



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:20 PM UTC

PDB ID : 7HVP / pdb_00007hvp
Title : X-RAY CRYSTALLOGRAPHIC STRUCTURE OF A COMPLEX BETWEEN A SYNTHETIC PROTEASE OF HUMAN IMMUNODEFICIENCY VIRUS 1 AND A SUBSTRATE-BASED HYDROXYETHYLAMINE INHIBITOR
Authors : Swain, A.L.; Miller, M.M.; Green, J.; Rich, D.H.; Schneider, J.; Kent, S.B.H.; Wlodawer, A.
Deposited on : 1990-09-13
Resolution : 2.40 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 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)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

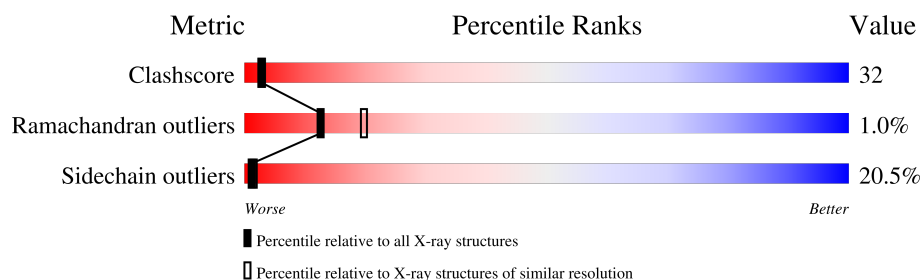
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 of 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	16% 53% 25% 6%
1	B	99	17% 45% 27% 10%
2	C	7	43% 29% 29%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	VME	C	6	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1672 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
1	A	99	Total	C	N	O	S	0	0	0
			758	490	131	135	2			
1	B	99	Total	C	N	O	S	0	0	0
			758	490	131	135	2			

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 a protein called INHIBITOR ACE-SER-LEU-ASN-PHE-PSI(CH(OH)-CH₂N)-PRO-ILE VME (JG-365).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			61	42	8	11			

- Molecule 3 is water.

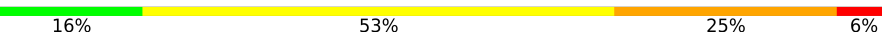
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	53	Total	O	0	0
			53	53		
3	C	4	Total	O	0	0
			4	4		

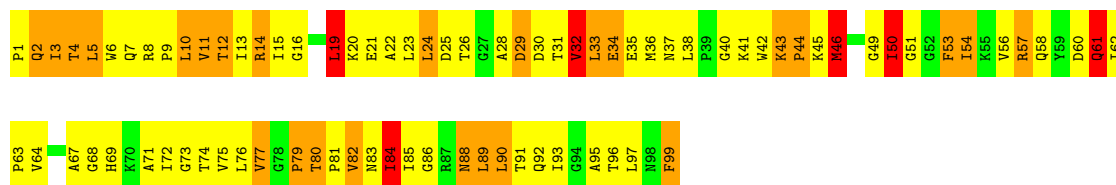
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

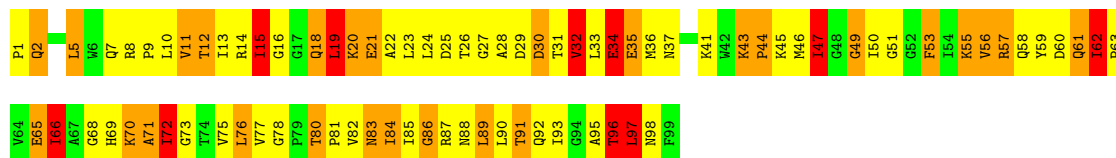
• Molecule 1: HIV-1 PROTEASE

Chain A: 



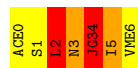
• Molecule 1: HIV-1 PROTEASE

Chain B: 



• Molecule 2: INHIBITOR ACE-SER-LEU-ASN-PHE-PSI(CH(OH)-CH2N)-PRO-ILE VME (JG-365)

Chain C: 



4 Data and refinement statistics

Xtriage (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	51.20Å 58.80Å 62.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.146 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1672	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ABA, ACE, VME, JG3

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	1.38	1/758 (0.1%)	3.26	130/1024 (12.7%)
1	B	1.32	0/758	2.97	95/1024 (9.3%)
2	C	1.05	0/29	3.48	5/37 (13.5%)
All	All	1.35	1/1545 (0.1%)	3.12	230/2085 (11.0%)

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 outliers	#Planarity outliers
2	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	LEU	CA-C	5.54	1.59	1.52

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	GLN	CA-CB-CG	15.97	146.03	114.10
1	A	50	ILE	N-CA-CB	13.14	128.41	110.54
1	B	25	ASP	CA-CB-CG	12.97	125.58	112.60
1	A	19	LEU	N-CA-CB	11.53	128.67	110.57
2	C	5	ILE	N-CA-CB	11.44	130.94	111.50
1	A	61	GLN	CB-CG-CD	10.91	131.15	112.60
1	B	20	LYS	CB-CG-CD	10.79	136.12	111.30
1	B	49	GLY	CA-C-O	-10.62	110.25	120.97
1	A	40	GLY	CA-C-O	10.54	130.04	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	THR	OG1-CB-CG2	-10.38	88.54	109.30
1	A	61	GLN	CA-C-N	10.24	132.24	123.33
1	A	61	GLN	C-N-CA	10.24	132.24	123.33
1	B	11	VAL	N-CA-CB	-10.02	97.43	112.35
1	A	14	ARG	N-CA-CB	9.92	126.13	110.55
1	A	2	GLN	CB-CA-C	9.80	125.94	109.48
1	B	62	ILE	O-C-N	9.77	130.20	121.12
1	B	56	VAL	O-C-N	9.74	133.44	122.82
1	B	32	VAL	CB-CA-C	9.61	124.36	110.33
1	B	35	GLU	CA-C-O	9.44	131.27	121.07
1	A	11	VAL	N-CA-CB	-9.39	96.67	112.44
1	A	57	ARG	CA-C-N	9.23	135.11	121.72
1	A	57	ARG	C-N-CA	9.23	135.11	121.72
1	A	62	ILE	CA-C-O	-9.19	113.81	119.51
1	A	4	THR	CA-CB-OG1	-9.14	95.90	109.60
1	A	7	GLN	OE1-CD-NE2	-9.03	113.57	122.60
1	B	72	ILE	CB-CG1-CD1	9.03	132.77	113.80
1	B	84	ILE	CB-CG1-CD1	8.66	131.99	113.80
1	B	25	ASP	N-CA-C	8.65	122.66	107.61
1	A	43	LYS	O-C-N	8.53	129.68	121.66
1	B	19	LEU	CB-CA-C	8.49	124.12	110.19
1	B	65	GLU	CA-CB-CG	8.38	130.86	114.10
1	A	46	MET	N-CA-C	8.37	123.60	107.44
1	B	97	LEU	N-CA-CB	8.36	124.06	110.43
1	A	77	VAL	O-C-N	8.33	132.01	123.10
1	B	37	ASN	CA-CB-CG	-8.22	104.38	112.60
1	A	26	THR	CA-CB-OG1	-8.17	97.34	109.60
1	A	44	PRO	CA-C-O	-8.15	110.74	120.85
1	A	33	LEU	CA-C-O	8.11	130.33	121.16
1	B	12	THR	CA-C-N	8.06	134.53	122.92
1	B	12	THR	C-N-CA	8.06	134.53	122.92
2	C	2	LEU	CB-CA-C	8.03	124.71	109.37
1	B	91	THR	O-C-N	8.02	133.17	122.43
1	B	2	GLN	CA-C-O	-7.98	109.42	120.52
1	B	66	ILE	CB-CA-C	7.94	127.48	111.60
1	A	20	LYS	CA-C-N	7.86	134.54	123.07
1	A	20	LYS	C-N-CA	7.86	134.54	123.07
1	A	2	GLN	CA-CB-CG	7.83	129.77	114.10
1	B	29	ASP	CA-C-O	-7.83	110.56	119.79
1	A	72	ILE	N-CA-CB	7.81	124.12	111.23
1	A	62	ILE	CA-C-N	7.78	128.07	119.90
1	A	62	ILE	C-N-CA	7.78	128.07	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	HIS	N-CA-CB	7.75	123.30	110.52
1	A	64	VAL	CA-C-O	-7.74	112.31	121.28
1	A	24	LEU	O-C-N	-7.71	111.78	122.41
1	A	32	VAL	CB-CA-C	7.70	122.02	110.63
1	B	96	THR	CA-CB-OG1	-7.67	98.10	109.60
1	A	43	LYS	N-CA-C	-7.64	98.60	110.14
1	A	24	LEU	CA-C-O	7.56	130.50	121.66
1	A	15	ILE	CB-CA-C	7.56	123.69	111.29
1	B	90	LEU	O-C-N	7.55	131.05	122.22
1	A	6	TRP	O-C-N	7.53	130.11	122.12
1	A	12	THR	O-C-N	7.50	131.77	123.22
1	A	54	ILE	N-CA-CB	7.43	125.81	111.92
1	A	29	ASP	CA-CB-CG	7.43	120.03	112.60
1	B	73	GLY	CA-C-O	-7.40	113.61	121.38
1	B	83	ASN	N-CA-CB	7.36	122.31	110.16
1	B	29	ASP	O-C-N	7.30	132.11	122.33
1	A	5	LEU	O-C-N	7.29	131.23	122.26
1	A	34	GLU	N-CA-C	-7.28	100.44	110.35
1	A	19	LEU	CA-CB-CG	7.27	141.73	116.30
1	B	29	ASP	N-CA-CB	7.26	121.48	110.30
1	A	10	LEU	O-C-N	7.21	131.42	123.27
1	A	69	HIS	N-CA-C	-7.20	97.96	109.76
1	B	57	ARG	CA-CB-CG	7.18	128.46	114.10
1	B	93	ILE	CA-C-O	7.16	127.44	119.92
1	A	71	ALA	CA-C-O	-7.14	113.33	121.40
1	A	4	THR	N-CA-CB	-7.12	99.88	110.85
1	B	20	LYS	CG-CD-CE	7.01	127.42	111.30
1	A	90	LEU	CA-C-O	6.97	127.98	119.97
1	A	83	ASN	CA-C-N	-6.96	114.56	123.19
1	A	83	ASN	C-N-CA	-6.96	114.56	123.19
1	B	47	ILE	CB-CA-C	6.93	121.50	110.82
1	A	69	HIS	CA-CB-CG	-6.91	106.89	113.80
1	B	19	LEU	N-CA-C	-6.90	97.28	108.52
1	A	58	GLN	N-CA-C	6.88	119.78	109.25
1	A	88	ASN	OD1-CG-ND2	-6.84	115.76	122.60
1	A	51	GLY	N-CA-C	6.79	122.37	114.16
1	A	88	ASN	CB-CG-ND2	6.79	126.58	116.40
1	A	43	LYS	CA-CB-CG	6.78	127.66	114.10
1	B	82	VAL	O-C-N	6.78	128.87	122.97
1	B	11	VAL	CA-CB-CG1	6.75	121.88	110.40
1	A	50	ILE	CA-C-O	-6.72	113.96	120.95
1	B	21	GLU	N-CA-CB	6.71	121.61	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ALA	O-C-N	6.70	131.28	123.17
1	A	57	ARG	CB-CA-C	6.68	120.37	110.62
1	B	30	ASP	O-C-N	6.67	132.48	122.94
1	B	36	MET	CA-C-O	6.67	128.22	120.75
1	A	6	TRP	N-CA-C	-6.66	104.02	111.28
1	A	6	TRP	CA-C-O	-6.66	113.49	120.55
1	B	45	LYS	N-CA-CB	6.64	122.91	111.69
1	B	57	ARG	N-CA-C	-6.64	98.42	109.24
1	B	89	LEU	CB-CA-C	6.59	120.77	109.24
1	B	44	PRO	N-CA-C	-6.58	101.33	111.13
1	A	8	ARG	CD-NE-CZ	-6.53	115.26	124.40
1	B	91	THR	CA-C-O	-6.50	111.39	119.38
1	B	5	LEU	N-CA-C	6.44	120.84	112.92
1	A	37	ASN	N-CA-CB	6.43	120.67	110.57
1	B	83	ASN	O-C-N	6.34	130.45	123.22
1	B	86	GLY	CA-C-O	-6.30	113.67	122.36
1	B	21	GLU	CA-CB-CG	6.29	126.69	114.10
1	A	3	ILE	CA-C-N	6.24	133.90	122.92
1	A	3	ILE	C-N-CA	6.24	133.90	122.92
1	B	51	GLY	CA-C-N	6.24	133.63	121.41
1	B	51	GLY	C-N-CA	6.24	133.63	121.41
1	A	50	ILE	CB-CA-C	-6.22	103.74	112.14
1	A	57	ARG	N-CA-C	-6.19	97.09	107.80
1	B	16	GLY	N-CA-C	-6.13	98.93	110.77
1	A	5	LEU	CA-C-O	-6.13	112.72	119.95
1	A	6	TRP	N-CA-CB	6.09	119.07	110.12
1	B	19	LEU	CA-C-O	-6.08	113.63	120.32
1	B	2	GLN	N-CA-CB	6.06	120.75	110.87
1	A	5	LEU	N-CA-C	6.06	119.98	112.59
1	A	38	LEU	O-C-N	6.04	127.18	121.38
1	B	25	ASP	N-CA-CB	-6.03	101.49	110.71
1	A	25	ASP	N-CA-CB	-6.01	100.31	110.46
1	A	75	VAL	CA-CB-CG2	6.00	120.61	110.40
1	A	82	VAL	CA-C-N	6.00	130.40	122.42
1	A	82	VAL	C-N-CA	6.00	130.40	122.42
1	A	61	GLN	CA-C-O	6.00	129.09	120.51
1	B	5	LEU	CA-C-N	5.97	128.88	120.28
1	B	5	LEU	C-N-CA	5.97	128.88	120.28
1	A	83	ASN	CA-C-O	-5.97	114.20	120.58
1	B	93	ILE	CB-CA-C	5.95	120.04	111.65
1	B	32	VAL	CA-C-O	5.94	126.66	120.36
1	A	71	ALA	CA-C-N	5.88	132.56	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ALA	C-N-CA	5.88	132.56	121.97
1	A	99	PHE	CA-CB-CG	5.88	119.68	113.80
1	B	77	VAL	CB-CA-C	5.87	119.58	110.83
1	B	72	ILE	CA-CB-CG1	5.87	120.38	110.40
1	A	61	GLN	CA-CB-CG	5.85	125.80	114.10
1	A	96	THR	CA-C-O	-5.85	110.86	120.80
1	A	4	THR	CB-CA-C	5.83	120.20	109.71
1	A	15	ILE	N-CA-C	-5.83	97.21	109.34
1	B	2	GLN	O-C-N	5.81	131.82	122.99
1	B	34	GLU	N-CA-CB	5.81	118.74	110.44
1	A	92	GLN	O-C-N	5.80	129.40	122.27
1	B	68	GLY	CA-C-N	5.79	130.37	122.84
1	B	68	GLY	C-N-CA	5.79	130.37	122.84
1	B	61	GLN	N-CA-C	5.78	119.32	111.17
1	B	15	ILE	O-C-N	5.78	129.18	123.00
1	B	5	LEU	N-CA-CB	-5.77	102.13	110.56
1	A	74	THR	N-CA-C	-5.75	101.89	110.23
1	B	69	HIS	CA-CB-CG	-5.74	108.06	113.80
1	B	76	LEU	N-CA-CB	-5.73	101.08	110.42
1	A	74	THR	CA-C-O	5.73	127.49	121.19
1	A	19	LEU	N-CA-C	-5.71	99.88	109.07
1	B	25	ASP	CA-C-O	5.70	127.96	120.15
1	B	71	ALA	CB-CA-C	5.70	124.02	111.09
1	B	66	ILE	CA-CB-CG2	5.69	120.17	110.50
1	B	89	LEU	N-CA-CB	-5.68	102.17	110.47
1	B	60	ASP	CA-C-O	-5.67	114.75	121.16
1	B	97	LEU	CB-CA-C	-5.66	100.42	109.75
1	A	80	THR	CB-CA-C	5.64	116.49	108.76
1	A	74	THR	N-CA-CB	5.62	118.32	109.83
1	A	58	GLN	CB-CG-CD	5.61	122.14	112.60
1	B	88	ASN	CB-CA-C	5.60	120.09	110.79
1	A	5	LEU	CB-CA-C	5.60	120.03	111.02
1	A	7	GLN	CB-CG-CD	5.60	122.11	112.60
1	A	84	ILE	O-C-N	-5.59	117.31	123.18
1	A	91	THR	N-CA-CB	5.59	118.94	110.28
1	B	73	GLY	O-C-N	5.58	130.04	123.62
1	B	35	GLU	CA-C-N	5.52	134.23	121.87
1	B	35	GLU	C-N-CA	5.52	134.23	121.87
1	A	11	VAL	CA-C-O	5.52	127.46	121.67
1	B	55	LYS	CA-C-N	-5.51	115.29	122.51
1	B	55	LYS	C-N-CA	-5.51	115.29	122.51
1	A	44	PRO	CB-CA-C	-5.50	106.39	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	PRO	CA-C-O	-5.50	114.76	121.03
1	A	2	GLN	N-CA-C	-5.50	100.74	109.76
1	B	37	ASN	N-CA-C	5.50	117.46	109.71
1	A	40	GLY	N-CA-C	5.49	117.64	112.04
1	B	55	LYS	CB-CA-C	5.49	118.89	109.51
1	B	7	GLN	CG-CD-OE1	5.48	131.77	120.80
1	A	53	PHE	CA-C-N	5.47	130.67	122.58
1	A	53	PHE	C-N-CA	5.47	130.67	122.58
1	A	72	ILE	CA-C-O	-5.46	113.95	120.78
1	A	92	GLN	CA-C-O	-5.45	113.70	119.97
1	A	14	ARG	O-C-N	5.45	129.70	123.27
1	A	25	ASP	N-CA-C	5.42	118.30	107.62
1	B	47	ILE	CA-CB-CG2	5.41	119.69	110.50
1	B	37	ASN	OD1-CG-ND2	5.40	128.00	122.60
1	A	82	VAL	CA-CB-CG2	5.40	119.58	110.40
1	A	73	GLY	N-CA-C	5.39	118.40	110.80
1	A	68	GLY	CA-C-N	-5.38	114.64	122.65
1	A	68	GLY	C-N-CA	-5.38	114.64	122.65
1	B	57	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	A	41	LYS	N-CA-C	-5.34	102.98	110.50
1	A	79	PRO	N-CA-CB	5.32	106.13	102.35
1	B	80	THR	N-CA-CB	-5.28	103.16	110.29
1	A	64	VAL	CA-CB-CG2	5.27	119.36	110.40
1	B	84	ILE	N-CA-C	5.27	115.49	108.11
1	B	46	MET	CA-CB-CG	-5.25	103.59	114.10
1	B	53	PHE	CA-CB-CG	-5.25	108.55	113.80
1	B	85	ILE	N-CA-CB	5.22	118.24	111.67
1	A	7	GLN	CG-CD-NE2	5.18	124.17	116.40
1	A	14	ARG	N-CA-C	-5.17	100.09	108.52
1	A	40	GLY	O-C-N	-5.17	117.06	123.21
1	A	53	PHE	N-CA-C	5.16	118.52	110.32
1	A	71	ALA	N-CA-CB	-5.15	102.73	111.69
1	B	34	GLU	CG-CD-OE2	-5.15	106.56	118.40
1	A	44	PRO	O-C-N	5.14	127.92	122.93
1	B	31	THR	N-CA-C	-5.14	101.32	109.76
1	A	34	GLU	CA-C-O	-5.14	116.10	121.55
1	A	84	ILE	CA-C-O	5.14	125.93	120.48
1	B	60	ASP	CB-CA-C	5.14	118.77	109.37
1	B	63	PRO	N-CA-CB	5.14	107.88	103.36
1	A	37	ASN	CA-CB-CG	5.13	117.73	112.60
2	C	3	ASN	OD1-CG-ND2	5.13	127.73	122.60
1	A	24	LEU	N-CA-CB	-5.12	103.19	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	MET	CA-C-N	5.12	127.75	122.27
1	A	46	MET	C-N-CA	5.12	127.75	122.27
2	C	0	ACE	O-C-N	-5.12	107.65	123.00
1	A	3	ILE	N-CA-C	-5.11	100.84	108.46
1	A	7	GLN	N-CA-CB	5.09	118.29	110.70
1	A	80	THR	CA-CB-CG2	5.05	119.08	110.50
1	A	92	GLN	OE1-CD-NE2	5.03	127.63	122.60
1	A	36	MET	CA-C-N	-5.03	116.07	123.00
1	A	36	MET	C-N-CA	-5.03	116.07	123.00
2	C	5	ILE	N-CA-C	-5.03	96.93	111.00
1	A	74	THR	CB-CA-C	5.02	118.05	109.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	4	JG3	Peptide,Mainchain

5.2 Too-close contacts ⓘ

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	53	0
1	B	758	0	804	71	0
2	C	61	0	61	7	0
3	A	38	0	0	3	0
3	B	53	0	0	4	0
3	C	4	0	0	1	0
All	All	1672	0	1668	105	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 32.

All (105) 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:HD12	1:B:47:ILE:HD12	1.61	0.83
1:A:50:ILE:HD13	2:C:5:ILE:HD12	1.60	0.82
1:B:56:VAL:HG12	1:B:78:GLY:HA3	1.64	0.80
1:A:2:GLN:HG3	1:B:96:THR:HG21	1.66	0.78
1:B:14:ARG:HB2	1:B:19:LEU:HD12	1.65	0.77
1:A:2:GLN:HB2	1:B:98:ASN:ND2	2.02	0.75
1:B:9:PRO:HD2	1:B:23:LEU:CD1	2.18	0.73
1:A:99:PHE:HB3	1:B:95:ABA:HA	1.71	0.71
1:B:26:THR:HG21	1:B:97:LEU:HD21	1.71	0.70
1:B:59:TYR:HB3	1:B:62:ILE:HD11	1.72	0.70
1:A:44:PRO:O	1:A:45:LYS:HD2	1.92	0.70
1:B:13:ILE:HA	1:B:65:GLU:O	1.93	0.69
1:B:9:PRO:HD2	1:B:23:LEU:HD11	1.73	0.69
1:A:3:ILE:O	1:B:96:THR:HG22	1.93	0.69
1:A:2:GLN:HG3	1:B:96:THR:CG2	2.24	0.68
1:A:9:PRO:HG2	1:B:26:THR:HB	1.76	0.68
1:A:32:VAL:HG13	1:A:84:ILE:HD11	1.76	0.68
1:B:34:GLU:HG2	1:B:35:GLU:H	1.58	0.67
1:A:34:GLU:HB3	3:A:306:HOH:O	1.94	0.67
1:B:57:ARG:NH1	1:B:59:TYR:OH	2.28	0.67
1:A:44:PRO:C	1:A:45:LYS:HD2	2.20	0.66
1:A:32:VAL:HG22	1:A:80:THR:HG21	1.78	0.66
1:B:44:PRO:HB2	1:B:55:LYS:HE2	1.77	0.66
1:A:99:PHE:CE1	1:B:1:PRO:HD2	2.31	0.65
1:B:15:ILE:CD1	1:B:20:LYS:HD3	2.27	0.64
1:A:28:ALA:HB1	2:C:3:ASN:HD22	1.61	0.64
1:A:54:ILE:HD12	1:A:79:PRO:HD2	1.79	0.64
1:B:8:ARG:HH22	2:C:2:LEU:HD22	1.63	0.63
1:A:13:ILE:HD13	1:A:85:ILE:HD11	1.79	0.63
1:A:43:LYS:NZ	1:A:60:ASP:OD2	2.33	0.61
1:A:23:LEU:HD21	1:B:27:GLY:HA2	1.83	0.61
1:A:2:GLN:HB2	1:B:98:ASN:HD21	1.65	0.60
1:A:32:VAL:HG22	1:A:80:THR:CG2	2.31	0.60
1:B:2:GLN:NE2	3:B:353:HOH:O	2.31	0.60
1:A:86:GLY:O	1:A:90:LEU:HG	2.02	0.59
1:A:32:VAL:HA	1:A:76:LEU:O	2.02	0.58
1:B:58:GLN:O	3:B:320:HOH:O	2.17	0.58
1:B:15:ILE:HD13	1:B:20:LYS:HD3	1.84	0.58
1:A:50:ILE:HA	2:C:4:JG3:H17	1.84	0.58
1:B:18:GLN:HB3	1:B:20:LYS:HD2	1.85	0.58
1:B:28:ALA:HB3	1:B:86:GLY:HA2	1.86	0.58
1:A:5:LEU:HD22	1:A:9:PRO:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLU:HB3	3:A:341:HOH:O	2.04	0.57
1:A:35:GLU:HG2	1:A:57:ARG:NH2	2.19	0.57
1:B:32:VAL:HG22	1:B:80:THR:HG21	1.86	0.57
1:B:26:THR:HG21	1:B:97:LEU:CD2	2.35	0.56
1:A:49:GLY:HA3	1:B:50:ILE:HB	1.89	0.55
1:B:32:VAL:O	1:B:33:LEU:HD23	2.07	0.55
1:B:53:PHE:HE2	3:C:388:HOH:O	1.90	0.54
1:B:47:ILE:HG21	1:B:76:LEU:CD1	2.37	0.54
1:A:2:GLN:CG	1:B:96:THR:HG21	2.37	0.54
1:A:30:ASP:H	2:C:3:ASN:HD21	1.56	0.52
1:A:30:ASP:O	1:A:86:GLY:HA3	2.10	0.52
1:B:14:ARG:HA	1:B:18:GLN:O	2.10	0.52
1:B:22:ALA:HA	1:B:83:ASN:HB2	1.92	0.51
1:A:14:ARG:HG2	1:A:19:LEU:HD13	1.91	0.51
1:B:43:LYS:HZ1	1:B:58:GLN:HE22	1.59	0.51
1:B:32:VAL:CG2	1:B:80:THR:HG21	2.40	0.50
1:A:50:ILE:HD12	1:B:47:ILE:CD1	2.36	0.50
1:B:59:TYR:HB3	1:B:62:ILE:CD1	2.40	0.49
1:A:4:THR:HG22	1:B:96:THR:HG23	1.94	0.49
1:B:81:PRO:HG2	2:C:4:JG3:H8	1.94	0.49
1:A:1:PRO:HD3	3:A:394:HOH:O	2.12	0.48
1:B:61:GLN:C	1:B:72:ILE:HD13	2.38	0.48
1:B:43:LYS:NZ	1:B:58:GLN:HE22	2.12	0.47
1:B:87:ARG:O	1:B:91:THR:HG23	2.14	0.47
1:A:12:THR:CG2	1:A:19:LEU:HD12	2.45	0.46
1:B:18:GLN:HB3	1:B:20:LYS:CD	2.46	0.46
1:A:46:MET:HG2	1:A:53:PHE:HD2	1.80	0.46
1:B:65:GLU:HA	1:B:70:LYS:HA	1.96	0.46
1:B:20:LYS:HG2	3:B:355:HOH:O	2.15	0.46
1:A:4:THR:HG22	1:B:96:THR:CG2	2.46	0.46
1:A:80:THR:HG23	1:A:82:VAL:O	2.16	0.46
1:B:43:LYS:NZ	1:B:58:GLN:NE2	2.64	0.46
1:A:46:MET:HG2	1:A:53:PHE:CD2	2.50	0.46
1:B:44:PRO:CB	1:B:55:LYS:HE2	2.45	0.46
1:B:71:ALA:HB1	1:B:92:GLN:OE1	2.17	0.45
1:B:30:ASP:HB3	3:B:308:HOH:O	2.15	0.45
1:A:34:GLU:O	1:A:34:GLU:HG3	2.17	0.45
1:B:34:GLU:HG2	1:B:35:GLU:N	2.28	0.45
1:B:15:ILE:N	1:B:18:GLN:O	2.50	0.44
1:B:11:VAL:O	1:B:21:GLU:HA	2.18	0.44
1:A:56:VAL:HG21	1:A:76:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLU:CG	1:B:35:GLU:H	2.28	0.44
1:B:15:ILE:O	1:B:18:GLN:N	2.51	0.44
1:B:13:ILE:HG22	1:B:66:ILE:HB	1.98	0.44
1:A:29:ASP:HB2	2:C:1:SER:HB3	1.99	0.43
1:A:97:LEU:HD22	1:B:95:ABA:CG	2.47	0.43
1:B:78:GLY:O	1:B:80:THR:HG22	2.18	0.43
1:A:9:PRO:HD3	1:B:87:ARG:HD3	2.01	0.42
1:B:11:VAL:CG1	1:B:66:ILE:HD12	2.49	0.42
1:B:49:GLY:O	1:B:50:ILE:C	2.61	0.42
1:B:34:GLU:O	1:B:35:GLU:C	2.62	0.42
1:A:32:VAL:HG13	1:A:84:ILE:CD1	2.44	0.42
1:B:12:THR:HA	1:B:20:LYS:O	2.19	0.42
1:A:80:THR:HA	1:A:81:PRO:HD3	1.95	0.42
1:B:34:GLU:CG	1:B:35:GLU:N	2.83	0.42
1:A:31:THR:OG1	1:A:89:LEU:HG	2.19	0.42
1:B:14:ARG:HH11	1:B:14:ARG:HG3	1.84	0.42
1:A:3:ILE:C	1:B:96:THR:HG22	2.45	0.41
1:A:99:PHE:HD2	1:B:95:ABA:HG3	1.84	0.41
1:B:56:VAL:HG21	1:B:76:LEU:HD13	2.03	0.41
1:A:42:TRP:CE2	1:A:57:ARG:HD3	2.56	0.41
1:A:5:LEU:CD2	1:A:9:PRO:HG3	2.50	0.41
1:A:88:ASN:ND2	1:A:89:LEU:HD23	2.36	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%)	86 (90%)	7 (7%)	2 (2%)	5	7
1	B	95/99 (96%)	91 (96%)	4 (4%)	0	100	100
2	C	4/7 (57%)	4 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	194/205 (95%)	181 (93%)	11 (6%)	2 (1%)	12	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	16	GLY

5.3.2 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 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%)	68 (84%)	13 (16%)	2	3
1	B	81/81 (100%)	61 (75%)	20 (25%)	1	1
2	C	4/4 (100%)	3 (75%)	1 (25%)	0	1
All	All	166/166 (100%)	132 (80%)	34 (20%)	1	1

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	11	VAL
1	A	19	LEU
1	A	24	LEU
1	A	32	VAL
1	A	33	LEU
1	A	46	MET
1	A	50	ILE
1	A	61	GLN
1	A	77	VAL
1	A	84	ILE
1	A	89	LEU
1	A	93	ILE
1	B	5	LEU

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Mol	Chain	Res	Type
1	B	10	LEU
1	B	15	ILE
1	B	18	GLN
1	B	19	LEU
1	B	24	LEU
1	B	32	VAL
1	B	34	GLU
1	B	41	LYS
1	B	43	LYS
1	B	47	ILE
1	B	62	ILE
1	B	66	ILE
1	B	70	LYS
1	B	72	ILE
1	B	75	VAL
1	B	84	ILE
1	B	89	LEU
1	B	96	THR
1	B	97	LEU
2	C	2	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	37	ASN
1	A	61	GLN
1	A	88	ASN
1	B	7	GLN
1	B	58	GLN
1	B	61	GLN
1	B	98	ASN
2	C	3	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	1.57	1 (25%)	1,5,7	0.17	0
1	ABA	B	95	1	4,5,6	0.78	0	1,5,7	1.03	0
1	ABA	A	95	1	4,5,6	1.16	1 (25%)	1,5,7	0.28	0
2	VME	C	6	2	6,8,8	4.18	3 (50%)	7,10,10	3.80	4 (57%)
1	ABA	B	67	1	4,5,6	0.81	0	1,5,7	1.42	0
2	JG3	C	4	2	19,20,21	1.22	3 (15%)	22,26,28	2.74	6 (27%)

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	-	1/3/4/6	-
1	ABA	B	95	1	-	0/3/4/6	-
1	ABA	A	95	1	-	1/3/4/6	-
2	VME	C	6	2	-	6/10/10/10	-
1	ABA	B	67	1	-	1/3/4/6	-
2	JG3	C	4	2	-	3/12/24/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	VME	O-C	6.83	1.38	1.21
2	C	6	VME	OXT-C	6.25	1.48	1.33
2	C	6	VME	OXT-CM	4.35	1.55	1.45
1	A	67	ABA	CB-CA	-2.66	1.45	1.53
2	C	4	JG3	C4-C1	2.59	1.56	1.52
2	C	4	JG3	C4-N2	2.53	1.52	1.47
1	A	95	ABA	O-C	2.12	1.28	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	JG3	C11-C8	2.01	1.57	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	JG3	C-C8-N2	9.87	121.30	112.28
2	C	6	VME	OXT-C-O	-7.55	109.15	123.85
2	C	6	VME	CB-CA-C	5.10	119.16	111.11
2	C	4	JG3	C10-CA-C1	3.81	117.90	111.86
2	C	4	JG3	C14-C10-CA	-3.40	106.25	113.48
2	C	6	VME	OXT-C-CA	3.15	121.44	111.62
2	C	4	JG3	C11-C8-N2	-3.10	94.19	101.38
2	C	6	VME	CG2-CB-CG1	2.79	118.25	110.58
2	C	4	JG3	O1-C1-CA	-2.50	104.73	109.48
2	C	4	JG3	C5-C13-C7	-2.26	117.45	120.24

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	95	ABA	C-CA-CB-CG
2	C	4	JG3	O1-C1-C4-N2
2	C	4	JG3	C1-C4-N2-C3
2	C	4	JG3	C1-C4-N2-C8
2	C	6	VME	N-CA-CB-CG1
2	C	6	VME	N-CA-CB-CG2
2	C	6	VME	C-CA-CB-CG1
2	C	6	VME	C-CA-CB-CG2
2	C	6	VME	CA-C-OXT-CM
2	C	6	VME	O-C-OXT-CM
1	B	67	ABA	C-CA-CB-CG
1	A	67	ABA	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	95	ABA	3	0
2	C	4	JG3	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.