wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1BVE
Title	:	HIV-1 PROTEASE-DMP323 COMPLEX IN SOLUTION, NMR, 28 STRUCTURES
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Deposited on	:	1996-01-16

This is a wwPDB NMR Structure Validation Summary 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 (i) symbol.

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

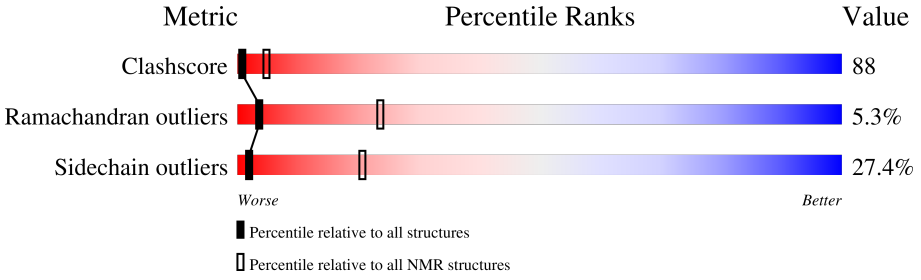
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	99	14% 65% 21%
1	B	99	15% 67% 18%

2 Ensemble composition and analysis (i)

This entry contains 28 models. Model 7 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:1-A:99, B:1-B:99 (198)	0.54	7

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 3, 9, 12, 14, 19, 22, 23, 27
2	7, 10, 15, 16, 18, 20, 24, 25, 26
3	4, 5, 6, 8, 21
4	2, 28
Single-model clusters	11; 13; 17

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3200 atoms, of which 1646 are hydrogens and 0 are deuteriums.

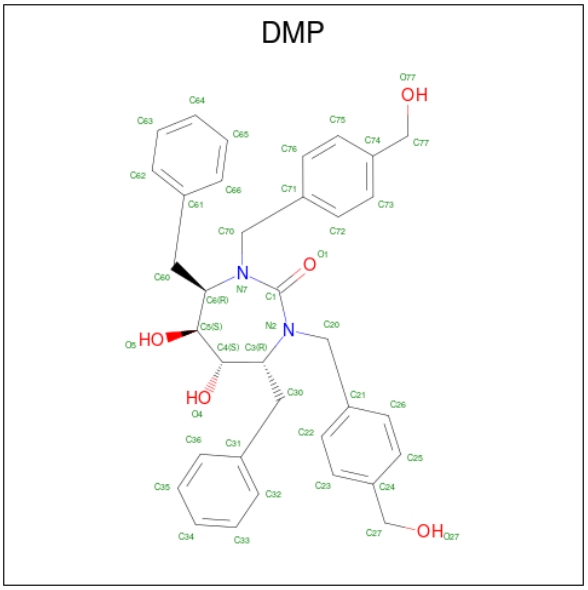
- Molecule 1 is a protein called HIV-1 PROTEASE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	99	1560	488	804	130	135	3	0
1	B	99	1560	488	804	130	135	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ALA	CYS	engineered mutation	UNP P04585
B	95	ALA	CYS	engineered mutation	UNP P04585

- Molecule 2 is [4-R-(-4-ALPHA,5-ALPHA,6-BETA,7-BETA)]-HEXAHYDRO-5,6-BIS(HYDROXY)-[1,3-BIS([4-HYDROXYMETHYL-PHENYL]METHYL)-4,7-BIS(PHEN YLMETHYL)]-2H-1,3-DIAZEPINONE (three-letter code: DMP) (formula: $C_{35}H_{38}N_2O_5$).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	B	1	80	35	38	2	5

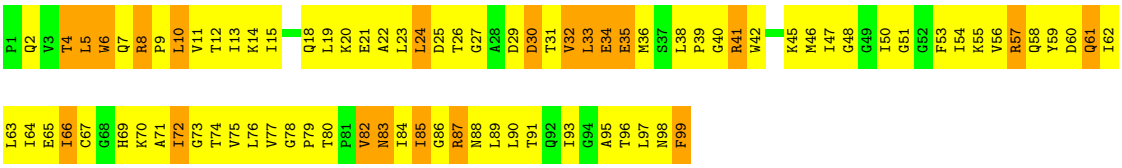
4 Residue-property plots (i)

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: HIV-1 PROTEASE

Chain A: 14% 65% 21%



• Molecule 1: HIV-1 PROTEASE

Chain B: 15% 67% 18%

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

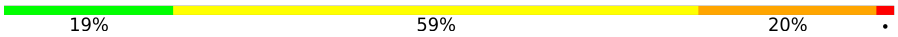
The representative model is number 7. Colouring as in section 4.1 above.

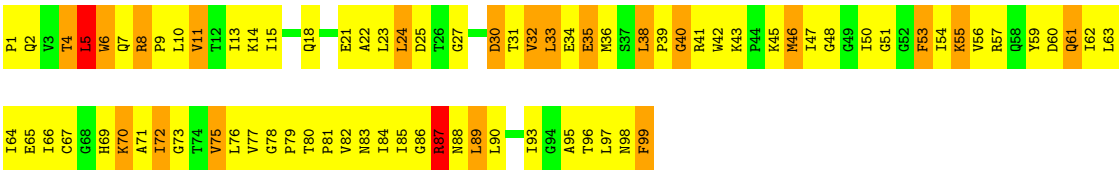
• Molecule 1: HIV-1 PROTEASE

Chain A: 22% 54% 24%

• Molecule 1: HIV-1 PROTEASE

Chain B:


19%
59%
20%


P1 Q2 V3 T4 L5 W6 Q7 R8 P9 L10 V11 T12 I13 K14 I15 Q18 E21 A22 L23 L24 D25 T26 G27 D30 T31 V32 L33 E34 E35 M36 S37 L38 P39 G40 R41 W42 K43 P44 K45 M46 I47 G48 G49 I50 G51 G52 F53 I54 K55 V56 R57 Q58 Y59 D60 Q61 I62 L63
I64 E65 I66 C67 G68 H69 K70 A71 I72 G73 T74 V75 L76 V77 G78 P79 T80 P81 V82 N83 I84 I85 G86 R87 N88 L89 L90 I93 G94 A95 T96 L97 N98 F99

5 Refinement protocol and experimental data overview (i)

Of the 28 calculated structures, 28 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
XPLOR	structure solution	3.1

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: DMP

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	3.8±0.4
1	B	0.0±0.0	3.7±0.5
All	All	0	211

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

5 of 8 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	8	ARG	Sidechain	28
1	B	8	ARG	Sidechain	28
1	A	57	ARG	Sidechain	27
1	B	41	ARG	Sidechain	27
1	A	41	ARG	Sidechain	26

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	756	804	804	159±13
1	B	756	804	804	160±14
2	B	42	38	38	17±4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	43512	46088	46088	7903

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 88.

5 of 2058 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:LEU:HD13	1:A:92:GLN:OE1	1.05	1.52	17	2
1:A:63:LEU:HD21	1:A:70:LYS:CG	1.04	1.82	7	11
1:B:33:LEU:HD13	1:B:75:VAL:CG1	1.03	1.82	14	28
1:B:63:LEU:HD21	1:B:70:LYS:CG	1.03	1.82	27	9
1:A:33:LEU:HD13	1:A:75:VAL:CG1	1.01	1.86	24	28

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/99 (98%)	77±2 (80±2%)	15±2 (15±2%)	5±1 (5±1%)	4	25
1	B	97/99 (98%)	77±3 (80±3%)	14±3 (15±3%)	5±2 (6±2%)	3	23
All	All	5432/5544 (98%)	4328 (80%)	818 (15%)	286 (5%)	3	23

5 of 35 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	34	GLU	22
1	B	5	LEU	21
1	A	6	TRP	20
1	B	34	GLU	20
1	B	6	TRP	19

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	82/82 (100%)	59±4 (72±4%)	23±4 (28±4%)	2 19
1	B	82/82 (100%)	60±3 (73±4%)	22±3 (27±4%)	2 21
All	All	4592/4592 (100%)	3334 (73%)	1258 (27%)	2 21

5 of 133 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	72	ILE	28
1	A	99	PHE	28
1	B	32	VAL	28
1	B	99	PHE	28
1	A	32	VAL	27

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

1 ligand 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	DMP	B	100	-	46,46,46	0.65±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
2	DMP	B	100	-	56,63,63	0.97±0.02	2±0 (3±0%)

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	DMP	B	100	-	-	0±0,20,48,48	0±0,5,5,5

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
2	B	100	DMP	C20-C21	2.31	1.47	1.51	5	5
2	B	100	DMP	C70-C71	2.16	1.47	1.51	26	3

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	100	DMP	C60-C6-C5	2.76	118.00	114.24	16	25
2	B	100	DMP	C30-C3-C4	2.53	117.67	114.24	21	27
2	B	100	DMP	C71-C70-N7	2.20	117.57	113.54	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	100	DMP	C5-C6-N7	2.04	116.17	112.76	25	4
2	B	100	DMP	C4-C3-N2	2.01	116.10	112.76	22	1

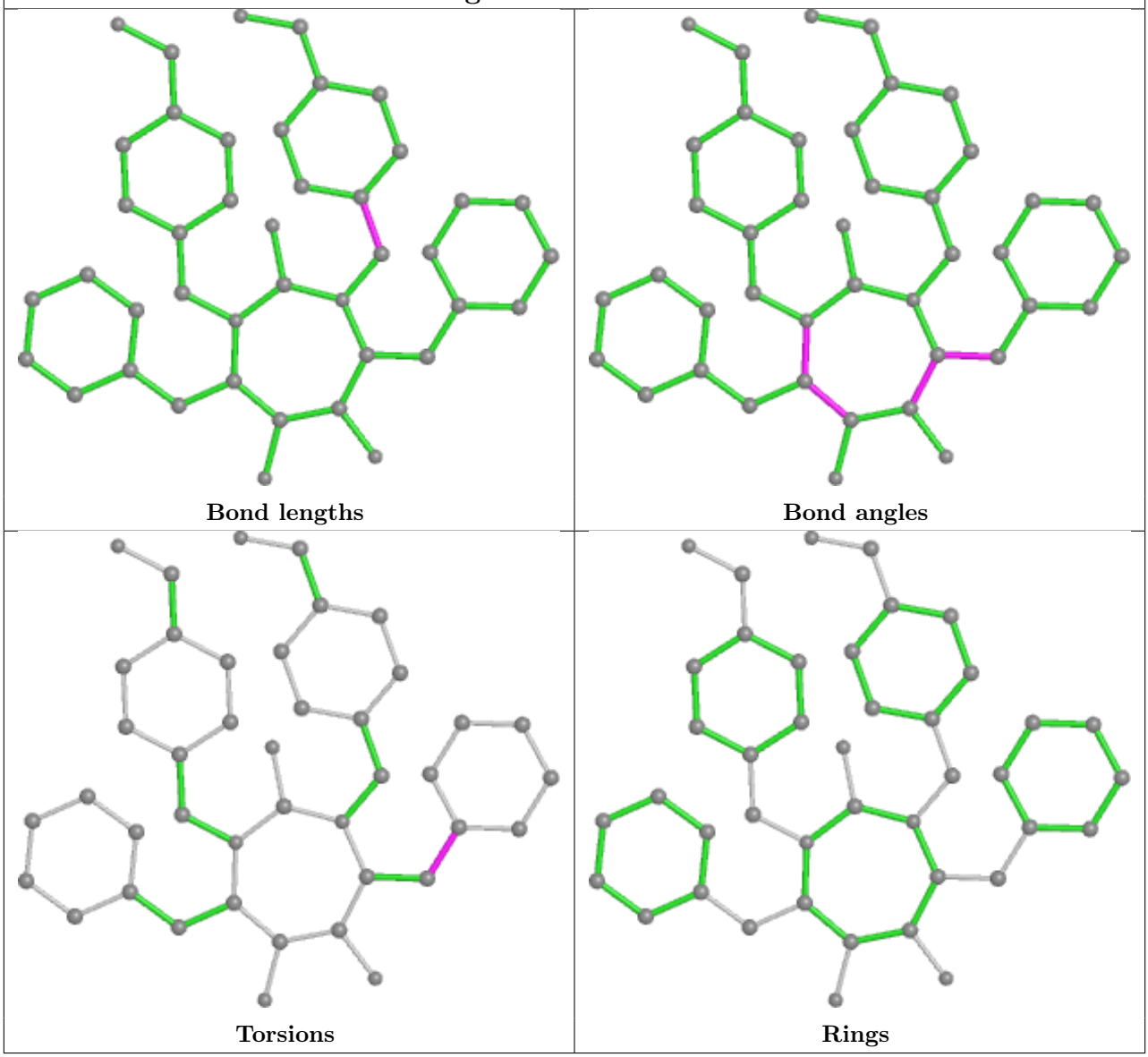
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DMP B 100



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 (i)

No chemical shift data were provided