	2.14	7	4
1:A:811:LYS:C	1:A:815:ILE:HD12	0.43	2.38	4	3
1:A:748:PHE:CE1	1:A:809:TYR:HB2	0.43	2.48	7	1
1:A:768:MET:CB	1:A:794:ARG:HB3	0.42	2.44	8	5
1:A:824:ILE:CB	1:A:829:LEU:CB	0.42	2.97	11	1
1:A:791:ASP:HA	1:A:794:ARG:CB	0.42	2.44	11	9
1:A:810:TYR:C	1:A:810:TYR:CD1	0.42	2.97	1	3
1:A:778:LYS:HZ2	1:A:778:LYS:HB2	0.42	1.74	3	1
1:A:776:ARG:HG3	1:A:776:ARG:HH11	0.42	1.73	6	1
1:A:789:MET:O	1:A:793:GLN:HB2	0.42	2.14	11	5
1:A:798:ASN:OD1	1:A:798:ASN:C	0.42	2.62	15	1
1:A:747:PRO:CG	1:A:809:TYR:HB3	0.42	2.45	18	3
1:A:778:LYS:HB2	1:A:778:LYS:NZ	0.42	2.28	9	4
1:A:747:PRO:HB2	1:A:748:PHE:CD1	0.42	2.50	19	1
1:A:821:PHE:CA	1:A:824:ILE:HD11	0.42	2.39	9	2
1:A:803:ASN:ND2	1:A:809:TYR:CE1	0.42	2.88	7	1
1:A:794:ARG:O	1:A:798:ASN:HB2	0.42	2.14	8	1
1:A:732:LEU:HD22	1:A:788:PHE:CB	0.42	2.45	11	1
1:A:800:LYS:HZ1	1:A:814:ASN:HA	0.42	1.74	18	1
1:A:742:HIS:CE1	1:A:744:SER:HB2	0.42	2.49	20	1
1:A:728:LEU:CD2	1:A:732:LEU:HD21	0.42	2.44	1	2
1:A:736:LEU:HD22	1:A:740:LYS:NZ	0.42	2.29	18	2
1:A:796:PHE:CE2	1:A:820:PHE:CE1	0.42	3.08	1	7
1:A:796:PHE:HE2	1:A:820:PHE:CE1	0.42	2.33	9	3
1:A:819:PHE:CD1	1:A:820:PHE:N	0.42	2.88	19	8
1:A:752:VAL:C	1:A:754:ARG:N	0.42	2.78	4	3
1:A:825:LYS:HG3	1:A:830:ILE:CD1	0.42	2.43	11	4
1:A:829:LEU:O	1:A:830:ILE:O	0.42	2.38	10	2
1:A:799:CYS:SG	1:A:809:TYR:O	0.42	2.77	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:773:MET:HE1	1:A:788:PHE:CG	0.42	2.50	2	8
1:A:739:VAL:CA	1:A:816:LEU:HD21	0.42	2.45	7	2
1:A:753:LYS:NZ	1:A:753:LYS:HB3	0.42	2.29	11	1
1:A:751:PRO:HA	1:A:769:ASP:CG	0.42	2.40	16	1
1:A:826:GLU:HG2	1:A:827:ALA:N	0.42	2.30	5	4
1:A:777:LEU:HA	1:A:782:TYR:HD2	0.42	1.75	6	2
1:A:805:PRO:HA	1:A:810:TYR:CG	0.42	2.50	6	1
1:A:785:LYS:HE2	1:A:828:GLY:O	0.42	2.15	8	2
1:A:752:VAL:CG2	1:A:753:LYS:N	0.41	2.83	12	2
1:A:776:ARG:O	1:A:781:TYR:CB	0.41	2.67	2	1
1:A:753:LYS:H	1:A:756:GLU:HG2	0.41	1.74	7	1
1:A:753:LYS:HB3	1:A:756:GLU:HG2	0.41	1.91	7	1
1:A:754:ARG:HG3	1:A:761:TYR:CD1	0.41	2.50	8	1
1:A:776:ARG:HB2	1:A:782:TYR:OH	0.41	2.15	9	1
1:A:752:VAL:HB	1:A:756:GLU:CD	0.41	2.40	17	1
1:A:746:TRP:CG	1:A:747:PRO:HD3	0.41	2.50	19	2
1:A:781:TYR:OH	1:A:787:LEU:HD22	0.41	2.16	10	2
1:A:802:TYR:CD1	1:A:802:TYR:O	0.41	2.73	17	1
1:A:805:PRO:N	1:A:810:TYR:CD2	0.41	2.88	17	1
1:A:740:LYS:HA	1:A:745:ALA:CB	0.41	2.44	19	1
1:A:782:TYR:CD1	1:A:788:PHE:CA	0.41	3.03	18	3
1:A:791:ASP:C	1:A:794:ARG:H	0.41	2.22	13	7
1:A:821:PHE:O	1:A:825:LYS:HE2	0.41	2.16	17	1
1:A:773:MET:CA	1:A:782:TYR:OH	0.41	2.67	7	5
1:A:736:LEU:HD21	1:A:773:MET:HB3	0.41	1.92	15	4
1:A:821:PHE:O	1:A:825:LYS:HE3	0.41	2.16	15	1
1:A:796:PHE:HA	1:A:813:ALA:HB1	0.41	1.93	19	1
1:A:781:TYR:O	1:A:783:VAL:N	0.41	2.54	8	1
1:A:742:HIS:ND1	1:A:744:SER:N	0.41	2.66	13	2
1:A:766:PHE:HB2	1:A:794:ARG:CD	0.41	2.46	20	3
1:A:762:GLU:CG	1:A:763:VAL:N	0.41	2.83	20	3
1:A:771:LYS:HE2	1:A:775:GLU:HG3	0.41	1.91	10	1
1:A:739:VAL:O	1:A:816:LEU:HD21	0.41	2.15	12	1
1:A:795:VAL:O	1:A:798:ASN:OD1	0.41	2.39	12	1
1:A:729:TYR:O	1:A:777:LEU:HD11	0.41	2.14	16	1
1:A:757:ALA:HA	1:A:758:PRO:HD2	0.41	1.76	9	1
1:A:829:LEU:HD23	1:A:829:LEU:N	0.41	2.31	19	1
1:A:794:ARG:HA	1:A:797:THR:HG22	0.41	1.91	3	1
1:A:759:GLY:O	1:A:760:TYR:C	0.41	2.64	10	2
1:A:763:VAL:HG21	1:A:802:TYR:CA	0.41	2.46	10	1
1:A:760:TYR:CE2	1:A:761:TYR:CE1	0.41	3.08	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:752:VAL:HG23	1:A:756:GLU:CG	0.41	2.45	16	1
1:A:789:MET:SD	1:A:830:ILE:HG23	0.41	2.56	2	1
1:A:759:GLY:O	1:A:763:VAL:CG1	0.41	2.69	19	1
1:A:760:TYR:CE2	1:A:761:TYR:HE1	0.40	2.34	17	5
1:A:724:ASP:CG	1:A:725:PRO:HD2	0.40	2.41	10	1
1:A:779:ASN:ND2	1:A:781:TYR:HB2	0.40	2.30	18	1
1:A:803:ASN:C	1:A:810:TYR:HD2	0.40	2.24	1	1
1:A:776:ARG:C	1:A:781:TYR:HB3	0.40	2.40	2	1
1:A:760:TYR:HD1	1:A:802:TYR:CE2	0.40	2.34	3	1
1:A:751:PRO:HG3	1:A:769:ASP:OD2	0.40	2.15	13	1
1:A:796:PHE:O	1:A:800:LYS:N	0.40	2.55	15	1
1:A:803:ASN:CG	1:A:809:TYR:CE2	0.40	2.99	19	1
1:A:807:SER:HB3	1:A:809:TYR:CE1	0.40	2.52	10	1
1:A:752:VAL:CG1	1:A:756:GLU:HG3	0.40	2.47	14	1
1:A:824:ILE:HG12	1:A:824:ILE:H	0.40	1.43	19	1
1:A:761:TYR:CE1	1:A:767:PRO:HG2	0.40	2.50	20	1
1:A:780:ARG:O	1:A:781:TYR:C	0.40	2.64	2	1
1:A:746:TRP:CH2	1:A:809:TYR:CE1	0.40	3.09	12	1
1:A:778:LYS:NZ	1:A:778:LYS:HB2	0.40	2.31	18	1
1:A:755:THR:O	1:A:756:GLU:C	0.40	2.63	20	1
1:A:776:ARG:HB2	1:A:782:TYR:CE2	0.40	2.51	2	1
1:A:820:PHE:CE1	1:A:824:ILE:HD13	0.40	2.51	17	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	107/118 (91%)	84±2 (78±2%)	19±2 (18±2%)	4±1 (4±1%)	4	30
2	B	0	-	-	-	-	-
All	All	2140/2620 (82%)	1672 (78%)	383 (18%)	85 (4%)	4	30

All 10 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	830	ILE	20
1	A	807	SER	16
1	A	829	LEU	15
1	A	808	GLU	13
1	A	724	ASP	6
1	A	752	VAL	6
1	A	758	PRO	4
1	A	805	PRO	3
1	A	767	PRO	1
1	A	782	TYR	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	100/110 (91%)	67±2 (67±2%)	33±2 (33±2%)	1 12
2	B	0	-	-	-
All	All	2000/2400 (83%)	1343 (67%)	657 (33%)	1 12

All 58 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	730	SER	20
1	A	731	THR	20
1	A	736	LEU	20
1	A	739	VAL	20
1	A	770	LEU	20
1	A	777	LEU	20
1	A	780	ARG	20
1	A	795	VAL	20
1	A	801	GLU	20
1	A	819	PHE	20
1	A	820	PHE	20
1	A	824	ILE	20
1	A	825	LYS	20
1	A	830	ILE	20
1	A	762	GLU	19

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Mol	Chain	Res	Type	Models (Total)
1	A	778	LYS	19
1	A	763	VAL	19
1	A	775	GLU	18
1	A	785	LYS	18
1	A	809	TYR	18
1	A	748	PHE	17
1	A	821	PHE	17
1	A	826	GLU	17
1	A	752	VAL	16
1	A	792	LEU	16
1	A	818	LYS	16
1	A	789	MET	15
1	A	740	LYS	13
1	A	811	LYS	12
1	A	798	ASN	12
1	A	817	GLU	11
1	A	784	SER	11
1	A	779	ASN	9
1	A	766	PHE	8
1	A	756	GLU	8
1	A	769	ASP	8
1	A	765	ARG	7
1	A	808	GLU	6
1	A	807	SER	6
1	A	794	ARG	5
1	A	802	TYR	5
1	A	800	LYS	5
1	A	823	LYS	4
1	A	750	GLU	3
1	A	806	GLU	3
1	A	803	ASN	2
1	A	753	LYS	2
1	A	786	LYS	2
1	A	749	MET	1
1	A	815	ILE	1
1	A	767	PRO	1
1	A	776	ARG	1
1	A	816	LEU	1
1	A	797	THR	1
1	A	799	CYS	1
1	A	737	GLN	1
1	A	754	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	812	CYS	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
2	ALY	B	36	2	10,11,12	0.65±0.04	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
2	ALY	B	36	2	7,12,14	1.03±0.11	0±0 (1±4%)

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
2	ALY	B	36	2	-	0±0,9,10,12	-

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)	Models	
								Worst	Total
2	B	36	ALY	OH-CH-CH3	2.14	118.24	122.05	6	2

There are no chirality outliers.

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	36	ALY	CH3-CH-NZ-CE	1

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided