



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:07 pm BST

PDB ID : 4HVP
Title : Structure of complex of synthetic HIV-1 protease with a substrate-based inhibitor at 2.3 Angstroms resolution
Authors : Miller, M.; Schneider, J.; Sathyanarayana, B.K.; Toth, M.V.; Marshall, G.R.; Clawson, L.; Selk, L.; Kent, S.B.H.; Wlodawer, A.
Deposited on : 1989-08-08
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

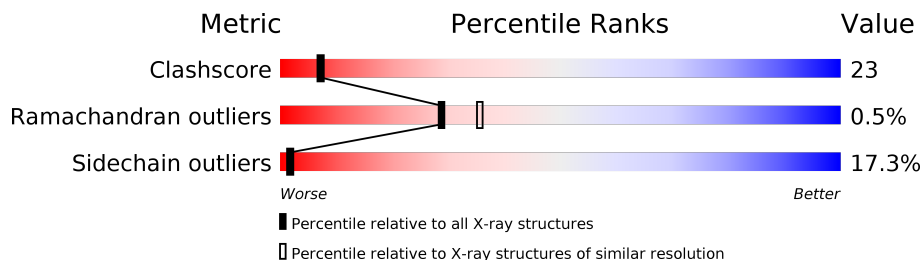
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	99	
1	B	99	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 1640 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

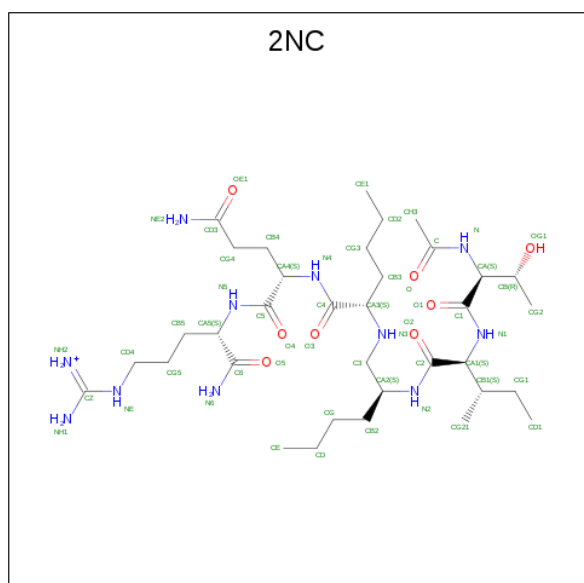
- Molecule 1 is a protein called HIV-1 PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	99	Total 758	C 490	N 131	O 135	S 2	0	0	0
1	B	99	Total 758	C 490	N 131	O 135	S 2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ABA	CYS	CONFLICT	UNP P03369
A	95	ABA	CYS	CONFLICT	UNP P03369
B	67	ABA	CYS	CONFLICT	UNP P03369
B	95	ABA	CYS	CONFLICT	UNP P03369

- Molecule 2 is N-((2S)-2-[(N-acetyl-L-threonyl-L-isoleucyl)amino]hexyl)-L-norleucyl-L-glutamyl-N 5 -[amino(iminio)methyl]-L-ornithinamide (three-letter code: 2NC) (formula: C₃₅H₆₈N₁₁O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	54	35	11	8	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	34	Total	O	0	0
			34	34		

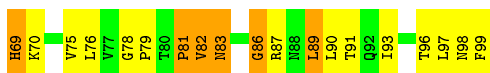
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

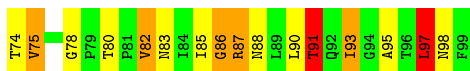
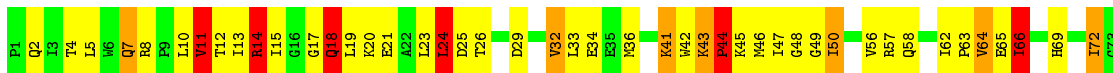
- Molecule 1: HIV-1 PROTEASE

Chain A: 



- Molecule 1: HIV-1 PROTEASE

Chain B: 



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.70Å 59.20Å 62.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1640	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2NC, ABA

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 root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.02	1/758 (0.1%)	2.76	65/1024 (6.3%)
1	B	1.06	0/758	2.77	64/1024 (6.2%)
All	All	1.04	1/1516 (0.1%)	2.77	129/2048 (6.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	GLU	CD-OE1	-5.45	1.19	1.25

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ARG	CD-NE-CZ	22.38	154.93	123.60
1	B	14	ARG	CD-NE-CZ	20.73	152.63	123.60
1	A	87	ARG	NE-CZ-NH1	18.34	129.47	120.30
1	A	34	GLU	CB-CG-CD	14.77	154.09	114.20
1	B	87	ARG	NE-CZ-NH2	14.71	127.66	120.30
1	B	14	ARG	NE-CZ-NH2	14.56	127.58	120.30
1	A	30	ASP	CB-CG-OD1	13.61	130.55	118.30
1	A	30	ASP	CB-CG-OD2	-13.53	106.13	118.30
1	A	57	ARG	NE-CZ-NH1	-12.80	113.90	120.30
1	B	57	ARG	CD-NE-CZ	11.91	140.27	123.60
1	A	29	ASP	CB-CG-OD2	-11.59	107.87	118.30
1	A	23	LEU	CA-CB-CG	11.23	141.12	115.30
1	A	8	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	A	7	GLN	CB-CG-CD	9.99	137.58	111.60
1	B	66	ILE	CB-CA-C	9.75	131.11	111.60
1	A	87	ARG	NH1-CZ-NH2	-9.72	108.70	119.40
1	B	43	LYS	CA-CB-CG	9.40	134.09	113.40
1	A	26	THR	N-CA-CB	-9.24	92.75	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	GLY	O-C-N	9.21	137.44	122.70
1	A	26	THR	CA-CB-CG2	9.16	125.22	112.40
1	A	82	VAL	CA-CB-CG2	9.06	124.49	110.90
1	A	8	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	B	87	ARG	NE-CZ-NH1	-8.71	115.95	120.30
1	A	17	GLY	N-CA-C	-8.69	91.38	113.10
1	A	57	ARG	NH1-CZ-NH2	8.66	128.93	119.40
1	B	11	VAL	N-CA-CB	-8.48	92.84	111.50
1	B	91	THR	N-CA-CB	-8.01	95.08	110.30
1	B	46	MET	CA-CB-CG	-8.00	99.69	113.30
1	B	88	ASN	CB-CG-OD1	8.00	137.60	121.60
1	B	17	GLY	CA-C-O	7.98	134.97	120.60
1	A	41	LYS	CB-CA-C	7.97	126.35	110.40
1	B	32	VAL	O-C-N	7.94	135.41	122.70
1	B	64	VAL	CA-CB-CG1	7.83	122.64	110.90
1	A	57	ARG	O-C-N	7.80	135.18	122.70
1	B	7	GLN	CG-CD-OE1	7.79	137.18	121.60
1	B	12	THR	N-CA-CB	7.69	124.92	110.30
1	A	14	ARG	N-CA-CB	7.68	124.42	110.60
1	B	7	GLN	CB-CG-CD	7.62	131.42	111.60
1	A	11	VAL	N-CA-CB	-7.53	94.92	111.50
1	B	41	LYS	CA-CB-CG	7.46	129.82	113.40
1	A	57	ARG	CB-CG-CD	-7.46	92.20	111.60
1	B	57	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	B	41	LYS	CB-CG-CD	7.30	130.57	111.60
1	B	29	ASP	CB-CG-OD1	7.25	124.83	118.30
1	B	93	ILE	C-N-CA	7.24	137.50	122.30
1	A	41	LYS	CA-CB-CG	7.24	129.32	113.40
1	B	15	ILE	CB-CA-C	-7.23	97.14	111.60
1	A	91	THR	CA-CB-CG2	7.17	122.44	112.40
1	A	87	ARG	CD-NE-CZ	7.17	133.63	123.60
1	A	22	ALA	N-CA-CB	7.08	120.02	110.10
1	A	18	GLN	O-C-N	-7.07	111.40	122.70
1	B	46	MET	CG-SD-CE	6.98	111.37	100.20
1	A	99	PHE	N-CA-CB	6.95	123.10	110.60
1	B	50	ILE	CB-CG1-CD1	6.89	133.21	113.90
1	A	11	VAL	CG1-CB-CG2	6.77	121.74	110.90
1	A	7	GLN	CA-CB-CG	6.76	128.27	113.40
1	A	82	VAL	CG1-CB-CG2	-6.72	100.15	110.90
1	A	17	GLY	CA-C-O	-6.69	108.56	120.60
1	B	57	ARG	CG-CD-NE	6.58	125.61	111.80
1	B	23	LEU	CB-CG-CD2	-6.51	99.93	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	GLY	CA-C-O	-6.42	109.04	120.60
1	B	97	LEU	N-CA-CB	6.41	123.23	110.40
1	A	35	GLU	CB-CA-C	6.35	123.10	110.40
1	B	43	LYS	CB-CG-CD	6.34	128.09	111.60
1	B	32	VAL	CA-CB-CG1	6.32	120.38	110.90
1	A	29	ASP	OD1-CG-OD2	6.27	135.21	123.30
1	A	57	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	66	ILE	CA-C-O	6.26	133.25	120.10
1	A	69	HIS	CA-CB-CG	-6.21	103.05	113.60
1	A	18	GLN	CA-C-O	6.13	132.98	120.10
1	A	69	HIS	N-CA-CB	6.13	121.63	110.60
1	A	15	ILE	N-CA-CB	6.09	124.80	110.80
1	B	15	ILE	N-CA-CB	6.04	124.69	110.80
1	B	11	VAL	CA-CB-CG1	6.02	119.93	110.90
1	A	30	ASP	O-C-N	5.99	132.28	122.70
1	B	5	LEU	CA-CB-CG	5.97	129.03	115.30
1	B	18	GLN	N-CA-CB	-5.94	99.91	110.60
1	B	72	ILE	CA-C-O	-5.92	107.67	120.10
1	B	74	THR	C-N-CA	5.90	136.45	121.70
1	A	18	GLN	C-N-CA	5.89	136.42	121.70
1	B	2	GLN	CB-CG-CD	5.87	126.87	111.60
1	B	14	ARG	CG-CD-NE	5.84	124.06	111.80
1	A	40	GLY	CA-C-O	5.82	131.08	120.60
1	B	82	VAL	O-C-N	5.82	132.02	122.70
1	A	46	MET	CA-C-O	-5.81	107.91	120.10
1	B	64	VAL	CG1-CB-CG2	-5.81	101.61	110.90
1	A	32	VAL	CA-C-O	5.77	132.22	120.10
1	B	24	LEU	N-CA-CB	-5.70	99.00	110.40
1	B	86	GLY	O-C-N	5.64	131.72	122.70
1	B	11	VAL	CB-CA-C	5.62	122.08	111.40
1	B	72	ILE	CB-CA-C	-5.59	100.42	111.60
1	B	19	LEU	O-C-N	5.58	131.62	122.70
1	B	91	THR	OG1-CB-CG2	5.57	122.81	110.00
1	A	65	GLU	OE1-CD-OE2	5.56	129.97	123.30
1	A	25	ASP	N-CA-CB	-5.55	100.60	110.60
1	B	14	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	86	GLY	CA-C-O	-5.50	110.70	120.60
1	A	6	TRP	N-CA-CB	5.50	120.49	110.60
1	B	44	PRO	N-CA-CB	-5.48	96.57	102.60
1	A	78	GLY	O-C-N	5.46	131.48	121.10
1	B	44	PRO	CB-CA-C	5.43	125.57	112.00
1	B	82	VAL	CB-CA-C	-5.41	101.12	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	GLN	N-CA-C	5.39	125.56	111.00
1	B	7	GLN	OE1-CD-NE2	-5.37	109.54	121.90
1	B	75	VAL	CA-CB-CG2	5.36	118.93	110.90
1	A	14	ARG	CD-NE-CZ	5.34	131.08	123.60
1	A	32	VAL	CB-CA-C	5.33	121.53	111.40
1	B	85	ILE	CG1-CB-CG2	5.32	123.10	111.40
1	B	8	ARG	N-CA-CB	-5.31	101.05	110.60
1	A	81	PRO	O-C-N	-5.30	114.22	122.70
1	B	21	GLU	CG-CD-OE1	5.29	128.88	118.30
1	A	10	LEU	CA-CB-CG	5.29	127.46	115.30
1	B	5	LEU	O-C-N	-5.27	114.26	122.70
1	A	33	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	91	THR	CA-CB-OG1	-5.23	98.02	109.00
1	A	10	LEU	CB-CG-CD2	-5.22	102.13	111.00
1	A	32	VAL	CA-CB-CG2	5.22	118.72	110.90
1	B	88	ASN	CB-CG-ND2	-5.21	104.20	116.70
1	B	15	ILE	CA-CB-CG1	5.19	120.87	111.00
1	A	89	LEU	CB-CG-CD1	5.18	119.80	111.00
1	B	8	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	83	ASN	CA-C-N	5.11	128.44	117.20
1	A	21	GLU	O-C-N	-5.09	114.56	122.70
1	A	89	LEU	CA-CB-CG	5.08	127.00	115.30
1	B	43	LYS	CG-CD-CE	5.06	127.07	111.90
1	B	91	THR	CA-CB-CG2	5.05	119.48	112.40
1	B	72	ILE	N-CA-CB	5.05	122.42	110.80
1	A	83	ASN	CA-C-O	-5.04	109.51	120.10
1	A	59	TYR	CG-CD1-CE1	5.03	125.32	121.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	758	0	803	43	0
1	B	758	0	803	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	54	0	63	13	0
3	A	36	0	0	2	0
3	B	34	0	0	0	0
All	All	1640	0	1669	73	0

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 23.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HD11	1:B:48:GLY:C	1.95	0.85
1:B:25:ASP:OD1	2:B:0:2NC:HC32	1.81	0.80
1:B:45:LYS:HE3	1:B:58:GLN:HE22	1.50	0.77
1:B:87:ARG:O	1:B:91:THR:HB	1.85	0.75
1:B:34:GLU:HG2	1:B:83:ASN:OD1	1.90	0.70
1:B:13:ILE:HG22	1:B:66:ILE:HB	1.74	0.70
1:A:63:PRO:HD2	3:A:603:HOH:O	1.93	0.69
1:A:15:ILE:HB	1:A:18:GLN:HE22	1.58	0.68
1:B:33:LEU:HD12	1:B:75:VAL:HG13	1.77	0.66
1:A:10:LEU:HD13	1:A:23:LEU:HD23	1.76	0.65
1:A:47:ILE:HB	2:B:0:2NC:HD11	1.79	0.65
1:A:42:TRP:CE3	1:A:57:ARG:HB2	2.33	0.62
1:A:97:LEU:HD23	1:B:97:LEU:HD13	1.80	0.62
1:A:28:ALA:HB1	2:B:0:2NC:HG26	1.80	0.62
1:A:50:ILE:HD11	1:B:48:GLY:O	2.01	0.60
1:B:26:THR:HG21	1:B:97:LEU:HD21	1.82	0.60
1:A:47:ILE:HD12	2:B:0:2NC:HD11	1.84	0.60
1:B:33:LEU:HD12	1:B:75:VAL:CG1	2.32	0.59
1:A:14:ARG:HD2	3:A:645:HOH:O	2.00	0.59
1:A:44:PRO:O	1:A:45:LYS:HD2	2.03	0.58
1:A:49:GLY:HA3	1:B:50:ILE:HB	1.87	0.57
1:A:81:PRO:HG2	2:B:0:2NC:HE11	1.86	0.56
1:B:45:LYS:HE3	1:B:58:GLN:NE2	2.20	0.56
1:A:38:LEU:HB3	1:A:39:PRO:HD2	1.88	0.55
1:A:82:VAL:HG12	2:B:0:2NC:HD21	1.89	0.54
1:A:98:ASN:O	1:B:95:ABA:HA	2.08	0.54
1:A:34:GLU:HG2	1:A:83:ASN:OD1	2.08	0.53
1:A:82:VAL:CG1	2:B:0:2NC:HD21	2.40	0.52
1:A:20:LYS:HE2	1:A:36:MET:HE1	1.91	0.52
1:B:66:ILE:HG13	1:B:93:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:OE2	1:A:57:ARG:NH1	2.43	0.51
1:B:25:ASP:OD1	2:B:0:2NC:C3	2.57	0.50
1:A:26:THR:HG22	1:B:24:LEU:O	2.12	0.50
1:A:86:GLY:O	1:A:90:LEU:HG	2.12	0.49
1:A:32:VAL:HA	1:A:76:LEU:O	2.13	0.49
1:B:24:LEU:HD11	1:B:66:ILE:CD1	2.43	0.48
1:A:43:LYS:NZ	1:A:58:GLN:O	2.46	0.48
1:A:47:ILE:CD1	2:B:0:2NC:HD11	2.43	0.48
1:B:56:VAL:HG12	1:B:78:GLY:HA3	1.95	0.48
1:A:12:THR:HA	1:A:20:LYS:O	2.15	0.47
1:A:48:GLY:O	2:B:0:2NC:HA	2.14	0.47
1:B:66:ILE:CG1	1:B:93:ILE:HD13	2.45	0.47
1:B:82:VAL:HG12	1:B:83:ASN:O	2.14	0.47
1:B:42:TRP:HZ3	1:B:44:PRO:HB3	1.81	0.46
1:A:33:LEU:HD22	1:A:75:VAL:HG13	1.96	0.46
2:B:0:2NC:HD13	2:B:0:2NC:HG24	1.80	0.45
1:A:65:GLU:HA	1:A:69:HIS:O	2.16	0.45
1:B:14:ARG:HA	1:B:18:GLN:O	2.16	0.45
1:B:20:LYS:HE2	1:B:36:MET:CE	2.47	0.44
2:B:0:2NC:HA5	2:B:0:2NC:CZ	2.48	0.44
1:B:13:ILE:HA	1:B:65:GLU:O	2.17	0.44
1:A:54:ILE:HD12	1:A:79:PRO:HD2	1.99	0.43
1:A:10:LEU:CD1	1:A:23:LEU:HD23	2.44	0.43
1:A:18:GLN:HG3	1:A:18:GLN:H	1.43	0.42
1:B:62:ILE:HA	1:B:63:PRO:HD3	1.78	0.42
1:A:20:LYS:HE2	1:A:36:MET:CE	2.50	0.42
1:B:58:GLN:HE21	1:B:58:GLN:HB2	1.62	0.42
1:B:86:GLY:O	1:B:90:LEU:HG	2.19	0.42
1:A:2:GLN:HB2	1:B:98:ASN:ND2	2.34	0.42
1:B:11:VAL:HG11	1:B:66:ILE:HD12	2.02	0.42
1:B:65:GLU:HA	1:B:69:HIS:O	2.19	0.42
1:A:96:THR:HG22	1:B:4:THR:HA	2.02	0.41
1:A:44:PRO:C	1:A:45:LYS:HD2	2.41	0.41
1:A:33:LEU:HD22	1:A:75:VAL:CG1	2.51	0.41
1:A:18:GLN:OE1	1:A:36:MET:HE1	2.21	0.41
2:B:0:2NC:O3	2:B:0:2NC:HB32	2.21	0.41
1:B:14:ARG:O	1:B:64:VAL:HA	2.20	0.41
1:A:50:ILE:HD11	1:B:49:GLY:N	2.33	0.40
1:A:9:PRO:HD2	1:A:23:LEU:HD22	2.03	0.40
1:A:50:ILE:H	1:A:50:ILE:HG12	1.71	0.40
1:A:8:ARG:HA	1:A:9:PRO:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:VAL:HG11	1:B:66:ILE:CD1	2.52	0.40
1:B:33:LEU:HD23	1:B:83:ASN:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	95/99 (96%)	89 (94%)	5 (5%)	1 (1%)	14	15
1	B	95/99 (96%)	90 (95%)	5 (5%)	0	100	100
All	All	190/198 (96%)	179 (94%)	10 (5%)	1 (0%)	29	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLY

5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	81/81 (100%)	69 (85%)	12 (15%)	3	3
1	B	81/81 (100%)	65 (80%)	16 (20%)	1	1
All	All	162/162 (100%)	134 (83%)	28 (17%)	2	2

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	12	THR
1	A	15	ILE
1	A	26	THR
1	A	36	MET
1	A	41	LYS
1	A	43	LYS
1	A	45	LYS
1	A	57	ARG
1	A	70	LYS
1	A	89	LEU
1	A	93	ILE
1	B	7	GLN
1	B	10	LEU
1	B	11	VAL
1	B	14	ARG
1	B	18	GLN
1	B	24	LEU
1	B	32	VAL
1	B	41	LYS
1	B	43	LYS
1	B	44	PRO
1	B	47	ILE
1	B	66	ILE
1	B	72	ILE
1	B	80	THR
1	B	91	THR
1	B	97	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	58	GLN
1	A	98	ASN
1	B	2	GLN
1	B	58	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	ABA	A	67	1	4,5,6	1.45	1 (25%)	1,5,7	1.95	0
1	ABA	A	95	1	4,5,6	1.11	0	1,5,7	1.65	0
1	ABA	B	95	1	4,5,6	0.83	0	1,5,7	1.85	0
1	ABA	B	67	1	4,5,6	0.84	0	1,5,7	0.39	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
1	ABA	A	67	1	-	0/3/4/6	-
1	ABA	A	95	1	-	2/3/4/6	-
1	ABA	B	95	1	-	1/3/4/6	-
1	ABA	B	67	1	-	0/3/4/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ABA	O-C	2.19	1.28	1.19

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	95	ABA	C-CA-CB-CG
1	B	95	ABA	C-CA-CB-CG
1	A	95	ABA	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	95	ABA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2NC	B	0	-	53,53,53	1.46	7 (13%)	64,68,68	4.52	39 (60%)

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	2NC	B	0	-	-	16/75/75/75	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	0	2NC	C6-N6	-4.18	1.22	1.32
2	B	0	2NC	CG21-CB1	3.62	1.61	1.53
2	B	0	2NC	CB4-CA4	-3.39	1.45	1.53
2	B	0	2NC	CA4-N4	2.83	1.51	1.45
2	B	0	2NC	CA1-N1	2.77	1.51	1.45
2	B	0	2NC	CA2-N2	2.70	1.52	1.46
2	B	0	2NC	CA5-N5	2.27	1.50	1.45

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	0	2NC	CG4-CB4-CA4	15.99	143.04	113.16
2	B	0	2NC	CB1-CA1-C2	14.58	138.95	111.62
2	B	0	2NC	CB4-CA4-C5	8.82	130.79	110.20
2	B	0	2NC	O5-C6-N6	-8.11	108.90	123.00
2	B	0	2NC	O3-C4-CA3	7.03	135.25	120.45
2	B	0	2NC	O2-C2-CA1	6.85	134.92	120.74
2	B	0	2NC	CA5-C6-N6	6.71	128.17	116.69
2	B	0	2NC	CG3-CB3-CA3	6.63	134.40	113.92
2	B	0	2NC	O4-C5-CA4	6.37	133.85	120.45
2	B	0	2NC	CB1-CA1-N1	-6.34	98.10	111.34
2	B	0	2NC	CB-CA-C1	5.77	123.99	111.28
2	B	0	2NC	CA4-C5-N5	-5.49	104.67	116.70
2	B	0	2NC	O2-C2-N2	-5.24	113.23	122.93
2	B	0	2NC	CB-CA-N	-5.23	98.34	111.72
2	B	0	2NC	CB2-CA2-C3	5.01	116.73	109.52
2	B	0	2NC	CG21-CB1-CG1	-4.83	99.55	111.78
2	B	0	2NC	O3-C4-N4	-4.80	114.04	122.93
2	B	0	2NC	CG-CB2-CA2	4.44	122.49	111.96
2	B	0	2NC	CB2-CA2-N2	4.01	116.19	110.54
2	B	0	2NC	CB5-CA5-N5	-3.94	102.91	110.88
2	B	0	2NC	CB4-CG4-CD3	-3.93	99.28	112.59
2	B	0	2NC	C5-CA4-N4	-3.91	100.51	111.16
2	B	0	2NC	CG2-CB-CA	3.86	120.07	112.29
2	B	0	2NC	CG4-CD3-NE2	-3.75	104.85	116.51
2	B	0	2NC	CG5-CD4-NE	3.52	122.28	112.21
2	B	0	2NC	OE1-CD3-NE2	3.10	130.97	122.50
2	B	0	2NC	O-C-CH3	2.83	127.31	122.06
2	B	0	2NC	CB5-CA5-C6	2.78	116.65	110.21
2	B	0	2NC	CB4-CA4-N4	-2.77	105.28	110.88
2	B	0	2NC	NH1-CZ-NE	2.76	125.56	119.19
2	B	0	2NC	CA3-C4-N4	-2.73	110.71	116.70
2	B	0	2NC	CH3-C-N	-2.59	111.72	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	0	2NC	O1-C1-CA	2.47	125.84	120.74
2	B	0	2NC	C6-CA5-N5	-2.42	104.32	110.18
2	B	0	2NC	CG21-CB1-CA1	2.38	116.91	111.02
2	B	0	2NC	C1-CA-N	-2.22	104.32	110.36
2	B	0	2NC	CA1-C2-N2	-2.16	111.83	116.48
2	B	0	2NC	NE-CZ-NH2	-2.15	116.92	120.70
2	B	0	2NC	OG1-CB-CA	-2.14	104.83	109.13

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	0	2NC	C1-CA-CB-CG2
2	B	0	2NC	CG21-CB1-CG1-CD1
2	B	0	2NC	CA4-CB4-CG4-CD3
2	B	0	2NC	CA3-CB3-CG3-CD2
2	B	0	2NC	CA1-CB1-CG1-CD1
2	B	0	2NC	N2-C2-CA1-N1
2	B	0	2NC	O2-C2-CA1-N1
2	B	0	2NC	N-CA-CB-CG2
2	B	0	2NC	C1-CA-CB-OG1
2	B	0	2NC	CE1-CD2-CG3-CB3
2	B	0	2NC	NE-CD4-CG5-CB5
2	B	0	2NC	N2-C2-CA1-CB1
2	B	0	2NC	O2-C2-CA1-CB1
2	B	0	2NC	CA2-C3-N3-CA3
2	B	0	2NC	N1-CA1-CB1-CG1
2	B	0	2NC	N3-C3-CA2-CB2

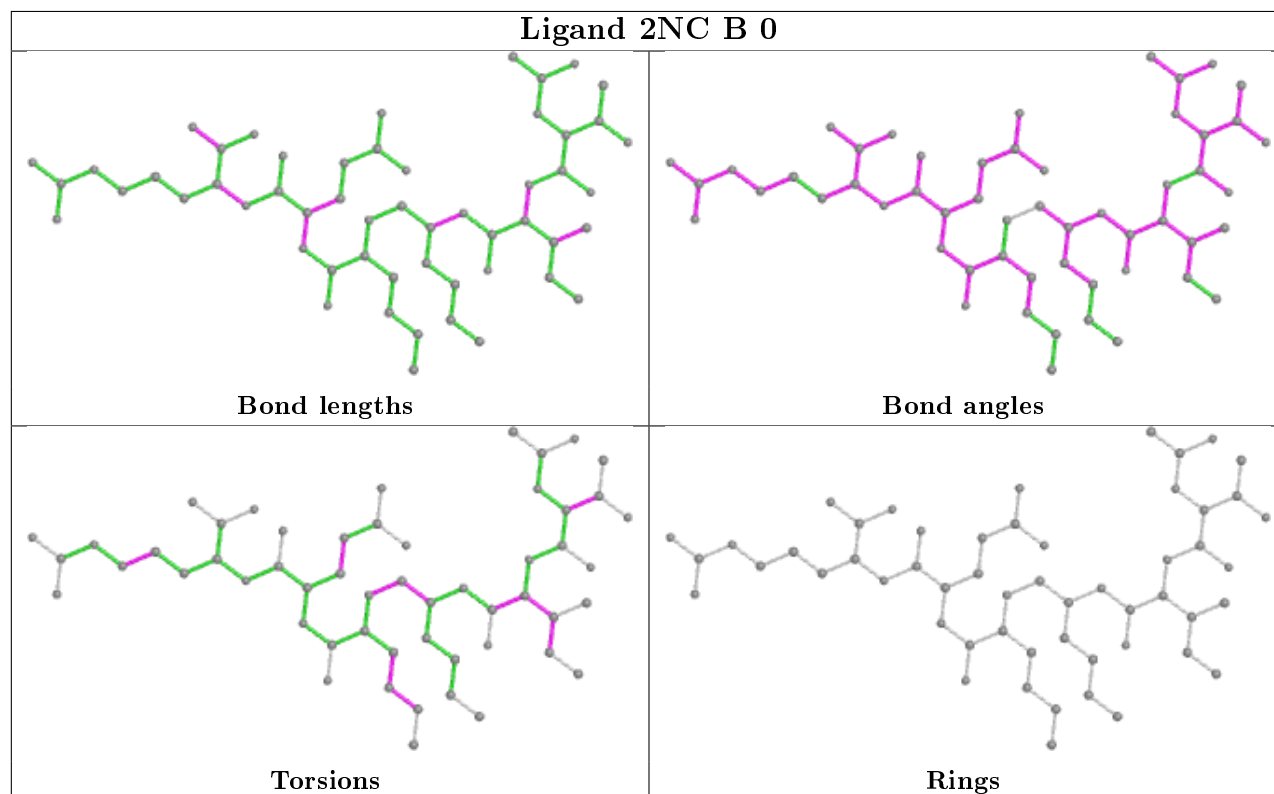
There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	0	2NC	13	0

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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.