



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:41 AM UTC

PDB ID : 1DIT / pdb_00001dit
Title : COMPLEX OF A DIVALENT INHIBITOR WITH THROMBIN
Authors : Tulinsky, A.; Krishnan, R.
Deposited on : 1995-07-20
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 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

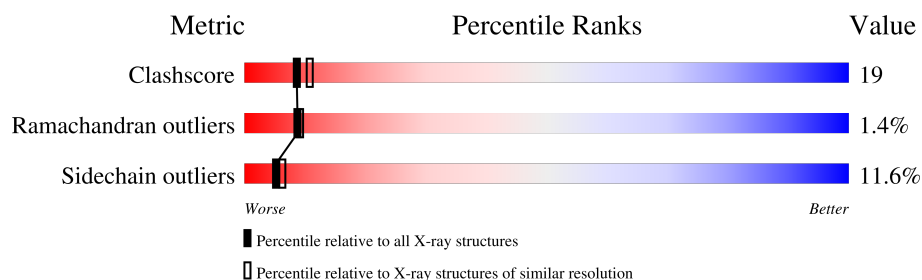
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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	L	36	
2	H	259	
3	P	20	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2530 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 ALPHA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	29	Total	C	N	O	S	0	0	0
			235	147	38	49	1			

- Molecule 2 is a protein called ALPHA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	251	Total	C	N	O	S	0	0	0
			2016	1287	352	363	14			

- Molecule 3 is a protein called PEPTIDE INHIBITOR CVS995.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	16	Total	C	N	O	0	0	0
			114	69	19	26			

- Molecule 4 is water.

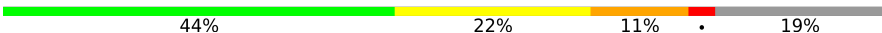
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	20	Total	O	0	0
			20	20		
4	H	138	Total	O	0	0
			138	138		
4	P	7	Total	O	0	0
			7	7		

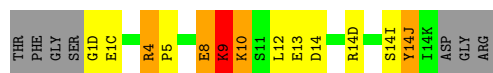
3 Residue-property plots [i](#)

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.

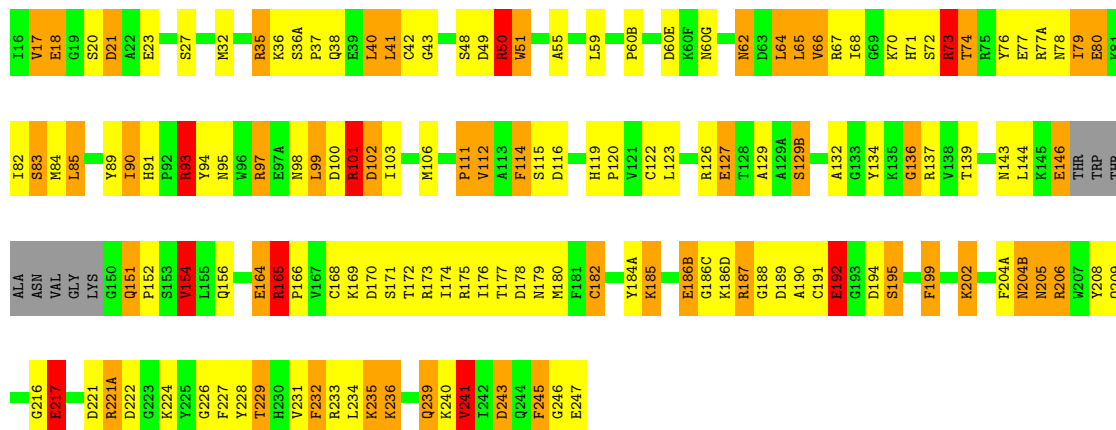
• Molecule 1: ALPHA-THROMBIN

Chain L: 

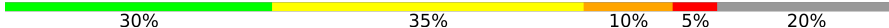


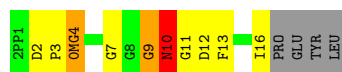
• Molecule 2: ALPHA-THROMBIN

Chain H: 



• Molecule 3: PEPTIDE INHIBITOR CVS995

Chain P: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.90Å 72.20Å 73.20Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30	Depositor
% Data completeness (in resolution range)	75.0 (7.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2530	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: 0MG, 2PP

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	L	1.48	1/237 (0.4%)	2.43	15/315 (4.8%)
2	H	1.88	22/2068 (1.1%)	2.82	188/2794 (6.7%)
3	P	1.36	0/92	1.90	3/120 (2.5%)
All	All	1.83	23/2397 (1.0%)	2.75	206/3229 (6.4%)

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
1	L	0	1
2	H	0	7
3	P	0	1
All	All	0	9

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	101	ARG	C-N	-35.17	0.84	1.33
2	H	191	CYS	C-N	19.73	1.61	1.33
1	L	12	LEU	C-N	-12.34	1.16	1.33
2	H	78	ASN	N-CA	12.09	1.60	1.46
2	H	192	GLU	C-N	10.56	1.46	1.33
2	H	100	ASP	C-N	9.81	1.47	1.33
2	H	174	ILE	CA-CB	8.16	1.64	1.54
2	H	93	ARG	CD-NE	7.43	1.56	1.46
2	H	216	GLY	N-CA	6.53	1.52	1.45
2	H	134	TYR	C-O	6.32	1.31	1.23
2	H	67	ARG	CD-NE	-5.87	1.38	1.46
2	H	154	VAL	N-CA	5.86	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	48	SER	C-O	5.78	1.29	1.24
2	H	77(A)	ARG	C-O	5.73	1.31	1.24
2	H	182	CYS	N-CA	5.65	1.53	1.45
2	H	187	ARG	NE-CZ	5.62	1.39	1.33
2	H	17	VAL	CA-CB	5.55	1.60	1.54
2	H	115	SER	C-N	-5.52	1.26	1.34
2	H	114	PHE	C-N	-5.39	1.26	1.33
2	H	137	ARG	C-O	5.33	1.30	1.24
2	H	27	SER	N-CA	5.15	1.52	1.46
2	H	55	ALA	C-O	5.10	1.30	1.24
2	H	129	ALA	C-O	5.02	1.29	1.24

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	67	ARG	CD-NE-CZ	31.97	169.16	124.40
2	H	205	ASN	OD1-CG-ND2	19.16	141.76	122.60
1	L	9	LYS	CB-CG-CD	15.46	146.85	111.30
2	H	192	GLU	CB-CG-CD	15.20	138.44	112.60
2	H	205	ASN	CA-CB-CG	-13.42	99.18	112.60
2	H	93	ARG	CD-NE-CZ	-12.87	106.38	124.40
2	H	67	ARG	CG-CD-NE	12.71	139.97	112.00
2	H	154	VAL	N-CA-CB	-12.63	96.30	112.60
2	H	245	PHE	CA-C-O	-12.43	104.51	119.18
2	H	18	GLU	CA-C-N	11.90	133.02	122.43
2	H	18	GLU	C-N-CA	11.90	133.02	122.43
2	H	77(A)	ARG	CA-C-N	-11.73	103.85	122.73
2	H	77(A)	ARG	C-N-CA	-11.73	103.85	122.73
2	H	67	ARG	NE-CZ-NH1	11.69	133.19	121.50
2	H	35	ARG	NE-CZ-NH2	-11.36	108.98	119.20
2	H	77	GLU	CA-C-O	11.27	136.04	122.41
2	H	186(B)	GLU	CB-CG-CD	10.72	130.83	112.60
2	H	93	ARG	NE-CZ-NH1	10.47	131.97	121.50
2	H	27	SER	N-CA-CB	-10.46	98.89	110.71
1	L	12	LEU	O-C-N	-10.04	111.56	123.10
2	H	77(A)	ARG	CA-C-O	-10.00	106.21	120.51
2	H	97	ARG	NE-CZ-NH2	-9.88	110.31	119.20
1	L	1(C)	GLU	N-CA-C	-9.75	99.56	113.21
2	H	101	ARG	O-C-N	-9.73	106.36	122.03
2	H	151	GLN	CB-CA-C	9.66	120.87	109.47
2	H	115	SER	CA-C-N	9.43	134.14	120.38
2	H	115	SER	C-N-CA	9.43	134.14	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	85	LEU	O-C-N	9.35	133.85	123.10
2	H	93	ARG	CB-CG-CD	9.17	132.40	111.30
2	H	60(G)	ASN	CB-CG-ND2	9.08	130.02	116.40
2	H	126	ARG	N-CA-CB	8.96	123.29	110.12
2	H	175	ARG	NE-CZ-NH1	-8.86	112.64	121.50
2	H	170	ASP	CA-CB-CG	-8.75	103.85	112.60
2	H	205	ASN	N-CA-CB	-8.72	99.29	112.28
1	L	1(D)	GLY	O-C-N	8.67	136.56	122.70
2	H	192	GLU	CB-CA-C	8.54	123.07	110.26
2	H	83	SER	O-C-N	8.53	134.63	122.94
2	H	101	ARG	CB-CA-C	8.51	125.46	111.26
2	H	178	ASP	CA-CB-CG	-8.48	104.12	112.60
2	H	74	THR	N-CA-C	8.35	123.60	113.41
2	H	74	THR	N-CA-CB	-8.35	98.27	110.47
2	H	112	VAL	O-C-N	8.00	131.41	122.93
2	H	205	ASN	CB-CG-OD1	-7.78	105.24	120.80
2	H	64	LEU	N-CA-C	7.72	122.04	109.85
2	H	93	ARG	CG-CD-NE	-7.67	95.13	112.00
2	H	20	SER	O-C-N	7.63	132.58	122.96
2	H	42	CYS	N-CA-CB	-7.59	98.82	111.57
2	H	231	VAL	O-C-N	7.57	129.21	121.87
2	H	154	VAL	CB-CA-C	7.55	121.53	111.19
2	H	73	ARG	CA-C-O	7.53	128.72	120.82
2	H	64	LEU	N-CA-CB	-7.49	99.06	111.20
2	H	66	VAL	N-CA-CB	-7.43	101.15	111.41
2	H	173	ARG	CA-C-O	-7.43	110.87	119.05
2	H	85	LEU	CA-C-O	-7.37	112.59	121.28
2	H	199	PHE	CB-CA-C	7.37	122.13	110.19
2	H	60(G)	ASN	OD1-CG-ND2	-7.34	115.26	122.60
2	H	119	HIS	O-C-N	-7.32	113.52	122.16
2	H	205	ASN	N-CA-C	7.29	121.50	112.47
2	H	221(A)	ARG	CD-NE-CZ	-7.25	114.25	124.40
2	H	127	GLU	CB-CG-CD	7.20	124.84	112.60
2	H	120	PRO	N-CA-CB	7.20	110.02	103.33
2	H	59	LEU	CA-C-N	7.18	133.06	122.86
2	H	59	LEU	C-N-CA	7.18	133.06	122.86
2	H	93	ARG	NE-CZ-NH2	-7.16	112.76	119.20
1	L	10	LYS	CA-CB-CG	7.05	128.21	114.10
2	H	97	ARG	NH1-CZ-NH2	7.05	128.47	119.30
2	H	67	ARG	CA-C-O	7.03	127.78	120.40
2	H	66	VAL	CA-C-N	7.03	133.33	123.07
2	H	66	VAL	C-N-CA	7.03	133.33	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	222	ASP	CA-C-N	7.01	133.61	121.07
2	H	222	ASP	C-N-CA	7.01	133.61	121.07
2	H	119	HIS	CA-C-N	6.98	126.90	119.85
2	H	119	HIS	C-N-CA	6.98	126.90	119.85
2	H	190	ALA	N-CA-C	-6.95	100.51	110.59
2	H	233	ARG	NE-CZ-NH1	-6.93	114.57	121.50
2	H	98	ASN	CA-C-O	-6.92	112.31	119.51
1	L	12	LEU	CA-C-N	6.87	132.89	122.93
1	L	12	LEU	C-N-CA	6.87	132.89	122.93
2	H	137	ARG	O-C-N	6.85	131.32	123.31
2	H	165	ARG	CA-C-N	6.79	126.30	119.24
2	H	165	ARG	C-N-CA	6.79	126.30	119.24
2	H	192	GLU	OE1-CD-OE2	-6.76	106.67	122.90
2	H	175	ARG	CA-C-N	6.73	130.95	121.66
2	H	175	ARG	C-N-CA	6.73	130.95	121.66
2	H	136	GLY	N-CA-C	-6.72	101.87	111.42
2	H	206	ARG	O-C-N	6.64	130.73	123.10
2	H	82	ILE	CA-C-O	-6.56	113.53	120.48
2	H	90	ILE	CB-CG1-CD1	6.49	127.44	113.80
2	H	71	HIS	CA-CB-CG	-6.45	107.35	113.80
2	H	199	PHE	O-C-N	-6.45	115.87	123.22
2	H	48	SER	CA-C-O	-6.41	114.28	120.94
2	H	77(A)	ARG	NE-CZ-NH2	-6.40	113.44	119.20
1	L	13	GLU	CA-C-O	-6.37	113.96	120.71
1	L	1(D)	GLY	CA-C-N	-6.36	103.21	117.20
2	H	179	ASN	CA-CB-CG	-6.35	106.25	112.60
3	P	2	ASP	CA-CB-CG	6.34	118.94	112.60
2	H	91	HIS	CA-C-N	6.33	126.54	119.32
2	H	91	HIS	C-N-CA	6.33	126.54	119.32
2	H	93	ARG	CA-C-O	6.31	127.29	119.78
2	H	232	PHE	CA-CB-CG	-6.31	107.49	113.80
2	H	229	THR	CA-CB-OG1	-6.30	100.15	109.60
2	H	74	THR	OG1-CB-CG2	6.30	121.90	109.30
2	H	90	ILE	O-C-N	6.28	129.55	123.14
2	H	136	GLY	O-C-N	-6.28	119.12	123.95
2	H	144	LEU	O-C-N	6.28	131.06	122.46
2	H	60(E)	ASP	CA-C-O	-6.26	112.93	120.32
2	H	115	SER	O-C-N	-6.26	115.59	122.92
2	H	71	HIS	CA-C-O	6.26	129.47	120.51
2	H	177	THR	CA-CB-OG1	-6.25	100.23	109.60
2	H	137	ARG	CA-C-O	-6.21	113.43	120.32
2	H	239	GLN	CA-C-O	6.20	127.54	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	116	ASP	O-C-N	6.20	129.27	122.20
2	H	171	SER	CA-C-N	-6.18	112.58	122.53
2	H	171	SER	C-N-CA	-6.18	112.58	122.53
2	H	221	ASP	CB-CA-C	6.18	121.27	111.51
2	H	97	ARG	N-CA-CB	6.16	119.00	110.07
2	H	78	ASN	CA-CB-CG	6.15	118.75	112.60
2	H	195	SER	O-C-N	6.14	130.49	123.12
2	H	93	ARG	O-C-N	-6.13	114.81	122.35
1	L	14(I)	SER	N-CA-C	-6.12	105.64	113.23
2	H	111	PRO	N-CA-CB	6.07	108.63	103.35
2	H	93	ARG	CA-CB-CG	-6.00	102.09	114.10
2	H	20	SER	CA-C-O	-5.99	114.80	121.51
2	H	97	ARG	CA-C-O	-5.99	114.53	120.70
2	H	233	ARG	NE-CZ-NH2	5.95	124.56	119.20
2	H	67	ARG	NE-CZ-NH2	-5.92	113.88	119.20
2	H	187	ARG	CD-NE-CZ	-5.91	116.12	124.40
2	H	95	ASN	OD1-CG-ND2	-5.85	116.75	122.60
2	H	175	ARG	NE-CZ-NH2	5.84	124.46	119.20
2	H	204(A)	PHE	CA-CB-CG	-5.84	107.96	113.80
2	H	231	VAL	CA-C-N	-5.84	112.45	120.28
2	H	231	VAL	C-N-CA	-5.84	112.45	120.28
2	H	91	HIS	ND1-CE1-NE2	-5.83	102.57	108.40
2	H	21	ASP	N-CA-CB	5.83	118.54	109.97
2	H	168	CYS	O-C-N	5.83	128.07	122.07
2	H	217	GLU	O-C-N	5.83	131.85	122.99
2	H	189	ASP	O-C-N	5.80	129.09	123.29
2	H	79	ILE	N-CA-C	5.80	116.93	111.48
2	H	166	PRO	O-C-N	5.78	128.43	122.18
2	H	35	ARG	CB-CG-CD	-5.77	98.04	111.30
2	H	139	THR	CA-CB-OG1	-5.75	100.97	109.60
2	H	143	ASN	CA-CB-CG	-5.73	106.87	112.60
2	H	241	VAL	N-CA-C	5.72	116.46	110.62
2	H	76	TYR	CA-C-O	-5.71	114.81	120.98
1	L	9	LYS	CG-CD-CE	5.70	124.40	111.30
2	H	229	THR	OG1-CB-CG2	5.69	120.68	109.30
2	H	180	MET	O-C-N	5.69	130.05	123.17
2	H	126	ARG	CB-CA-C	-5.67	101.38	110.79
2	H	101	ARG	NE-CZ-NH2	5.65	124.28	119.20
2	H	77(A)	ARG	CD-NE-CZ	5.64	132.30	124.40
2	H	126	ARG	O-C-N	5.64	128.09	122.12
2	H	173	ARG	N-CA-C	-5.63	106.40	113.72
2	H	73	ARG	CA-C-N	5.62	132.15	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	73	ARG	C-N-CA	5.62	132.15	122.09
2	H	123	LEU	N-CA-CB	5.61	119.37	110.11
2	H	43	GLY	N-CA-C	-5.61	104.02	112.60
2	H	50	ARG	NE-CZ-NH2	-5.60	114.16	119.20
3	P	16	ILE	CA-C-O	-5.57	111.33	120.80
2	H	168	CYS	N-CA-CB	5.57	118.08	110.01
2	H	74	THR	CA-CB-OG1	-5.56	101.26	109.60
1	L	8	GLU	O-C-N	5.55	127.86	122.09
2	H	146	GLU	CA-C-O	5.55	130.24	120.80
2	H	192	GLU	O-C-N	-5.55	115.97	122.96
2	H	173	ARG	O-C-N	5.52	129.15	122.35
2	H	94	TYR	N-CA-CB	-5.51	101.25	109.69
2	H	18	GLU	CB-CA-C	-5.50	102.86	111.39
2	H	101	ARG	N-CA-CB	-5.49	103.80	112.63
2	H	80	GLU	CG-CD-OE1	-5.48	105.79	118.40
1	L	9	LYS	O-C-N	-5.48	115.21	122.33
2	H	246	GLY	N-CA-C	5.47	126.15	113.18
2	H	202	LYS	CA-C-O	-5.46	114.52	120.36
2	H	231	VAL	CA-C-O	-5.42	115.31	120.95
2	H	217	GLU	N-CA-CB	5.42	119.71	110.87
2	H	185	LYS	CA-CB-CG	-5.42	103.26	114.10
1	L	14(D)	ARG	NE-CZ-NH2	5.40	124.06	119.20
2	H	186(C)	GLY	C-N-CA	5.40	135.19	121.70
2	H	129(B)	SER	CA-C-O	-5.38	112.78	119.18
2	H	93	ARG	CB-CA-C	-5.37	102.07	110.94
2	H	91	HIS	CB-CA-C	5.36	117.70	109.50
2	H	80	GLU	CA-C-O	-5.34	115.74	121.56
2	H	99	LEU	CA-C-O	5.33	127.41	120.81
2	H	60(B)	PRO	CB-CA-C	5.30	117.39	110.92
2	H	221(A)	ARG	CA-C-O	-5.30	114.65	120.69
2	H	132	ALA	CA-C-O	-5.27	114.91	120.92
2	H	89	TYR	CA-C-O	5.25	126.15	120.32
2	H	101	ARG	CA-C-O	5.25	126.16	120.12
2	H	184(A)	TYR	CA-C-O	5.25	127.50	121.47
2	H	204(B)	ASN	CA-C-N	5.24	130.78	122.61
2	H	204(B)	ASN	C-N-CA	5.24	130.78	122.61
2	H	186(D)	LYS	N-CA-C	-5.20	99.86	108.75
2	H	243	ASP	CA-CB-CG	5.19	117.79	112.60
2	H	35	ARG	NH1-CZ-NH2	5.19	126.04	119.30
2	H	228	TYR	CA-C-O	-5.19	114.70	120.66
2	H	83	SER	N-CA-CB	5.18	119.67	111.43
3	P	10	ASN	N-CA-C	-5.17	105.08	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	50	ARG	NH1-CZ-NH2	5.15	126.00	119.30
2	H	137	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	H	51	TRP	CD2-CE3-CZ3	-5.13	111.93	118.60
2	H	84	MET	CA-CB-CG	-5.10	103.89	114.10
2	H	202	LYS	O-C-N	5.10	129.03	123.22
2	H	156	GLN	OE1-CD-NE2	-5.09	117.51	122.60
2	H	229	THR	CA-CB-CG2	5.07	119.12	110.50
2	H	209	GLN	CA-C-O	-5.06	114.89	120.60
2	H	51	TRP	N-CA-C	5.05	116.62	108.34
1	L	4	ARG	NE-CZ-NH2	5.03	123.73	119.20
2	H	186(D)	LYS	CA-C-O	-5.01	114.37	120.54

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	101	ARG	Mainchain,Sidechain
2	H	192	GLU	Mainchain
2	H	221(A)	ARG	Sidechain
2	H	50	ARG	Sidechain
2	H	73	ARG	Sidechain
2	H	93	ARG	Sidechain
1	L	4	ARG	Sidechain
3	P	3	PRO	Peptide

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	L	235	0	233	5	0
2	H	2016	0	1974	79	0
3	P	114	0	95	7	0
4	H	138	0	0	5	0
4	L	20	0	0	1	0
4	P	7	0	0	0	0
All	All	2530	0	2302	83	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 19.

All (83) 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)
2:H:101:ARG:C	2:H:102:ASP:CA	2.09	1.26
2:H:101:ARG:O	2:H:102:ASP:N	1.67	1.22
2:H:101:ARG:CA	2:H:102:ASP:N	2.13	1.12
2:H:236:LYS:H	2:H:236:LYS:HD2	0.93	1.04
2:H:236:LYS:H	2:H:236:LYS:CD	1.74	1.00
2:H:236:LYS:HD2	2:H:236:LYS:N	1.77	1.00
2:H:101:ARG:O	2:H:102:ASP:CA	2.09	0.96
2:H:101:ARG:C	2:H:102:ASP:N	0.84	0.94
2:H:85:LEU:CD1	2:H:106:MET:HE2	1.99	0.92
2:H:217:GLU:HG3	2:H:224:LYS:HD2	1.56	0.87
2:H:50:ARG:HD3	2:H:111:PRO:HD3	1.61	0.82
2:H:101:ARG:O	2:H:103:ILE:N	2.12	0.82
2:H:151:GLN:NE2	3:P:7:GLY:O	2.12	0.81
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.62	0.80
2:H:36:LYS:HE2	2:H:62:ASN:O	1.82	0.79
2:H:50:ARG:HD3	2:H:111:PRO:CD	2.12	0.79
2:H:85:LEU:HD11	2:H:106:MET:HE2	1.66	0.76
2:H:93:ARG:O	2:H:101:ARG:HD3	1.86	0.75
2:H:73:ARG:NH2	4:H:565:HOH:O	1.87	0.73
2:H:50:ARG:HG2	2:H:111:PRO:HA	1.72	0.72
2:H:101:ARG:O	2:H:102:ASP:C	2.33	0.71
2:H:235:LYS:HB3	2:H:236:LYS:HE3	1.71	0.71
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	1.98	0.70
2:H:172:THR:O	4:H:420:HOH:O	2.08	0.70
2:H:36(A):SER:HA	2:H:37:PRO:C	2.17	0.67
2:H:195:SER:OG	3:P:4:0MG:C	2.44	0.65
2:H:235:LYS:CB	2:H:236:LYS:HE3	2.28	0.64
2:H:165:ARG:HD3	2:H:169:LYS:HZ1	1.63	0.63
2:H:70:LYS:HE3	2:H:72:SER:O	1.99	0.62
2:H:195:SER:CB	3:P:4:0MG:CA	2.76	0.62
2:H:93:ARG:O	2:H:101:ARG:CD	2.48	0.62
2:H:36:LYS:O	2:H:38:GLN:HG2	2.01	0.60
2:H:165:ARG:HD3	2:H:169:LYS:NZ	2.16	0.60
2:H:17:VAL:O	2:H:188:GLY:HA2	2.01	0.60
2:H:85:LEU:HD11	2:H:106:MET:CE	2.30	0.59
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.38	0.58
2:H:17:VAL:O	2:H:18:GLU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:MET:HG3	2:H:40:LEU:HD23	1.85	0.57
2:H:236:LYS:CD	2:H:236:LYS:N	2.49	0.56
2:H:32:MET:HG3	2:H:40:LEU:CD2	2.36	0.56
2:H:129(B):SER:HB2	4:H:550:HOH:O	2.07	0.54
2:H:70:LYS:NZ	2:H:80:GLU:OE2	2.37	0.54
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.66	0.54
3:P:11:GLY:O	3:P:13:PHE:N	2.33	0.53
2:H:50:ARG:HD3	2:H:111:PRO:N	2.23	0.52
2:H:194:ASP:O	2:H:195:SER:C	2.52	0.52
2:H:18:GLU:HG3	2:H:187:ARG:HB2	1.91	0.52
2:H:112:VAL:HG13	2:H:114:PHE:CE1	2.44	0.52
2:H:41:LEU:HD23	2:H:64:LEU:CD2	2.39	0.51
2:H:241:VAL:O	2:H:245:PHE:HD1	1.93	0.51
2:H:112:VAL:HG13	2:H:114:PHE:HE1	1.75	0.50
2:H:112:VAL:CG1	2:H:114:PHE:HE1	2.25	0.50
2:H:37:PRO:HB2	3:P:10:ASN:OD1	2.12	0.50
2:H:101:ARG:C	2:H:102:ASP:C	2.78	0.49
2:H:36:LYS:CE	2:H:62:ASN:O	2.57	0.49
3:P:9:GLY:C	3:P:11:GLY:N	2.63	0.49
2:H:176:ILE:HD12	2:H:227:PHE:CE2	2.48	0.49
2:H:185:LYS:O	2:H:186(B):GLU:HB2	2.13	0.48
2:H:37:PRO:CB	3:P:10:ASN:OD1	2.62	0.48
2:H:165:ARG:CD	2:H:169:LYS:HZ1	2.25	0.48
1:L:5:PRO:HA	1:L:9:LYS:HE3	1.96	0.48
1:L:14(J):TYR:HE2	2:H:202:LYS:O	1.96	0.48
1:L:8:GLU:OE2	2:H:202:LYS:NZ	2.30	0.47
2:H:21:ASP:HB3	2:H:154:VAL:CG1	2.45	0.47
2:H:229:THR:HG22	2:H:234:LEU:HD12	1.96	0.47
2:H:35:ARG:O	2:H:38:GLN:HA	2.16	0.46
2:H:146:GLU:C	4:H:519:HOH:O	2.59	0.46
2:H:50:ARG:HG2	2:H:111:PRO:CA	2.45	0.45
2:H:122:CYS:HB2	2:H:208:TYR:CD1	2.52	0.45
2:H:70:LYS:CE	2:H:72:SER:O	2.65	0.44
2:H:36(A):SER:CA	2:H:37:PRO:C	2.86	0.44
2:H:151:GLN:HA	2:H:152:PRO:HD3	1.91	0.44
2:H:85:LEU:HD22	2:H:106:MET:HB3	2.00	0.43
2:H:114:PHE:N	2:H:114:PHE:CD1	2.84	0.42
2:H:204(B):ASN:HD21	2:H:206:ARG:HB2	1.85	0.41
2:H:97:ARG:HG3	4:H:452:HOH:O	2.21	0.41
2:H:164:GLU:CD	2:H:164:GLU:H	2.28	0.41
2:H:182:CYS:HA	2:H:226:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:10:LYS:HE2	4:L:777:HOH:O	2.20	0.41
2:H:65:LEU:HD12	2:H:65:LEU:HA	1.72	0.41
2:H:232:PHE:O	2:H:235:LYS:HB2	2.20	0.41
2:H:49:ASP:HA	2:H:112:VAL:HG12	2.03	0.40
1:L:14:ASP:HB2	2:H:23:GLU:OE2	2.22	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	L	27/36 (75%)	23 (85%)	3 (11%)	1 (4%)	2	1
2	H	247/259 (95%)	233 (94%)	13 (5%)	1 (0%)	30	38
3	P	12/20 (60%)	6 (50%)	4 (33%)	2 (17%)	0	0
All	All	286/315 (91%)	262 (92%)	20 (7%)	4 (1%)	9	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	102	ASP
3	P	12	ASP
1	L	14(J)	TYR
3	P	9	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	L	26/31 (84%)	25 (96%)	1 (4%)	29	44
2	H	216/225 (96%)	189 (88%)	27 (12%)	4	5
3	P	8/12 (67%)	7 (88%)	1 (12%)	4	5
All	All	250/268 (93%)	221 (88%)	29 (12%)	5	6

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	LYS
2	H	40	LEU
2	H	41	LEU
2	H	51	TRP
2	H	62	ASN
2	H	65	LEU
2	H	66	VAL
2	H	68	ILE
2	H	74	THR
2	H	79	ILE
2	H	83	SER
2	H	90	ILE
2	H	99	LEU
2	H	101	ARG
2	H	127	GLU
2	H	154	VAL
2	H	164	GLU
2	H	165	ARG
2	H	192	GLU
2	H	205	ASN
2	H	217	GLU
2	H	235	LYS
2	H	236	LYS
2	H	239	GLN
2	H	240	LYS
2	H	241	VAL
2	H	243	ASP
2	H	247	GLU
3	P	10	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	156	GLN
2	H	204(B)	ASN
2	H	239	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 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 (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
3	0MG	P	4	2,3	12,12,13	2.69	6 (50%)	10,14,16	3.29	6 (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
3	0MG	P	4	2,3	-	1/9/13/15	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	4	0MG	O1-CA	5.32	1.30	1.22
3	P	4	0MG	C6-N4	3.66	1.45	1.32
3	P	4	0MG	C-CA	3.49	1.55	1.46
3	P	4	0MG	C5-N2	-3.13	1.39	1.46
3	P	4	0MG	C4-C5	-2.95	1.39	1.51
3	P	4	0MG	C6-N2	-2.89	1.27	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	4	0MG	C3-C4-C5	5.72	128.57	112.07
3	P	4	0MG	N2-C6-N4	-5.16	111.81	120.67
3	P	4	0MG	O1-CA-C	-4.59	112.62	123.51
3	P	4	0MG	C3-CB-N	3.27	118.63	110.12
3	P	4	0MG	N3-C6-N4	2.61	127.50	120.07
3	P	4	0MG	C4-C5-N2	2.49	119.17	112.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	4	0MG	O1-CA-CB-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	4	0MG	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	2

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Mol	Chain	Number of breaks
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	191:CYS	C	192:GLU	N	1.61
1	L	12:LEU	C	13:GLU	N	1.16
1	H	101:ARG	C	102:ASP	N	0.84

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.