



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:45 PM UTC

PDB ID : 1GNS / pdb_00001gns
Title : SUBTILISIN BPN'
Authors : Almog, O.; Gallagher, D.T.; Ladner, J.E.; Strausberg, S.; Alexander, P.
Deposited on : 2001-10-06
Resolution : 1.80 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

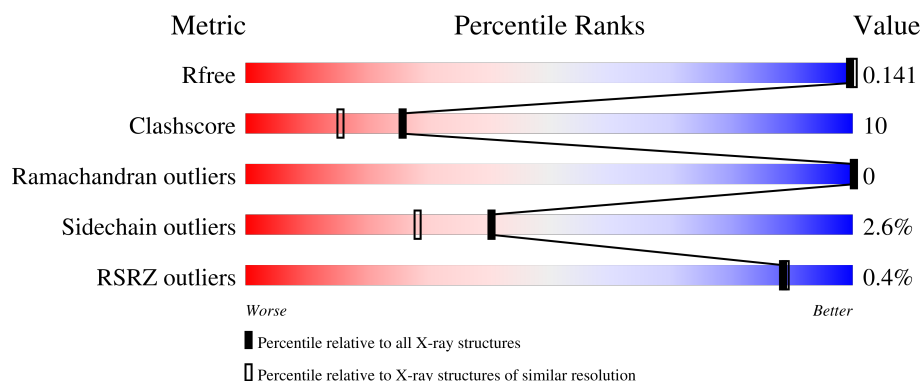
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	263	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2017 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.

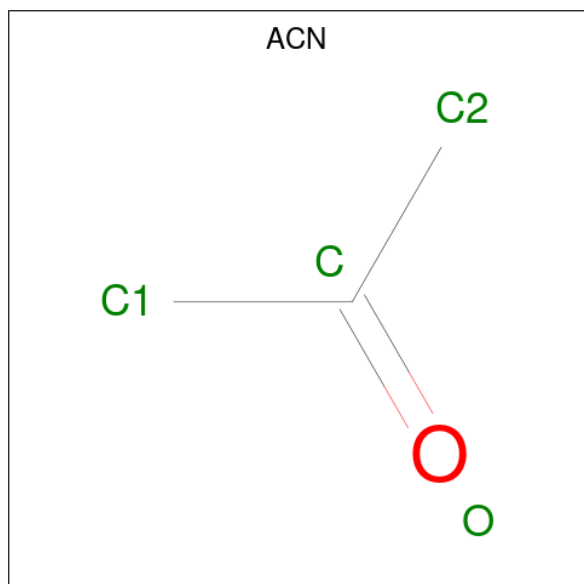
- Molecule 1 is a protein called SUBTILISIN BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	1858	1160	319	374	5	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLY	VAL	conflict	UNP P00782
A	41	ALA	ASP	engineered mutation	UNP P00782
A	50	PHE	MET	engineered mutation	UNP P00782
A	73	LEU	ALA	engineered mutation	UNP P00782
A	206	TRP	GLN	engineered mutation	UNP P00782
A	217	LYS	TYR	engineered mutation	UNP P00782
A	218	SER	ASN	engineered mutation	UNP P00782
A	221	CSO	SER	engineered mutation	UNP P00782
A	271	GLU	GLN	engineered mutation	UNP P00782

- Molecule 2 is ACETONE (CCD ID: ACN) (formula: C₃H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	3	1		

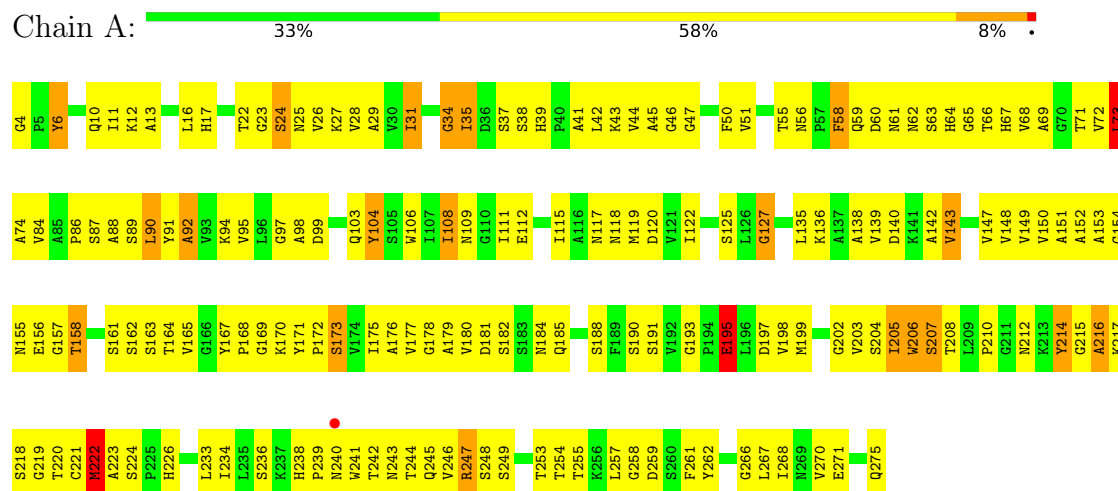
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total	O	0	0
			155	155		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: SUBTILISIN BPN'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.17Å 78.06Å 36.70Å 90.00° 114.60° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80 8.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	77.0 (8.00-1.80) 78.9 (8.00-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.80Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.165 , (Not available) (Not available) , 0.141	Depositor DCC
R_{free} test set	505 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å ²)	10.3	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.045 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2017	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ACN, CSO

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	2.51	99/1890 (5.2%)	2.85	216/2578 (8.4%)

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	HIS	CE1-NE2	13.67	1.46	1.32
1	A	222	MET	CG-SD	-12.17	1.50	1.80
1	A	222	MET	SD-CE	-9.89	1.54	1.79
1	A	181	ASP	N-CA	8.97	1.56	1.45
1	A	68	VAL	N-CA	8.96	1.57	1.46
1	A	245	GLN	C-O	-8.71	1.14	1.24
1	A	246	VAL	N-CA	8.27	1.56	1.46
1	A	248	SER	CA-CB	7.99	1.65	1.53
1	A	69	ALA	CA-C	-7.92	1.42	1.52
1	A	217	LYS	CA-C	7.90	1.62	1.52
1	A	111	ILE	N-CA	7.85	1.55	1.46
1	A	63	SER	C-N	7.85	1.43	1.33
1	A	35	ILE	CA-C	7.81	1.62	1.52
1	A	207	SER	C-O	7.75	1.32	1.23
1	A	71	THR	CB-OG1	7.61	1.55	1.43
1	A	178	GLY	CA-C	7.42	1.62	1.52
1	A	148	VAL	CA-C	7.41	1.61	1.52
1	A	226	HIS	ND1-CE1	7.34	1.39	1.32
1	A	4	GLY	N-CA	7.15	1.56	1.45
1	A	244	THR	CA-CB	7.14	1.64	1.53
1	A	219	GLY	N-CA	7.13	1.53	1.45
1	A	17	HIS	CE1-NE2	-7.04	1.25	1.32
1	A	127	GLY	N-CA	7.02	1.52	1.45
1	A	197	ASP	CA-C	-6.97	1.44	1.53
1	A	153	ALA	N-CA	6.95	1.55	1.46
1	A	255	THR	CA-CB	6.92	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	THR	CA-CB	6.91	1.64	1.53
1	A	206	TRP	C-N	6.88	1.42	1.33
1	A	139	VAL	C-O	-6.84	1.16	1.24
1	A	218	SER	N-CA	6.75	1.54	1.45
1	A	195	GLU	C-O	6.69	1.32	1.24
1	A	28	VAL	C-O	6.68	1.31	1.24
1	A	97	GLY	C-O	6.66	1.31	1.23
1	A	125	SER	CA-C	-6.63	1.45	1.53
1	A	226	HIS	CG-ND1	-6.62	1.30	1.38
1	A	95	VAL	N-CA	6.62	1.54	1.46
1	A	171	TYR	CA-C	-6.61	1.45	1.53
1	A	205	ILE	C-O	-6.54	1.17	1.24
1	A	22	THR	CA-CB	6.53	1.63	1.53
1	A	185	GLN	N-CA	-6.52	1.37	1.46
1	A	29	ALA	C-N	6.40	1.41	1.33
1	A	193	GLY	N-CA	6.36	1.53	1.44
1	A	199	MET	C-O	-6.34	1.15	1.23
1	A	31	ILE	CA-CB	6.33	1.60	1.53
1	A	254	THR	CA-CB	6.33	1.63	1.53
1	A	214	TYR	C-O	6.24	1.31	1.23
1	A	67	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	191	SER	CA-C	6.18	1.60	1.52
1	A	108	ILE	N-CA	6.18	1.53	1.46
1	A	22	THR	N-CA	6.17	1.52	1.46
1	A	38	SER	C-O	6.08	1.31	1.24
1	A	197	ASP	C-N	6.07	1.41	1.33
1	A	193	GLY	C-N	6.04	1.41	1.33
1	A	177	VAL	N-CA	6.03	1.53	1.46
1	A	39	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	203	VAL	CA-C	5.96	1.60	1.52
1	A	92	ALA	CA-CB	5.94	1.60	1.53
1	A	98	ALA	N-CA	5.93	1.53	1.46
1	A	169	GLY	CA-C	5.92	1.58	1.52
1	A	181	ASP	C-N	5.92	1.42	1.33
1	A	44	VAL	N-CA	5.91	1.53	1.46
1	A	136	LYS	N-CA	5.87	1.53	1.46
1	A	157	GLY	CA-C	5.85	1.59	1.52
1	A	90	LEU	CB-CG	-5.85	1.41	1.53
1	A	207	SER	C-N	-5.82	1.25	1.33
1	A	106	TRP	N-CA	5.78	1.53	1.46
1	A	179	ALA	N-CA	5.78	1.53	1.46
1	A	86	PRO	C-O	5.76	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	ASN	N-CA	5.74	1.53	1.46
1	A	242	THR	C-N	-5.68	1.26	1.34
1	A	203	VAL	N-CA	5.63	1.52	1.46
1	A	164	THR	N-CA	5.63	1.53	1.46
1	A	169	GLY	C-N	-5.60	1.26	1.33
1	A	226	HIS	C-O	-5.59	1.17	1.24
1	A	148	VAL	C-O	-5.58	1.18	1.24
1	A	22	THR	CA-C	-5.57	1.46	1.52
1	A	220	THR	N-CA	5.56	1.56	1.46
1	A	234	ILE	C-N	-5.51	1.26	1.34
1	A	158	THR	N-CA	5.50	1.52	1.45
1	A	205	ILE	CA-C	5.47	1.59	1.52
1	A	152	ALA	C-O	-5.46	1.17	1.23
1	A	104	TYR	CA-CB	5.44	1.61	1.53
1	A	94	LYS	C-O	-5.42	1.17	1.24
1	A	261	PHE	CA-C	5.42	1.60	1.52
1	A	245	GLN	CA-C	5.39	1.59	1.52
1	A	64	HIS	N-CA	5.32	1.52	1.46
1	A	261	PHE	C-O	-5.30	1.17	1.24
1	A	242	THR	CA-CB	5.20	1.61	1.53
1	A	29	ALA	N-CA	-5.19	1.39	1.46
1	A	84	VAL	N-CA	5.19	1.52	1.46
1	A	112	GLU	C-N	5.17	1.40	1.33
1	A	158	THR	C-O	5.12	1.29	1.23
1	A	224	SER	CA-CB	5.11	1.61	1.53
1	A	226	HIS	CE1-NE2	-5.10	1.27	1.32
1	A	72	VAL	C-N	5.09	1.40	1.34
1	A	42	LEU	CA-C	-5.08	1.46	1.52
1	A	243	ASN	C-N	5.08	1.40	1.33
1	A	234	ILE	N-CA	5.06	1.52	1.46
1	A	268	ILE	CB-CG1	5.01	1.63	1.53

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ASN	CA-CB-CG	11.53	124.13	112.60
1	A	181	ASP	CA-CB-CG	10.62	123.22	112.60
1	A	243	ASN	OD1-CG-ND2	10.47	133.07	122.60
1	A	139	VAL	N-CA-CB	10.42	122.74	110.55
1	A	117	ASN	OD1-CG-ND2	10.35	132.95	122.60
1	A	205	ILE	O-C-N	10.18	134.24	122.83
1	A	109	ASN	CA-CB-CG	10.14	122.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	SER	CA-C-O	9.73	131.10	120.20
1	A	222	MET	CG-SD-CE	9.73	122.30	100.90
1	A	216	ALA	CA-C-O	9.61	132.62	121.28
1	A	247	ARG	NE-CZ-NH1	9.33	130.83	121.50
1	A	157	GLY	O-C-N	9.29	132.89	122.67
1	A	26	VAL	N-CA-CB	8.91	121.63	111.21
1	A	66	THR	CA-CB-OG1	-8.89	96.26	109.60
1	A	22	THR	CA-C-O	8.77	129.95	119.78
1	A	169	GLY	O-C-N	8.55	130.46	122.17
1	A	117	ASN	CA-C-O	8.45	129.66	119.43
1	A	135	LEU	O-C-N	8.36	130.68	122.07
1	A	35	ILE	O-C-N	8.30	132.26	123.05
1	A	207	SER	CA-C-N	8.19	132.50	120.87
1	A	207	SER	C-N-CA	8.19	132.50	120.87
1	A	244	THR	CA-CB-OG1	-8.19	97.32	109.60
1	A	214	TYR	CA-C-O	7.89	130.21	121.06
1	A	84	VAL	CA-C-O	-7.85	112.31	120.71
1	A	27	LYS	CA-C-O	7.82	128.72	120.36
1	A	181	ASP	CA-C-O	7.79	131.24	121.50
1	A	165	VAL	CA-C-O	7.70	129.81	121.04
1	A	6	TYR	O-C-N	7.66	130.24	122.12
1	A	248	SER	CA-CB-OG	-7.66	95.79	111.10
1	A	43	LYS	N-CA-CB	7.62	122.74	110.77
1	A	150	VAL	CA-CB-CG2	7.61	123.34	110.40
1	A	39	HIS	CA-C-O	7.58	126.94	119.51
1	A	112	GLU	CA-C-O	7.58	128.59	120.55
1	A	155	ASN	OD1-CG-ND2	7.55	130.15	122.60
1	A	185	GLN	CB-CG-CD	7.48	125.32	112.60
1	A	29	ALA	N-CA-CB	7.43	122.53	110.42
1	A	87	SER	O-C-N	-7.40	113.09	122.34
1	A	243	ASN	CA-C-O	7.40	128.46	120.10
1	A	87	SER	CA-C-O	7.36	127.96	119.35
1	A	118	ASN	CA-CB-CG	7.34	119.94	112.60
1	A	212	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	A	68	VAL	CB-CA-C	7.33	121.36	111.97
1	A	261	PHE	CA-CB-CG	7.25	121.05	113.80
1	A	73	LEU	CB-CA-C	7.23	124.01	110.63
1	A	184	ASN	CA-CB-CG	7.23	119.83	112.60
1	A	188	SER	N-CA-C	7.20	120.96	111.75
1	A	87	SER	CA-C-N	7.19	132.23	120.94
1	A	87	SER	C-N-CA	7.19	132.23	120.94
1	A	176	ALA	CA-C-O	7.15	128.01	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ASP	CB-CA-C	7.04	123.49	110.11
1	A	169	GLY	CA-C-O	-7.03	113.91	120.80
1	A	203	VAL	N-CA-C	-6.98	98.34	108.11
1	A	10	GLN	O-C-N	6.95	130.81	122.27
1	A	143	VAL	CB-CA-C	6.91	120.82	111.97
1	A	45	ALA	CA-C-N	6.91	128.94	120.51
1	A	45	ALA	C-N-CA	6.91	128.94	120.51
1	A	99	ASP	CA-CB-CG	6.90	119.50	112.60
1	A	178	GLY	CA-C-N	-6.88	112.61	122.94
1	A	178	GLY	C-N-CA	-6.88	112.61	122.94
1	A	68	VAL	N-CA-CB	-6.88	102.50	110.55
1	A	94	LYS	CA-C-O	6.87	127.93	120.58
1	A	195	GLU	CB-CG-CD	6.86	124.25	112.60
1	A	154	GLY	N-CA-C	-6.84	105.18	112.08
1	A	17	HIS	CB-CG-CD2	6.83	140.08	131.20
1	A	212	ASN	CA-CB-CG	6.83	119.43	112.60
1	A	12	LYS	CA-C-O	6.81	127.95	120.12
1	A	255	THR	CA-CB-OG1	-6.81	99.38	109.60
1	A	223	ALA	CA-C-O	-6.79	113.22	120.42
1	A	67	HIS	O-C-N	6.76	129.39	122.09
1	A	56	ASN	CA-CB-CG	6.75	119.35	112.60
1	A	51	VAL	N-CA-C	-6.74	100.88	107.55
1	A	203	VAL	CA-C-O	6.73	127.45	120.39
1	A	233	LEU	O-C-N	6.71	129.23	122.12
1	A	244	THR	CA-C-N	6.66	129.50	120.44
1	A	244	THR	C-N-CA	6.66	129.50	120.44
1	A	193	GLY	CA-C-O	6.65	131.03	121.52
1	A	202	GLY	CA-C-N	-6.61	114.47	123.14
1	A	202	GLY	C-N-CA	-6.61	114.47	123.14
1	A	197	ASP	N-CA-C	6.58	121.52	112.04
1	A	118	ASN	CA-C-O	6.51	129.27	121.65
1	A	215	GLY	O-C-N	6.51	131.08	123.66
1	A	63	SER	N-CA-CB	6.50	121.47	110.49
1	A	161	SER	CA-C-N	6.48	132.14	121.39
1	A	161	SER	C-N-CA	6.48	132.14	121.39
1	A	22	THR	O-C-N	-6.47	113.39	122.26
1	A	89	SER	CA-C-O	6.43	127.46	120.58
1	A	58	PHE	CA-CB-CG	6.42	120.22	113.80
1	A	188	SER	O-C-N	-6.42	114.89	122.20
1	A	259	ASP	OD1-CG-OD2	6.41	138.28	122.90
1	A	24	SER	N-CA-CB	-6.39	100.18	109.83
1	A	257	LEU	CB-CA-C	6.37	123.09	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	THR	OG1-CB-CG2	6.35	122.01	109.30
1	A	214	TYR	O-C-N	-6.34	115.91	123.27
1	A	64	HIS	CA-C-O	-6.32	114.18	120.82
1	A	163	SER	CB-CA-C	6.32	120.00	109.89
1	A	261	PHE	O-C-N	6.29	129.57	122.22
1	A	64	HIS	O-C-N	6.25	128.51	122.07
1	A	179	ALA	CA-C-O	6.25	127.45	120.70
1	A	223	ALA	N-CA-CB	-6.23	100.94	110.16
1	A	181	ASP	N-CA-CB	-6.16	100.60	110.39
1	A	29	ALA	CA-C-N	-6.15	115.32	122.95
1	A	29	ALA	C-N-CA	-6.15	115.32	122.95
1	A	154	GLY	CA-C-O	6.15	126.86	122.37
1	A	61	ASN	CA-C-O	6.13	126.48	119.18
1	A	103	GLN	CB-CG-CD	6.12	123.01	112.60
1	A	151	ALA	CA-C-O	6.09	128.13	121.06
1	A	199	MET	CA-C-O	6.09	128.00	121.11
1	A	191	SER	CA-C-O	6.09	128.00	121.55
1	A	91	TYR	CA-C-O	6.09	126.94	120.36
1	A	112	GLU	CG-CD-OE2	-6.07	104.43	118.40
1	A	143	VAL	CA-CB-CG1	6.07	120.72	110.40
1	A	31	ILE	CA-C-O	6.07	128.19	120.97
1	A	62	ASN	CA-C-N	6.07	133.13	121.54
1	A	62	ASN	C-N-CA	6.07	133.13	121.54
1	A	271	GLU	CG-CD-OE1	6.04	132.30	118.40
1	A	173	SER	O-C-N	6.01	130.75	122.46
1	A	239	PRO	CA-C-N	6.00	131.65	121.14
1	A	239	PRO	C-N-CA	6.00	131.65	121.14
1	A	143	VAL	O-C-N	5.97	127.77	121.91
1	A	46	GLY	CA-C-O	5.96	127.75	121.08
1	A	168	PRO	CA-C-N	5.92	126.66	120.03
1	A	168	PRO	C-N-CA	5.92	126.66	120.03
1	A	244	THR	CA-CB-CG2	5.90	120.53	110.50
1	A	197	ASP	CA-C-O	5.88	127.66	120.31
1	A	271	GLU	CG-CD-OE2	-5.88	104.89	118.40
1	A	117	ASN	O-C-N	-5.87	114.81	122.39
1	A	254	THR	OG1-CB-CG2	5.87	121.05	109.30
1	A	208	THR	CA-C-O	5.85	127.71	121.16
1	A	268	ILE	N-CA-CB	5.84	119.94	110.13
1	A	135	LEU	CA-C-N	-5.84	112.00	120.29
1	A	135	LEU	C-N-CA	-5.84	112.00	120.29
1	A	16	LEU	CB-CA-C	5.82	120.74	110.85
1	A	238	HIS	CA-CB-CG	5.81	119.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ALA	CA-C-O	5.81	126.64	119.79
1	A	35	ILE	N-CA-CB	5.78	120.92	111.45
1	A	241	TRP	CA-C-O	5.78	127.63	121.16
1	A	60	ASP	O-C-N	5.76	130.38	123.13
1	A	210	PRO	O-C-N	5.75	129.99	123.03
1	A	29	ALA	CA-C-O	5.75	126.51	120.36
1	A	156	GLU	N-CA-C	5.75	120.01	112.89
1	A	163	SER	N-CA-CB	-5.73	101.32	109.85
1	A	87	SER	N-CA-C	5.70	120.35	113.17
1	A	104	TYR	N-CA-C	5.69	118.22	111.33
1	A	25	ASN	CA-CB-CG	5.69	118.29	112.60
1	A	198	VAL	O-C-N	5.69	129.44	123.02
1	A	176	ALA	CA-C-N	-5.68	116.15	123.19
1	A	176	ALA	C-N-CA	-5.68	116.15	123.19
1	A	271	GLU	CA-C-O	-5.67	114.86	120.82
1	A	177	VAL	CA-C-O	5.65	126.47	120.48
1	A	266	GLY	CA-C-O	5.63	127.83	122.25
1	A	148	VAL	CA-CB-CG2	5.63	119.96	110.40
1	A	255	THR	N-CA-C	-5.59	100.70	109.25
1	A	161	SER	O-C-N	-5.58	116.15	122.23
1	A	184	ASN	CA-C-N	5.58	129.40	121.42
1	A	184	ASN	C-N-CA	5.58	129.40	121.42
1	A	43	LYS	CA-C-N	-5.57	116.28	123.19
1	A	43	LYS	C-N-CA	-5.57	116.28	123.19
1	A	245	GLN	N-CA-CB	5.57	118.15	110.07
1	A	218	SER	N-CA-CB	-5.56	101.58	111.08
1	A	149	VAL	CB-CA-C	5.55	118.66	110.77
1	A	212	ASN	CA-C-O	5.55	128.28	121.84
1	A	55	THR	CA-C-O	5.55	126.20	119.38
1	A	61	ASN	CA-CB-CG	5.54	118.14	112.60
1	A	190	SER	O-C-N	5.54	130.38	123.01
1	A	74	ALA	CA-C-O	5.54	126.42	120.55
1	A	258	GLY	CA-C-O	5.52	127.38	121.64
1	A	10	GLN	CA-C-O	-5.51	113.63	119.97
1	A	156	GLU	CG-CD-OE2	-5.51	105.73	118.40
1	A	71	THR	CA-CB-OG1	-5.49	101.36	109.60
1	A	64	HIS	CB-CA-C	5.46	119.46	110.88
1	A	103	GLN	CA-CB-CG	5.46	125.02	114.10
1	A	245	GLN	CG-CD-OE1	5.43	131.67	120.80
1	A	125	SER	CA-C-O	5.43	130.47	122.38
1	A	242	THR	CA-CB-OG1	-5.42	101.46	109.60
1	A	161	SER	CA-C-O	5.42	125.16	119.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ALA	CA-C-N	5.42	130.72	122.65
1	A	41	ALA	C-N-CA	5.42	130.72	122.65
1	A	28	VAL	N-CA-CB	5.42	118.68	111.64
1	A	246	VAL	N-CA-CB	-5.42	103.18	110.54
1	A	245	GLN	O-C-N	5.41	127.93	122.09
1	A	241	TRP	CA-CB-CG	5.41	123.87	113.60
1	A	255	THR	CA-C-O	5.40	126.76	120.49
1	A	162	SER	O-C-N	5.40	129.06	122.96
1	A	246	VAL	CA-C-N	5.40	127.78	120.65
1	A	246	VAL	C-N-CA	5.40	127.78	120.65
1	A	245	GLN	CG-CD-NE2	-5.38	108.33	116.40
1	A	171	TYR	CA-CB-CG	5.37	123.57	113.90
1	A	72	VAL	CA-C-O	5.34	126.96	121.41
1	A	37	SER	O-C-N	5.33	129.58	122.43
1	A	138	ALA	CA-C-N	5.30	127.24	120.56
1	A	138	ALA	C-N-CA	5.30	127.24	120.56
1	A	247	ARG	O-C-N	5.28	127.52	122.03
1	A	61	ASN	CB-CA-C	5.28	119.85	109.72
1	A	43	LYS	CB-CA-C	5.25	118.54	110.14
1	A	50	PHE	CA-C-O	5.25	125.67	119.48
1	A	120	ASP	CA-C-O	5.19	125.91	119.79
1	A	34	GLY	O-C-N	-5.18	116.31	122.68
1	A	71	THR	CA-C-O	-5.18	115.36	120.70
1	A	271	GLU	O-C-N	5.17	127.40	122.07
1	A	216	ALA	O-C-N	-5.15	117.18	123.10
1	A	206	TRP	CB-CA-C	5.12	118.20	109.80
1	A	104	TYR	CA-C-N	5.11	127.12	120.28
1	A	104	TYR	C-N-CA	5.11	127.12	120.28
1	A	59	GLN	O-C-N	5.09	129.17	123.27
1	A	136	LYS	CG-CD-CE	-5.08	99.61	111.30
1	A	217	LYS	O-C-N	5.07	129.16	123.27
1	A	55	THR	CA-CB-CG2	5.06	119.10	110.50
1	A	42	LEU	N-CA-C	5.06	118.06	109.76
1	A	44	VAL	CB-CA-C	5.05	118.36	110.83
1	A	234	ILE	CA-C-O	-5.05	115.82	121.17
1	A	13	ALA	N-CA-C	5.04	119.81	113.25
1	A	111	ILE	N-CA-C	-5.04	105.63	110.72
1	A	140	ASP	CB-CG-OD1	5.03	129.97	118.40
1	A	165	VAL	CA-CB-CG2	5.01	118.92	110.40
1	A	68	VAL	CA-C-N	5.00	127.23	120.38
1	A	68	VAL	C-N-CA	5.00	127.23	120.38

There are no chirality outliers.

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	1858	0	1817	35	0
2	A	4	0	6	0	0
3	A	155	0	0	8	0
All	All	2017	0	1823	35	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 10.

All (35) 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:221:CSO:SG	1:A:222:MET:HE2	2.16	0.86
1:A:73:LEU:HD13	1:A:90:LEU:HD22	1.61	0.81
1:A:104:TYR:HD2	3:A:2068:HOH:O	1.71	0.72
1:A:206:TRP:CD1	1:A:216:ALA:HB2	2.29	0.67
1:A:73:LEU:HD22	3:A:2026:HOH:O	2.00	0.61
1:A:240:ASN:HB3	3:A:2132:HOH:O	2.02	0.58
1:A:23:GLY:HA2	1:A:236:SER:HB3	1.86	0.58
1:A:108:ILE:HD11	3:A:2068:HOH:O	2.03	0.58
1:A:240:ASN:HA	3:A:2131:HOH:O	2.04	0.56
1:A:31:ILE:HD12	1:A:122:ILE:HG23	1.87	0.56
1:A:115:ILE:HG12	1:A:142:ALA:HA	1.90	0.52
1:A:31:ILE:HD12	1:A:122:ILE:CG2	2.41	0.50
1:A:205:ILE:O	1:A:216:ALA:HA	2.11	0.50
1:A:73:LEU:CD1	1:A:90:LEU:HD22	2.38	0.50
1:A:122:ILE:HD12	1:A:147:VAL:HG11	1.94	0.50
1:A:158:THR:HG22	1:A:262:TYR:HE1	1.77	0.49
1:A:34:GLY:O	1:A:65:GLY:HA3	2.13	0.48
1:A:11:ILE:O	1:A:270:VAL:HG12	2.14	0.48
1:A:175:ILE:HG12	1:A:247:ARG:HG3	1.95	0.47
1:A:104:TYR:HB3	3:A:2068:HOH:O	2.16	0.45
1:A:207:SER:O	1:A:214:TYR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LYS:HE3	1:A:195:GLU:OE1	2.18	0.44
1:A:170:LYS:HG2	1:A:195:GLU:HG2	2.00	0.44
1:A:73:LEU:HD11	1:A:88:ALA:O	2.18	0.43
1:A:6:TYR:CE1	1:A:182:SER:HB2	2.53	0.43
1:A:180:VAL:HG21	1:A:267:LEU:HD13	2.01	0.43
1:A:119:MET:O	1:A:147:VAL:HG22	2.18	0.43
1:A:195:GLU:HB3	3:A:2095:HOH:O	2.19	0.42
1:A:249:SER:OG	1:A:275:GLN:NE2	2.53	0.42
1:A:127:GLY:HA2	1:A:167:TYR:O	2.21	0.41
1:A:143:VAL:HG21	1:A:173:SER:HB2	2.02	0.41
1:A:73:LEU:HD21	3:A:2040:HOH:O	2.21	0.41
1:A:172:PRO:O	1:A:247:ARG:NH1	2.47	0.41
1:A:47:GLY:HA3	1:A:92:ALA:O	2.21	0.40
1:A:35:ILE:O	1:A:58:PHE:HA	2.21	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	16/263 (6%)	15 (94%)	1 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	194/194 (100%)	189 (97%)	5 (3%)	40	28

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	73	LEU
1	A	195	GLU
1	A	204	SER
1	A	222	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	123	ASN
1	A	252	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	CSO	A	221	1	3,6,7	0.95	0	1,6,8	1.76	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	CSO	A	221	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	221	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	221	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	ACN	A	298	-	3,3,3	0.80	0	3,3,3	1.32	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	262/263 (99%)	-0.68	1 (0%) 88 89	4, 8, 17, 24	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	ASN	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSO	A	221	7/8	0.91	0.06	4,5,11,13	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACN	A	298	4/4	0.95	0.08	16,17,17,17	1

6.5 Other polymers [i](#)

There are no such residues in this entry.