



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:55 PM UTC

PDB ID : 1GNV / pdb_00001gnv
Title : CALCIUM INDEPENDENT SUBTILISIN BPN' MUTANT
Authors : Almog, O.; Gilliland, G.L.
Deposited on : 2001-10-10
Resolution : 1.90 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

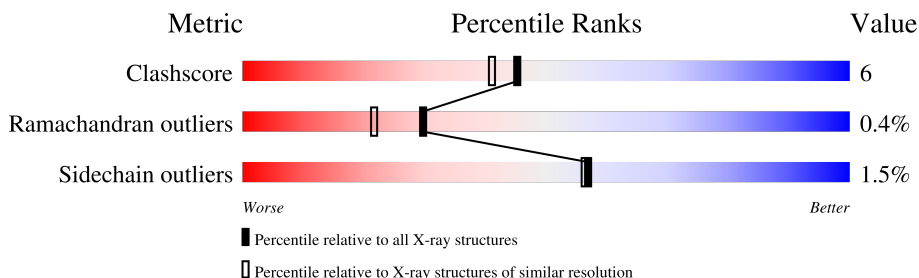
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	266	36% 56% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2014 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 SUBTILISIN BPN'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	266	1881	1167	322	385	1	6	0	1	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LYS	GLU	engineered mutation	UNP P00782
A	3	CYS	SER	engineered mutation	UNP P00782
A	5	SER	PRO	engineered mutation	UNP P00782
A	43	ASN	LYS	engineered mutation	UNP P00782
A	50	PHE	MET	engineered mutation	UNP P00782
A	73	LEU	ALA	engineered mutation	UNP P00782
A	206	CYS	GLU	engineered mutation	UNP P00782
A	217	LYS	TYR	engineered mutation	UNP P00782
A	218	SER	ASN	engineered mutation	UNP P00782
A	221	MIS	SER	engineered mutation	UNP P00782
A	271	GLU	GLN	engineered mutation	UNP P00782

- Molecule 2 is water.

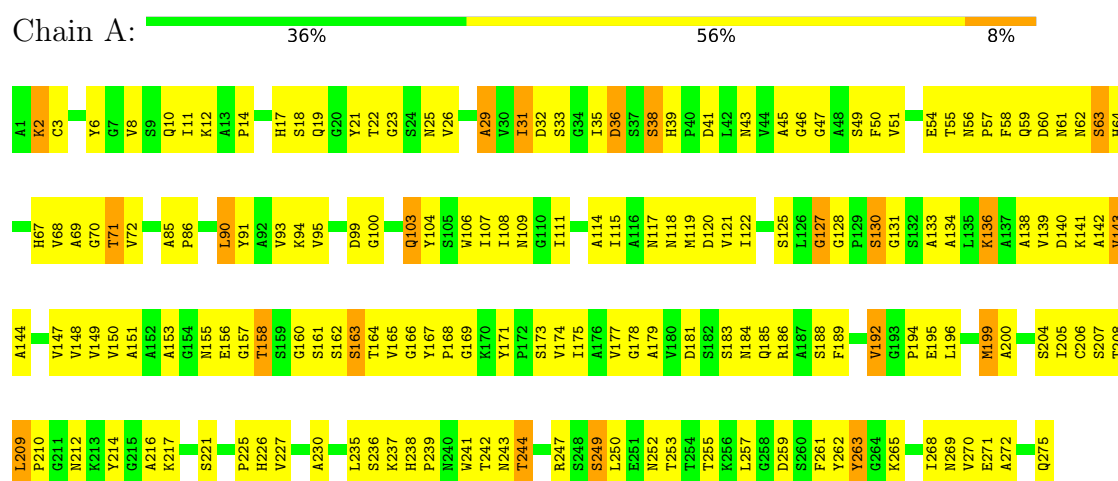
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	133	Total	O	0	0
			133	133		

3 Residue-property plots

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: SUBTILISIN BPN'



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	54.20Å 60.40Å 82.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90	Depositor
% Data completeness (in resolution range)	86.0 (8.00-1.90)	Depositor
R_{merge}	0.09	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.	Xtriage
Total number of atoms	2014	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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: MIS

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	2.03	42/1909 (2.2%)	3.07	263/2602 (10.1%)

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	A	1	0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	ASP	CA-CB	9.43	1.63	1.54
1	A	68	VAL	C-O	7.57	1.32	1.24
1	A	22	THR	CA-CB	7.43	1.64	1.53
1	A	209	LEU	N-CA	7.20	1.51	1.45
1	A	111	ILE	N-CA	6.95	1.54	1.46
1	A	166	GLY	N-CA	6.56	1.51	1.44
1	A	50	PHE	CA-CB	6.54	1.63	1.53
1	A	31	ILE	N-CA	6.50	1.54	1.46
1	A	157	GLY	CA-C	6.45	1.60	1.51
1	A	268	ILE	N-CA	5.93	1.53	1.46
1	A	6	TYR	N-CA	5.93	1.53	1.46
1	A	91	TYR	CA-C	-5.84	1.45	1.52
1	A	35	ILE	CA-CB	5.81	1.62	1.54
1	A	178	GLY	N-CA	5.79	1.50	1.44
1	A	271	GLU	C-O	5.71	1.30	1.24
1	A	39	HIS	ND1-CE1	5.58	1.38	1.32
1	A	153	ALA	C-O	5.53	1.31	1.24
1	A	17	HIS	ND1-CE1	-5.50	1.27	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	TYR	C-O	5.49	1.31	1.24
1	A	181	ASP	N-CA	5.48	1.52	1.45
1	A	238	HIS	CA-CB	5.47	1.60	1.53
1	A	189	PHE	CA-CB	5.45	1.62	1.53
1	A	158	THR	CB-OG1	5.45	1.52	1.43
1	A	127	GLY	C-O	-5.44	1.18	1.24
1	A	62	ASN	N-CA	-5.44	1.39	1.46
1	A	143	VAL	C-O	5.40	1.30	1.24
1	A	95	VAL	N-CA	5.37	1.53	1.46
1	A	247	ARG	C-N	-5.36	1.27	1.33
1	A	226	HIS	N-CA	5.36	1.52	1.46
1	A	209	LEU	C-O	5.34	1.29	1.24
1	A	114	ALA	C-N	5.33	1.40	1.33
1	A	49	SER	CA-C	5.33	1.59	1.52
1	A	250	LEU	C-N	-5.33	1.26	1.33
1	A	208	THR	CA-CB	5.28	1.62	1.53
1	A	235	LEU	C-O	5.18	1.30	1.24
1	A	253	THR	C-O	5.13	1.31	1.24
1	A	150	VAL	N-CA	5.13	1.52	1.46
1	A	200	ALA	N-CA	5.11	1.50	1.45
1	A	43	ASN	CG-OD1	5.08	1.33	1.23
1	A	242	THR	N-CA	5.05	1.52	1.45
1	A	141	LYS	N-CA	5.04	1.52	1.46
1	A	134	ALA	C-O	5.02	1.29	1.24

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ASN	CA-CB-CG	11.42	124.02	112.60
1	A	99	ASP	CA-CB-CG	11.06	123.66	112.60
1	A	140	ASP	CA-CB-CG	10.94	123.54	112.60
1	A	195	GLU	CA-C-N	10.87	136.89	121.24
1	A	195	GLU	C-N-CA	10.87	136.89	121.24
1	A	247	ARG	NE-CZ-NH2	-10.65	109.62	119.20
1	A	185	GLN	CB-CG-CD	10.62	130.65	112.60
1	A	181	ASP	CA-CB-CG	10.29	122.89	112.60
1	A	25	ASN	OD1-CG-ND2	10.18	132.78	122.60
1	A	26	VAL	CA-C-N	9.99	135.83	122.84
1	A	26	VAL	C-N-CA	9.99	135.83	122.84
1	A	244	THR	OG1-CB-CG2	9.83	128.95	109.30
1	A	244	THR	CA-CB-CG2	9.74	127.06	110.50
1	A	59	GLN	OE1-CD-NE2	-9.62	112.98	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ASP	O-C-N	-9.59	115.92	123.11
1	A	175	ILE	N-CA-CB	9.52	121.39	110.82
1	A	94	LYS	CA-C-O	9.11	130.63	120.43
1	A	133	ALA	CA-C-N	8.81	131.89	120.44
1	A	133	ALA	C-N-CA	8.81	131.89	120.44
1	A	243	ASN	CA-CB-CG	8.72	121.32	112.60
1	A	184	ASN	CA-C-O	8.72	131.01	119.59
1	A	179	ALA	CA-C-O	8.68	129.84	120.38
1	A	179	ALA	N-CA-C	8.53	122.80	109.07
1	A	59	GLN	CB-CG-CD	8.52	127.08	112.60
1	A	257	LEU	CA-C-O	-8.50	114.37	119.55
1	A	151	ALA	CA-C-O	8.27	130.26	121.33
1	A	41	ASP	CA-CB-CG	8.24	120.84	112.60
1	A	242	THR	CA-CB-CG2	8.22	124.47	110.50
1	A	43	ASN	OD1-CG-ND2	-8.17	114.43	122.60
1	A	200	ALA	O-C-N	-8.15	115.70	121.65
1	A	14	PRO	CA-C-N	8.03	131.04	120.28
1	A	14	PRO	C-N-CA	8.03	131.04	120.28
1	A	57	PRO	CA-C-N	8.03	136.37	122.56
1	A	57	PRO	C-N-CA	8.03	136.37	122.56
1	A	271	GLU	CB-CG-CD	8.00	126.19	112.60
1	A	153	ALA	CA-C-N	7.99	133.33	122.63
1	A	153	ALA	C-N-CA	7.99	133.33	122.63
1	A	100	GLY	CA-C-N	7.96	136.18	122.64
1	A	100	GLY	C-N-CA	7.96	136.18	122.64
1	A	253	THR	O-C-N	-7.96	112.78	122.25
1	A	253	THR	CA-C-O	7.93	128.95	119.59
1	A	64	HIS	CA-CB-CG	7.92	121.72	113.80
1	A	3	CYS	CA-C-N	7.90	133.92	122.94
1	A	3	CYS	C-N-CA	7.90	133.92	122.94
1	A	155	ASN	CA-CB-CG	7.90	120.50	112.60
1	A	51	VAL	CA-C-O	7.77	125.15	119.25
1	A	156	GLU	CA-C-O	7.76	128.67	119.28
1	A	186	ARG	CD-NE-CZ	7.69	135.16	124.40
1	A	70	GLY	CA-C-N	7.66	130.85	120.44
1	A	70	GLY	C-N-CA	7.66	130.85	120.44
1	A	63	SER	N-CA-CB	7.65	123.41	110.49
1	A	106	TRP	CA-C-N	7.63	130.18	120.56
1	A	106	TRP	C-N-CA	7.63	130.18	120.56
1	A	136	LYS	CA-C-O	-7.61	111.22	119.97
1	A	72	VAL	O-C-N	7.56	129.31	121.91
1	A	109	ASN	CA-CB-CG	7.53	120.13	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	LEU	CA-C-N	7.51	130.96	120.29
1	A	250	LEU	C-N-CA	7.51	130.96	120.29
1	A	32	ASP	N-CA-C	7.49	117.11	108.49
1	A	168	PRO	CA-C-N	7.46	128.42	119.99
1	A	168	PRO	C-N-CA	7.46	128.42	119.99
1	A	192	VAL	CA-CB-CG2	7.45	123.07	110.40
1	A	151	ALA	O-C-N	-7.41	114.80	123.25
1	A	212	ASN	CB-CA-C	7.41	122.41	111.89
1	A	17	HIS	CA-CB-CG	7.40	121.20	113.80
1	A	107	ILE	CA-C-N	7.39	129.87	120.56
1	A	107	ILE	C-N-CA	7.39	129.87	120.56
1	A	206	CYS	CA-C-O	7.37	128.24	120.36
1	A	257	LEU	O-C-N	-7.29	114.15	120.71
1	A	61	ASN	CA-CB-CG	7.28	119.88	112.60
1	A	205	ILE	CB-CA-C	7.25	119.74	110.96
1	A	49	SER	CA-C-O	7.25	128.39	120.71
1	A	125	SER	CA-C-N	7.22	134.84	121.62
1	A	125	SER	C-N-CA	7.22	134.84	121.62
1	A	71	THR	CA-C-N	7.20	129.63	120.56
1	A	71	THR	C-N-CA	7.20	129.63	120.56
1	A	207	SER	CA-C-N	7.17	131.06	120.87
1	A	207	SER	C-N-CA	7.17	131.06	120.87
1	A	200	ALA	CA-C-O	7.16	126.92	120.34
1	A	33	SER	CA-C-N	7.11	134.09	122.21
1	A	33	SER	C-N-CA	7.11	134.09	122.21
1	A	19	GLN	CA-C-N	7.11	132.32	121.51
1	A	19	GLN	C-N-CA	7.11	132.32	121.51
1	A	104	TYR	CA-CB-CG	7.10	126.68	113.90
1	A	272	ALA	CB-CA-C	7.07	121.98	110.88
1	A	54	GLU	CA-CB-CG	7.01	128.11	114.10
1	A	45	ALA	O-C-N	-7.00	112.81	122.46
1	A	31	ILE	CA-C-N	6.99	132.20	120.81
1	A	31	ILE	C-N-CA	6.99	132.20	120.81
1	A	23	GLY	CA-C-N	6.93	130.59	120.82
1	A	23	GLY	C-N-CA	6.93	130.59	120.82
1	A	270	VAL	CB-CA-C	6.91	121.75	112.22
1	A	91	TYR	O-C-N	-6.89	115.28	123.27
1	A	188	SER	CB-CA-C	6.89	122.39	110.68
1	A	56	ASN	OD1-CG-ND2	-6.87	115.73	122.60
1	A	265	LYS	CA-C-O	6.84	127.79	119.38
1	A	64	HIS	CA-C-N	6.83	127.56	119.98
1	A	64	HIS	C-N-CA	6.83	127.56	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	GLN	CB-CA-C	6.80	123.02	110.10
1	A	117	ASN	O-C-N	-6.78	113.65	122.39
1	A	259	ASP	CA-C-N	6.77	130.26	120.38
1	A	259	ASP	C-N-CA	6.77	130.26	120.38
1	A	2	LYS	CA-C-O	6.74	128.31	120.89
1	A	51	VAL	N-CA-C	-6.74	100.88	107.55
1	A	31	ILE	CA-C-O	6.72	128.97	120.97
1	A	103	GLN	CB-CG-CD	6.71	124.02	112.60
1	A	158	THR	CA-CB-CG2	6.70	121.89	110.50
1	A	12	LYS	CA-C-N	6.70	128.46	120.09
1	A	12	LYS	C-N-CA	6.70	128.46	120.09
1	A	184	ASN	CA-CB-CG	6.69	119.29	112.60
1	A	156	GLU	N-CA-C	6.69	121.45	113.16
1	A	109	ASN	OD1-CG-ND2	-6.68	115.92	122.60
1	A	21	TYR	CB-CA-C	6.67	121.66	110.79
1	A	227	VAL	CB-CA-C	6.64	120.74	112.04
1	A	35	ILE	O-C-N	6.64	130.24	123.07
1	A	161	SER	CA-C-N	6.64	130.91	121.42
1	A	161	SER	C-N-CA	6.64	130.91	121.42
1	A	130	SER	CB-CA-C	6.63	122.40	109.33
1	A	85	ALA	CA-C-N	6.62	127.15	119.47
1	A	85	ALA	C-N-CA	6.62	127.15	119.47
1	A	265	LYS	O-C-N	-6.60	113.58	122.43
1	A	32	ASP	N-CA-CB	-6.60	102.78	109.51
1	A	32	ASP	CA-C-O	6.57	124.92	120.19
1	A	169	GLY	O-C-N	6.51	128.58	122.13
1	A	19	GLN	O-C-N	-6.50	112.95	122.43
1	A	36	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	25	ASN	CA-CB-CG	6.46	119.06	112.60
1	A	62	ASN	CA-C-N	6.43	133.82	121.54
1	A	62	ASN	C-N-CA	6.43	133.82	121.54
1	A	45	ALA	CA-C-O	6.38	127.22	119.31
1	A	205	ILE	CA-CB-CG2	6.33	121.25	110.50
1	A	118	ASN	CA-C-O	6.31	128.79	121.28
1	A	54	GLU	CA-C-N	6.30	131.24	120.72
1	A	54	GLU	C-N-CA	6.30	131.24	120.72
1	A	107	ILE	N-CA-CB	6.26	117.88	110.55
1	A	139	VAL	N-CA-CB	6.24	119.03	110.54
1	A	184	ASN	O-C-N	-6.24	114.21	122.00
1	A	120	ASP	N-CA-CB	6.21	119.46	110.20
1	A	50	PHE	O-C-N	-6.16	114.73	122.19
1	A	261	PHE	CA-C-O	6.15	127.04	119.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ALA	O-C-N	-6.14	116.22	123.22
1	A	164	THR	CA-CB-CG2	6.12	120.90	110.50
1	A	56	ASN	CB-CA-C	6.03	116.72	109.85
1	A	255	THR	N-CA-CB	6.03	119.80	110.21
1	A	128	GLY	CA-C-N	6.02	125.64	119.56
1	A	128	GLY	C-N-CA	6.02	125.64	119.56
1	A	117	ASN	CA-C-N	6.01	130.66	122.19
1	A	117	ASN	C-N-CA	6.01	130.66	122.19
1	A	178	GLY	O-C-N	-6.00	114.27	123.03
1	A	272	ALA	CA-C-N	6.00	128.32	120.28
1	A	272	ALA	C-N-CA	6.00	128.32	120.28
1	A	3	CYS	O-C-N	-5.99	115.92	123.17
1	A	117	ASN	CA-C-O	5.98	126.67	119.43
1	A	238	HIS	CA-C-N	5.98	125.86	119.28
1	A	238	HIS	C-N-CA	5.98	125.86	119.28
1	A	91	TYR	CB-CA-C	5.97	120.08	110.16
1	A	47	GLY	CA-C-O	5.96	127.38	121.48
1	A	177	VAL	CA-CB-CG2	5.94	120.50	110.40
1	A	239	PRO	CA-C-N	5.94	131.53	121.14
1	A	239	PRO	C-N-CA	5.94	131.53	121.14
1	A	196	LEU	O-C-N	5.93	130.44	122.96
1	A	230	ALA	CA-C-N	5.93	128.23	120.28
1	A	230	ALA	C-N-CA	5.93	128.23	120.28
1	A	104	TYR	CB-CG-CD1	5.89	129.64	120.80
1	A	252	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	10	GLN	N-CA-C	5.85	118.44	111.71
1	A	249	SER	CA-CB-OG	-5.85	99.40	111.10
1	A	61	ASN	CA-C-N	5.85	131.48	122.42
1	A	61	ASN	C-N-CA	5.85	131.48	122.42
1	A	155	ASN	CA-C-O	5.84	128.41	121.17
1	A	156	GLU	O-C-N	-5.83	114.33	122.37
1	A	46	GLY	CA-C-O	5.81	127.45	121.35
1	A	91	TYR	CA-C-O	5.78	126.48	120.30
1	A	204	SER	CA-C-O	5.76	129.29	122.14
1	A	50	PHE	CA-C-N	5.74	129.39	122.85
1	A	50	PHE	C-N-CA	5.74	129.39	122.85
1	A	162	SER	CA-C-O	5.74	127.59	121.05
1	A	216	ALA	CA-C-O	5.72	127.50	120.92
1	A	10	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	A	244	THR	CB-CA-C	5.70	120.25	110.79
1	A	163[A]	SER	N-CA-CB	5.66	118.60	110.06
1	A	163[B]	SER	N-CA-CB	5.66	118.60	110.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ILE	O-C-N	-5.65	115.86	122.07
1	A	253	THR	CA-CB-OG1	-5.64	101.14	109.60
1	A	51	VAL	CB-CA-C	5.61	117.66	111.04
1	A	151	ALA	CA-C-N	5.60	128.82	120.87
1	A	151	ALA	C-N-CA	5.60	128.82	120.87
1	A	39	HIS	CA-CB-CG	5.60	119.40	113.80
1	A	165	VAL	CA-C-N	-5.59	115.79	122.16
1	A	165	VAL	C-N-CA	-5.59	115.79	122.16
1	A	58	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	55	THR	N-CA-C	5.58	119.35	112.54
1	A	95	VAL	CA-CB-CG2	5.58	119.88	110.40
1	A	269	ASN	OD1-CG-ND2	-5.58	117.03	122.60
1	A	60	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	125	SER	CA-C-O	5.57	129.97	122.51
1	A	247	ARG	NH1-CZ-NH2	5.57	126.54	119.30
1	A	45	ALA	CA-C-N	5.53	128.54	120.91
1	A	45	ALA	C-N-CA	5.53	128.54	120.91
1	A	54	GLU	CA-C-O	5.52	127.93	120.47
1	A	11	ILE	CA-C-O	5.52	126.43	119.48
1	A	237	LYS	CA-C-O	-5.51	114.12	120.24
1	A	107	ILE	CA-C-O	-5.50	115.34	121.17
1	A	138	ALA	CA-C-N	5.48	127.96	120.46
1	A	138	ALA	C-N-CA	5.48	127.96	120.46
1	A	252	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	149	VAL	CA-C-O	5.45	126.06	120.39
1	A	25	ASN	CB-CG-OD1	-5.45	109.91	120.80
1	A	144	ALA	O-C-N	-5.44	115.85	122.22
1	A	50	PHE	CA-C-O	5.42	125.88	119.48
1	A	115	ILE	CA-C-O	-5.42	115.03	121.05
1	A	161	SER	CB-CA-C	5.42	119.14	110.09
1	A	205	ILE	CA-CB-CG1	5.39	119.57	110.40
1	A	108	ILE	CB-CA-C	5.39	118.87	111.97
1	A	169	GLY	CA-C-N	5.39	128.04	120.28
1	A	169	GLY	C-N-CA	5.39	128.04	120.28
1	A	18	SER	CB-CA-C	5.39	121.01	110.67
1	A	157	GLY	O-C-N	5.39	128.70	122.61
1	A	183	SER	O-C-N	-5.39	115.72	122.35
1	A	68	VAL	CB-CA-C	5.38	119.06	112.02
1	A	50	PHE	CB-CG-CD2	-5.37	111.58	120.70
1	A	247	ARG	CA-C-N	5.36	127.41	120.44
1	A	247	ARG	C-N-CA	5.36	127.41	120.44
1	A	174	VAL	CA-C-N	5.36	129.21	121.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	VAL	C-N-CA	5.36	129.21	121.18
1	A	59	GLN	CG-CD-OE1	5.34	131.49	120.80
1	A	93	VAL	CB-CA-C	5.32	120.01	111.29
1	A	106	TRP	CA-CB-CG	5.30	123.66	113.60
1	A	143	VAL	CB-CA-C	5.29	118.94	112.02
1	A	155	ASN	O-C-N	-5.27	114.86	121.97
1	A	208	THR	CA-C-O	5.27	127.06	121.16
1	A	131	GLY	O-C-N	-5.26	116.91	123.12
1	A	115	ILE	CA-CB-CG1	5.25	119.33	110.40
1	A	160	GLY	CA-C-N	5.25	131.20	122.54
1	A	160	GLY	C-N-CA	5.25	131.20	122.54
1	A	199	MET	O-C-N	-5.23	116.42	123.23
1	A	144	ALA	CA-C-O	5.23	126.01	120.10
1	A	33	SER	O-C-N	-5.21	114.02	122.42
1	A	241	TRP	CA-CB-CG	5.21	123.50	113.60
1	A	259	ASP	CA-C-O	-5.20	115.47	121.19
1	A	148	VAL	N-CA-CB	5.19	116.92	111.00
1	A	121	VAL	CA-CB-CG2	5.17	119.19	110.40
1	A	142	ALA	CA-C-N	5.15	127.15	120.56
1	A	142	ALA	C-N-CA	5.15	127.15	120.56
1	A	58	PHE	CB-CA-C	5.14	119.51	110.37
1	A	67	HIS	CA-C-N	5.13	127.13	120.56
1	A	67	HIS	C-N-CA	5.13	127.13	120.56
1	A	150	VAL	CA-CB-CG2	5.13	119.12	110.40
1	A	262	TYR	N-CA-C	5.12	119.56	112.45
1	A	207	SER	CA-C-O	5.10	126.77	121.36
1	A	271	GLU	CB-CA-C	5.09	118.88	110.88
1	A	90	LEU	CA-C-O	5.09	126.45	120.80
1	A	86	PRO	N-CA-C	5.09	121.19	113.81
1	A	51	VAL	N-CA-CB	5.09	117.31	111.31
1	A	103	GLN	CA-CB-CG	5.06	124.21	114.10
1	A	50	PHE	CB-CG-CD1	5.04	129.27	120.70
1	A	125	SER	N-CA-CB	5.04	116.00	110.35
1	A	19	GLN	CA-C-O	5.04	125.56	119.11
1	A	39	HIS	CA-C-N	5.03	125.06	119.32
1	A	39	HIS	C-N-CA	5.03	125.06	119.32
1	A	38	SER	CA-C-O	5.02	125.57	119.49
1	A	95	VAL	CA-CB-CG1	5.02	118.94	110.40
1	A	8	VAL	CA-CB-CG1	5.01	118.92	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	244	THR	CB

There are no planarity outliers.

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	1881	0	1839	22	0
2	A	133	0	0	5	0
All	All	2014	0	1839	22	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 6.

All (22) 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:31:ILE:HD12	1:A:122:ILE:HG23	1.77	0.66
1:A:69:ALA:HB1	1:A:90:LEU:HD21	1.81	0.62
1:A:136:LYS:HG3	1:A:171:TYR:CD1	2.37	0.60
1:A:103:GLN:HG3	2:A:2057:HOH:O	2.04	0.58
1:A:2:LYS:HG3	1:A:214:TYR:CZ	2.39	0.57
1:A:31:ILE:HD12	1:A:122:ILE:CG2	2.35	0.56
1:A:143:VAL:HG21	1:A:173:SER:HB2	1.87	0.55
1:A:199:MET:HG2	1:A:263:TYR:O	2.06	0.55
1:A:236:SER:HA	2:A:2019:HOH:O	2.07	0.55
1:A:163[A]:SER:HB2	1:A:194:PRO:HD2	1.92	0.51
1:A:158:THR:HG22	1:A:192:VAL:HG21	1.93	0.51
1:A:163[B]:SER:HB3	1:A:194:PRO:HD2	1.92	0.50
1:A:158:THR:HB	2:A:2088:HOH:O	2.14	0.46
1:A:71:THR:HG21	1:A:225:PRO:HG2	1.97	0.45
1:A:29:ALA:HB2	1:A:119:MET:HG3	1.99	0.45
1:A:122:ILE:HD12	1:A:147:VAL:HG11	1.99	0.44
1:A:2:LYS:N	2:A:2001:HOH:O	2.51	0.43
1:A:209:LEU:HD21	1:A:217:LYS:HE2	2.00	0.43
1:A:36:ASP:OD2	1:A:210:PRO:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLY:HA2	1:A:167:TYR:O	2.20	0.41
1:A:130:SER:HB3	2:A:2068:HOH:O	2.21	0.41
1:A:31:ILE:CD1	1:A:122:ILE:HG23	2.49	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	264/266 (99%)	259 (98%)	4 (2%)	1 (0%)	30 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	SER

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	199/198 (100%)	196 (98%)	3 (2%)	57 56

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	244	THR
1	A	249	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	275	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	$\# Z > 2$
1	MIS	A	221	1	11,12,13	1.97	4 (36%)	11,16,18	1.55	3 (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	MIS	A	221	1	-	1/11/13/15	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	MIS	P-O1P	-3.64	1.38	1.55
1	A	221	MIS	P-O2P	-3.19	1.39	1.50
1	A	221	MIS	P-O3P	2.86	1.68	1.59
1	A	221	MIS	C3-C1	2.30	1.61	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	MIS	O3P-C1-C3	-2.60	98.74	107.72
1	A	221	MIS	O3P-C1-C2	2.58	116.62	107.72
1	A	221	MIS	OG-P-O2P	2.06	117.10	108.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	221	MIS	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

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.