



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:47 AM UTC

PDB ID : 1SBC / pdb_00001sbc
Title : THE REFINED CRYSTAL STRUCTURE OF SUBTILISIN CARLSBERG
AT 2.5 ANGSTROMS RESOLUTION
Authors : Neidhart, D.J.; Petsko, G.A.
Deposited on : 1988-05-13
Resolution : 2.50 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
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

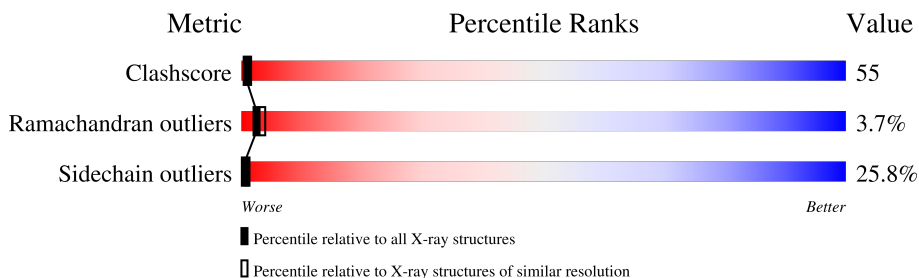
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	274	24% 41% 24% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1921 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 CARLSBERG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			1920	1190	332	393	5			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	SER	THR	conflict	UNP P00780
A	129	ALA	PRO	conflict	UNP P00780
A	158	ASN	SER	conflict	UNP P00780
A	161	SER	ASN	conflict	UNP P00780
A	212	ASN	SER	conflict	UNP P00780

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

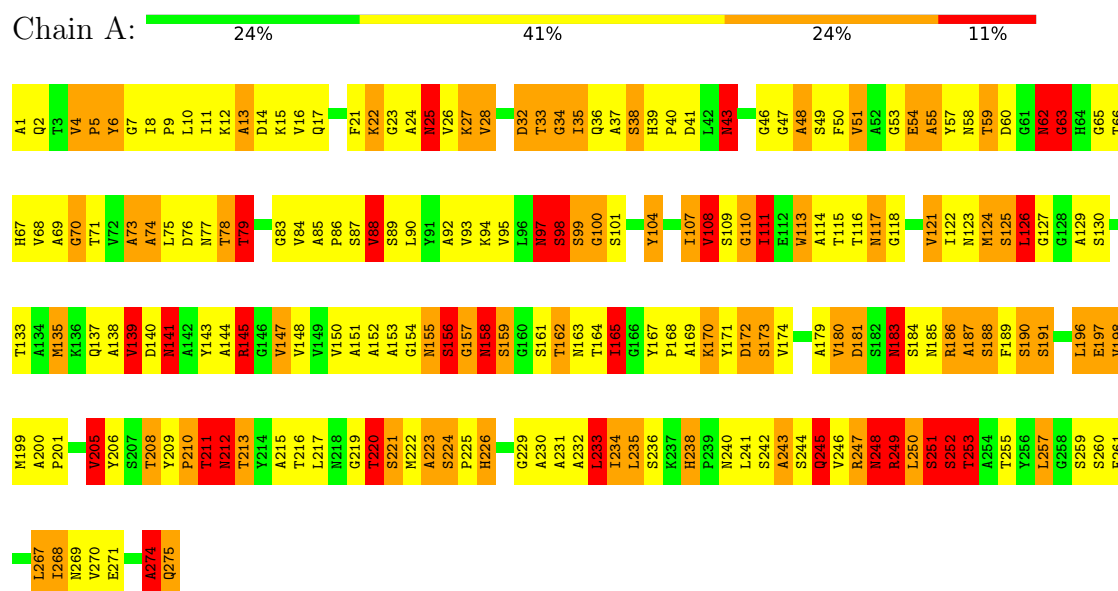
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

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 CARLSBERG



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	76.67Å 55.65Å 53.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.206 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1921	wwPDB-VP
Average B, all atoms (Å ²)	9.0	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: CA

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	1.11	1/1952 (0.1%)	2.77	186/2662 (7.0%)

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
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	GLY	N-CA	5.18	1.52	1.45

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ASN	CA-CB-CG	23.82	136.42	112.60
1	A	76	ASP	CA-CB-CG	14.76	127.36	112.60
1	A	247	ARG	CD-NE-CZ	14.09	144.13	124.40
1	A	97	ASN	CA-CB-CG	13.76	126.36	112.60
1	A	139	VAL	N-CA-C	-12.16	100.14	111.45
1	A	139	VAL	CB-CA-C	11.93	127.55	111.92
1	A	248	ASN	CA-CB-CG	11.41	124.01	112.60
1	A	187	ALA	CA-C-N	10.27	134.45	120.38
1	A	187	ALA	C-N-CA	10.27	134.45	120.38
1	A	248	ASN	OD1-CG-ND2	-10.20	112.40	122.60
1	A	173	SER	N-CA-C	-9.80	101.33	113.28
1	A	77	ASN	CA-CB-CG	9.76	122.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	PHE	CA-C-O	9.69	130.67	120.30
1	A	245	GLN	OE1-CD-NE2	-9.36	113.24	122.60
1	A	223	ALA	CA-C-N	9.08	132.57	120.58
1	A	223	ALA	C-N-CA	9.08	132.57	120.58
1	A	250	LEU	N-CA-C	-9.01	100.40	111.40
1	A	156	SER	N-CA-C	-8.90	98.53	110.55
1	A	43	ASN	CA-CB-CG	-8.73	103.87	112.60
1	A	163	ASN	OD1-CG-ND2	-8.68	113.92	122.60
1	A	181	ASP	CA-CB-CG	8.57	121.17	112.60
1	A	90	LEU	N-CA-C	8.56	122.20	108.41
1	A	25	ASN	OD1-CG-ND2	8.54	131.14	122.60
1	A	109	SER	CA-C-N	8.53	129.44	119.98
1	A	109	SER	C-N-CA	8.53	129.44	119.98
1	A	60	ASP	CA-CB-CG	8.45	121.05	112.60
1	A	275	GLN	N-CA-CB	8.38	124.74	110.50
1	A	25	ASN	CA-CB-CG	-8.32	104.28	112.60
1	A	165	ILE	N-CA-CB	8.28	119.56	110.53
1	A	55	ALA	N-CA-C	8.23	121.36	111.82
1	A	213	THR	CA-CB-OG1	-8.11	97.43	109.60
1	A	162	THR	O-C-N	8.06	131.97	122.94
1	A	141	ASN	OD1-CG-ND2	8.05	130.65	122.60
1	A	68	VAL	CA-C-N	8.03	131.04	120.28
1	A	68	VAL	C-N-CA	8.03	131.04	120.28
1	A	153	ALA	N-CA-C	7.86	119.84	111.28
1	A	70	GLY	O-C-N	7.79	130.77	122.28
1	A	113	TRP	CB-CA-C	7.78	123.09	110.88
1	A	4	VAL	CA-C-O	7.73	126.14	120.88
1	A	71	THR	N-CA-C	-7.68	102.91	111.82
1	A	252	SER	CA-C-O	-7.68	109.53	120.51
1	A	39	HIS	CA-CB-CG	-7.51	106.29	113.80
1	A	226	HIS	CA-CB-CG	7.47	121.27	113.80
1	A	157	GLY	N-CA-C	-7.44	95.54	113.18
1	A	205	VAL	CA-C-N	7.44	132.68	122.19
1	A	205	VAL	C-N-CA	7.44	132.68	122.19
1	A	39	HIS	O-C-N	7.42	128.08	121.18
1	A	249	ARG	NE-CZ-NH1	7.36	128.86	121.50
1	A	73	ALA	CA-C-O	-7.31	111.30	119.78
1	A	268	ILE	CA-C-N	7.30	133.22	122.86
1	A	268	ILE	C-N-CA	7.30	133.22	122.86
1	A	34	GLY	CA-C-O	-7.29	114.94	122.01
1	A	205	VAL	N-CA-CB	7.26	121.08	111.64
1	A	87	SER	CA-C-N	7.25	130.49	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	SER	C-N-CA	7.25	130.49	120.49
1	A	274	ALA	CA-C-N	7.23	134.71	121.70
1	A	274	ALA	C-N-CA	7.23	134.71	121.70
1	A	162	THR	CA-C-O	-7.22	113.20	121.72
1	A	77	ASN	OD1-CG-ND2	-7.16	115.44	122.60
1	A	190	SER	CA-CB-OG	-7.16	96.78	111.10
1	A	97	ASN	N-CA-C	-7.14	98.41	109.76
1	A	2	GLN	OE1-CD-NE2	-7.12	115.48	122.60
1	A	238	HIS	O-C-N	7.12	127.78	121.37
1	A	144	ALA	N-CA-C	-7.11	103.57	111.82
1	A	210	PRO	CA-C-N	7.00	134.92	121.54
1	A	210	PRO	C-N-CA	7.00	134.92	121.54
1	A	156	SER	CA-C-O	-6.97	113.58	121.81
1	A	186	ARG	CD-NE-CZ	6.96	134.14	124.40
1	A	100	GLY	N-CA-C	6.94	124.24	115.21
1	A	196	LEU	CB-CA-C	6.93	120.23	109.84
1	A	224	SER	CA-C-N	6.92	126.53	119.19
1	A	224	SER	C-N-CA	6.92	126.53	119.19
1	A	53	GLY	CA-C-N	6.87	131.55	122.42
1	A	53	GLY	C-N-CA	6.87	131.55	122.42
1	A	216	THR	CA-CB-OG1	-6.83	99.35	109.60
1	A	253	THR	CA-C-N	6.83	134.77	121.66
1	A	253	THR	C-N-CA	6.83	134.77	121.66
1	A	107	ILE	O-C-N	6.82	129.00	121.90
1	A	70	GLY	CA-C-O	-6.82	112.80	120.30
1	A	79	THR	N-CA-CB	-6.82	100.96	111.46
1	A	161	SER	CB-CA-C	6.81	122.02	110.85
1	A	4	VAL	CB-CA-C	6.80	117.54	111.08
1	A	125	SER	N-CA-CB	6.78	118.15	110.35
1	A	245	GLN	CA-C-N	6.78	130.05	120.42
1	A	245	GLN	C-N-CA	6.78	130.05	120.42
1	A	226	HIS	N-CA-C	-6.73	103.87	111.07
1	A	83	GLY	CA-C-N	6.71	129.15	120.56
1	A	83	GLY	C-N-CA	6.71	129.15	120.56
1	A	54	GLU	CB-CA-C	-6.68	99.79	110.81
1	A	47	GLY	CA-C-O	6.68	128.84	121.02
1	A	139	VAL	CA-C-N	6.66	129.75	120.29
1	A	139	VAL	C-N-CA	6.66	129.75	120.29
1	A	205	VAL	CA-C-O	6.64	127.30	120.39
1	A	158	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	A	253	THR	N-CA-CB	6.51	121.50	110.49
1	A	253	THR	CA-CB-CG2	6.49	121.54	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ASN	OD1-CG-ND2	-6.42	116.18	122.60
1	A	269	ASN	CA-C-N	6.41	129.52	120.42
1	A	269	ASN	C-N-CA	6.41	129.52	120.42
1	A	155	ASN	CB-CA-C	6.40	121.44	111.13
1	A	121	VAL	CA-C-O	6.35	127.69	120.90
1	A	104	TYR	CA-C-O	-6.34	114.11	120.90
1	A	260	SER	CA-CB-OG	6.28	123.67	111.10
1	A	212	ASN	CA-C-O	6.24	129.44	120.51
1	A	77	ASN	CA-C-N	6.20	132.22	122.49
1	A	77	ASN	C-N-CA	6.20	132.22	122.49
1	A	63	GLY	CA-C-N	6.17	129.02	120.63
1	A	63	GLY	C-N-CA	6.17	129.02	120.63
1	A	172	ASP	CB-CA-C	6.13	122.62	110.42
1	A	73	ALA	N-CA-C	6.13	120.64	112.30
1	A	75	LEU	CA-C-N	6.13	131.84	122.77
1	A	75	LEU	C-N-CA	6.13	131.84	122.77
1	A	145	ARG	CD-NE-CZ	6.13	132.98	124.40
1	A	148	VAL	N-CA-CB	6.11	118.36	111.21
1	A	249	ARG	NE-CZ-NH2	-6.07	113.74	119.20
1	A	247	ARG	CA-C-N	6.06	128.68	120.38
1	A	247	ARG	C-N-CA	6.06	128.68	120.38
1	A	39	HIS	ND1-CG-CD2	6.04	112.14	106.10
1	A	10	LEU	CA-C-O	-6.02	114.46	120.90
1	A	122	ILE	O-C-N	6.00	129.42	123.18
1	A	59	THR	CA-C-O	-5.98	113.78	120.66
1	A	261	PHE	O-C-N	5.98	128.31	122.09
1	A	210	PRO	CA-C-O	5.97	131.47	120.60
1	A	125	SER	N-CA-C	-5.96	103.14	110.65
1	A	211	THR	CA-CB-OG1	-5.95	100.67	109.60
1	A	257	LEU	CA-C-N	5.91	129.51	121.83
1	A	257	LEU	C-N-CA	5.91	129.51	121.83
1	A	110	GLY	CA-C-N	5.87	127.95	120.56
1	A	110	GLY	C-N-CA	5.87	127.95	120.56
1	A	220	THR	N-CA-C	-5.82	105.07	111.82
1	A	74	ALA	CB-CA-C	5.81	118.14	110.06
1	A	71	THR	O-C-N	5.79	129.40	122.27
1	A	108	VAL	CB-CA-C	5.75	119.90	112.14
1	A	213	THR	CA-CB-CG2	5.69	120.17	110.50
1	A	88	VAL	N-CA-C	5.67	117.62	109.51
1	A	17	GLN	N-CA-C	-5.67	105.01	111.07
1	A	78	THR	N-CA-CB	-5.56	102.02	111.20
1	A	248	ASN	CA-C-N	5.56	128.76	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ASN	C-N-CA	5.56	128.76	120.31
1	A	159	SER	N-CA-CB	5.52	119.83	110.49
1	A	168	PRO	CA-C-N	5.52	128.44	120.38
1	A	168	PRO	C-N-CA	5.52	128.44	120.38
1	A	126	LEU	O-C-N	5.51	130.11	122.78
1	A	140	ASP	CB-CA-C	-5.50	101.51	110.85
1	A	245	GLN	N-CA-C	-5.50	105.19	111.07
1	A	69	ALA	CA-C-N	5.48	127.18	120.22
1	A	69	ALA	C-N-CA	5.48	127.18	120.22
1	A	250	LEU	CB-CA-C	5.47	119.98	110.79
1	A	5	PRO	CB-CA-C	5.47	120.59	111.56
1	A	252	SER	O-C-N	5.47	129.87	122.59
1	A	35	ILE	CA-C-O	-5.43	114.51	120.43
1	A	188	SER	N-CA-C	5.42	117.89	111.33
1	A	267	LEU	CA-C-O	5.42	126.87	120.69
1	A	187	ALA	CB-CA-C	5.39	118.67	109.72
1	A	21	PHE	CB-CA-C	5.36	119.05	110.16
1	A	208	THR	CA-C-N	5.29	131.85	122.48
1	A	208	THR	C-N-CA	5.29	131.85	122.48
1	A	43	ASN	CA-C-N	5.28	129.19	122.37
1	A	43	ASN	C-N-CA	5.28	129.19	122.37
1	A	162	THR	N-CA-C	-5.28	102.70	110.52
1	A	129	ALA	CB-CA-C	5.28	119.85	109.72
1	A	133	THR	CA-C-N	5.27	127.35	120.28
1	A	133	THR	C-N-CA	5.27	127.35	120.28
1	A	233	LEU	O-C-N	5.27	127.72	122.08
1	A	163	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	111	ILE	N-CA-C	-5.23	105.40	110.42
1	A	62	ASN	N-CA-CB	-5.22	101.66	110.49
1	A	38	SER	CA-C-N	5.22	129.62	121.17
1	A	38	SER	C-N-CA	5.22	129.62	121.17
1	A	87	SER	CA-C-O	5.18	124.59	118.90
1	A	117	ASN	CA-C-N	5.17	127.92	120.11
1	A	117	ASN	C-N-CA	5.17	127.92	120.11
1	A	98	SER	N-CA-C	5.14	121.75	110.80
1	A	59	THR	O-C-N	5.13	129.53	123.27
1	A	161	SER	CA-C-O	5.12	125.72	119.78
1	A	183	ASN	N-CA-C	-5.12	106.88	112.72
1	A	74	ALA	N-CA-C	-5.10	102.65	110.30
1	A	99	SER	N-CA-CB	5.10	118.31	110.46
1	A	147	VAL	N-CA-C	-5.08	102.39	109.45
1	A	51	VAL	N-CA-C	-5.08	101.10	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	VAL	CA-C-N	5.07	129.39	122.90
1	A	147	VAL	C-N-CA	5.07	129.39	122.90
1	A	13	ALA	CA-C-O	5.06	125.79	120.42
1	A	48	ALA	O-C-N	5.06	128.47	123.46
1	A	17	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	A	123	ASN	OD1-CG-ND2	-5.05	117.55	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	ARG	Sidechain

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	1920	0	1881	209	0
2	A	1	0	0	0	0
All	All	1921	0	1881	209	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 55.

All (209) 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:159:SER:O	1:A:162:THR:HG22	1.47	1.10
1:A:152:ALA:HB1	1:A:220:THR:HG23	1.35	1.08
1:A:183:ASN:HD22	1:A:183:ASN:N	1.51	1.07
1:A:238:HIS:HE1	1:A:275:GLN:HB2	1.31	0.96
1:A:36:GLN:NE2	1:A:211:THR:H	1.64	0.96
1:A:238:HIS:CE1	1:A:275:GLN:HB2	2.04	0.93
1:A:55:ALA:O	1:A:57:TYR:HB3	1.65	0.93
1:A:241:LEU:HA	1:A:245:GLN:NE2	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLY:HA2	1:A:210:PRO:HG3	1.53	0.89
1:A:183:ASN:H	1:A:183:ASN:ND2	1.71	0.87
1:A:183:ASN:N	1:A:183:ASN:ND2	2.15	0.87
1:A:8:ILE:HG13	1:A:9:PRO:HD3	1.58	0.84
1:A:183:ASN:HD22	1:A:183:ASN:H	0.88	0.84
1:A:159:SER:HB3	1:A:164:THR:HG22	1.58	0.84
1:A:205:VAL:HG13	1:A:222:MET:HG2	1.60	0.82
1:A:8:ILE:CD1	1:A:14:ASP:HB3	2.09	0.82
1:A:249:ARG:NH2	1:A:253:THR:HG22	1.95	0.81
1:A:16:VAL:HG21	1:A:270:VAL:HG12	1.62	0.81
1:A:51:VAL:HG11	1:A:54:GLU:HG3	1.64	0.80
1:A:137:GLN:O	1:A:141:ASN:HB2	1.81	0.79
1:A:251:SER:OG	1:A:252:SER:N	2.13	0.79
1:A:167:TYR:CZ	1:A:170:LYS:HD2	2.18	0.79
1:A:217:LEU:HD23	1:A:222:MET:HE1	1.64	0.79
1:A:8:ILE:HD12	1:A:14:ASP:HB3	1.63	0.78
1:A:33:THR:O	1:A:94:LYS:HE2	1.84	0.76
1:A:156:SER:O	1:A:189:PHE:O	2.04	0.76
1:A:57:TYR:HE1	1:A:92:ALA:HB3	1.52	0.75
1:A:255:THR:O	1:A:257:LEU:HD12	1.86	0.74
1:A:57:TYR:O	1:A:58:ASN:HB2	1.86	0.74
1:A:271:GLU:O	1:A:274:ALA:HB3	1.88	0.74
1:A:115:THR:HG22	1:A:145:ARG:HE	1.55	0.72
1:A:115:THR:O	1:A:145:ARG:NH2	2.20	0.71
1:A:113:TRP:O	1:A:117:ASN:ND2	2.20	0.71
1:A:51:VAL:CG1	1:A:54:GLU:HG3	2.20	0.71
1:A:241:LEU:HD22	1:A:245:GLN:HE21	1.56	0.69
1:A:35:ILE:HD12	1:A:92:ALA:HB2	1.74	0.69
1:A:180:VAL:HG13	1:A:199:MET:HB3	1.75	0.69
1:A:49:SER:HB2	1:A:57:TYR:HB2	1.75	0.68
1:A:242:SER:O	1:A:246:VAL:HG23	1.93	0.68
1:A:127:GLY:HA2	1:A:167:TYR:O	1.93	0.68
1:A:27:LYS:NZ	1:A:118:GLY:O	2.27	0.68
1:A:22:LYS:HZ3	1:A:86:PRO:HG2	1.59	0.67
1:A:8:ILE:N	1:A:9:PRO:HD2	2.10	0.67
1:A:252:SER:O	1:A:253:THR:HG22	1.95	0.66
1:A:63:GLY:CA	1:A:210:PRO:HG3	2.24	0.66
1:A:205:VAL:HG11	1:A:222:MET:HB3	1.77	0.66
1:A:165:ILE:HD11	1:A:169:ALA:C	2.20	0.66
1:A:217:LEU:HD23	1:A:222:MET:CE	2.25	0.65
1:A:249:ARG:CZ	1:A:253:THR:HG21	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LYS:HD3	1:A:271:GLU:OE1	1.97	0.64
1:A:270:VAL:O	1:A:274:ALA:HB2	1.97	0.64
1:A:183:ASN:HB2	1:A:185:ASN:OD1	1.97	0.64
1:A:231:ALA:O	1:A:235:LEU:HB2	1.98	0.64
1:A:165:ILE:O	1:A:170:LYS:NZ	2.31	0.64
1:A:63:GLY:HA2	1:A:210:PRO:CG	2.27	0.64
1:A:111:ILE:CG2	1:A:138:ALA:HB1	2.28	0.64
1:A:249:ARG:HA	1:A:249:ARG:NE	2.10	0.64
1:A:241:LEU:HD22	1:A:245:GLN:NE2	2.13	0.63
1:A:249:ARG:O	1:A:253:THR:HG23	1.98	0.63
1:A:179:ALA:HA	1:A:200:ALA:O	1.99	0.63
1:A:165:ILE:HD12	1:A:169:ALA:HB3	1.79	0.62
1:A:34:GLY:O	1:A:65:GLY:HA3	1.98	0.62
1:A:51:VAL:HG13	1:A:97:ASN:OD1	1.98	0.62
1:A:36:GLN:HE21	1:A:211:THR:H	1.47	0.62
1:A:51:VAL:HG12	1:A:54:GLU:CG	2.30	0.62
1:A:249:ARG:CZ	1:A:253:THR:CG2	2.78	0.61
1:A:55:ALA:O	1:A:57:TYR:CB	2.45	0.61
1:A:8:ILE:N	1:A:9:PRO:CD	2.63	0.61
1:A:206:TYR:HA	1:A:215:ALA:O	2.01	0.61
1:A:249:ARG:NH2	1:A:253:THR:CG2	2.64	0.61
1:A:224:SER:N	1:A:225:PRO:HD2	2.16	0.60
1:A:158:ASN:N	1:A:158:ASN:ND2	2.48	0.60
1:A:57:TYR:CE1	1:A:92:ALA:HB3	2.36	0.60
1:A:165:ILE:HD11	1:A:170:LYS:N	2.16	0.59
1:A:36:GLN:HE22	1:A:212:ASN:H	1.49	0.59
1:A:249:ARG:HA	1:A:249:ARG:HE	1.66	0.59
1:A:241:LEU:HA	1:A:245:GLN:HE22	1.63	0.59
1:A:234:ILE:HG22	1:A:235:LEU:N	2.16	0.59
1:A:51:VAL:CG1	1:A:54:GLU:CG	2.81	0.59
1:A:197:GLU:HG3	1:A:247:ARG:HH11	1.67	0.58
1:A:230:ALA:HB1	1:A:270:VAL:HG22	1.83	0.58
1:A:180:VAL:HG23	1:A:181:ASP:O	2.04	0.58
1:A:198:VAL:O	1:A:199:MET:HE2	2.03	0.58
1:A:242:SER:H	1:A:245:GLN:HB2	1.69	0.57
1:A:11:ILE:HG21	1:A:268:ILE:HD11	1.87	0.57
1:A:238:HIS:CB	1:A:241:LEU:HG	2.34	0.57
1:A:124:MET:HG2	1:A:126:LEU:HD11	1.87	0.57
1:A:171:TYR:O	1:A:174:VAL:N	2.30	0.57
1:A:158:ASN:N	1:A:158:ASN:HD22	2.03	0.56
1:A:209:TYR:CG	1:A:210:PRO:HD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ALA:C	1:A:225:PRO:HD2	2.31	0.56
1:A:43:ASN:ND2	1:A:43:ASN:O	2.39	0.56
1:A:62:ASN:O	1:A:62:ASN:ND2	2.39	0.56
1:A:135:MET:O	1:A:139:VAL:HB	2.06	0.56
1:A:40:PRO:HD2	1:A:212:ASN:HB3	1.88	0.56
1:A:35:ILE:CD1	1:A:92:ALA:HB2	2.37	0.55
1:A:85:ALA:O	1:A:88:VAL:HB	2.06	0.55
1:A:51:VAL:HG13	1:A:97:ASN:CG	2.32	0.55
1:A:107:ILE:HG21	1:A:135:MET:HE2	1.88	0.55
1:A:57:TYR:H	1:A:94:LYS:HZ2	1.55	0.54
1:A:143:TYR:HD1	1:A:147:VAL:O	1.91	0.54
1:A:189:PHE:CE1	1:A:219:GLY:HA2	2.42	0.54
1:A:84:VAL:CG1	1:A:229:GLY:HA3	2.37	0.54
1:A:238:HIS:HB3	1:A:241:LEU:HG	1.87	0.54
1:A:6:TYR:CD1	1:A:6:TYR:C	2.86	0.54
1:A:184:SER:O	1:A:257:LEU:HD23	2.07	0.54
1:A:234:ILE:HG21	1:A:246:VAL:HG13	1.90	0.54
1:A:171:TYR:O	1:A:173:SER:N	2.40	0.54
1:A:180:VAL:HG23	1:A:181:ASP:N	2.22	0.54
1:A:36:GLN:NE2	1:A:211:THR:N	2.46	0.54
1:A:37:ALA:CB	1:A:58:ASN:OD1	2.56	0.53
1:A:155:ASN:OD1	1:A:220:THR:HB	2.08	0.53
1:A:243:ALA:O	1:A:246:VAL:N	2.41	0.53
1:A:28:VAL:HG13	1:A:121:VAL:HB	1.89	0.53
1:A:26:VAL:O	1:A:88:VAL:HG22	2.08	0.53
1:A:171:TYR:C	1:A:173:SER:H	2.16	0.53
1:A:16:VAL:CG2	1:A:270:VAL:HG12	2.35	0.52
1:A:270:VAL:O	1:A:274:ALA:N	2.41	0.52
1:A:222:MET:C	1:A:225:PRO:HD2	2.35	0.52
1:A:37:ALA:HB2	1:A:58:ASN:OD1	2.09	0.52
1:A:98:SER:C	1:A:100:GLY:H	2.16	0.52
1:A:186:ARG:HG2	1:A:187:ALA:O	2.10	0.52
1:A:93:VAL:HG12	1:A:95:VAL:HG13	1.91	0.52
1:A:49:SER:HB2	1:A:57:TYR:CB	2.40	0.51
1:A:104:TYR:O	1:A:108:VAL:HG13	2.09	0.51
1:A:158:ASN:C	1:A:164:THR:HG21	2.36	0.51
1:A:159:SER:HB3	1:A:164:THR:CG2	2.35	0.51
1:A:73:ALA:O	1:A:74:ALA:C	2.52	0.51
1:A:111:ILE:HG21	1:A:138:ALA:HB1	1.92	0.51
1:A:40:PRO:CD	1:A:212:ASN:HB3	2.41	0.51
1:A:67:HIS:HA	1:A:208:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLN:HE21	1:A:210:PRO:HA	1.76	0.51
1:A:191:SER:O	1:A:196:LEU:HD22	2.10	0.51
1:A:111:ILE:HG22	1:A:138:ALA:HB1	1.93	0.50
1:A:78:THR:C	1:A:79:THR:HG22	2.35	0.50
1:A:154:GLY:H	1:A:220:THR:HG21	1.75	0.50
1:A:46:GLY:O	1:A:57:TYR:OH	2.28	0.50
1:A:51:VAL:HG11	1:A:97:ASN:HA	1.94	0.50
1:A:238:HIS:NE2	1:A:275:GLN:OE1	2.44	0.50
1:A:46:GLY:C	1:A:57:TYR:OH	2.54	0.50
1:A:242:SER:H	1:A:245:GLN:CB	2.25	0.50
1:A:11:ILE:HD12	1:A:270:VAL:HG21	1.94	0.49
1:A:23:GLY:HA2	1:A:236:SER:HB3	1.92	0.49
1:A:57:TYR:CD1	1:A:58:ASN:N	2.80	0.49
1:A:115:THR:CG2	1:A:145:ARG:HD3	2.42	0.49
1:A:187:ALA:O	1:A:190:SER:OG	2.21	0.49
1:A:16:VAL:HG21	1:A:270:VAL:CG1	2.36	0.49
1:A:5:PRO:C	1:A:7:GLY:H	2.21	0.49
1:A:26:VAL:O	1:A:89:SER:N	2.39	0.49
1:A:157:GLY:C	1:A:158:ASN:HD22	2.21	0.49
1:A:111:ILE:HG21	1:A:138:ALA:CB	2.43	0.48
1:A:248:ASN:C	1:A:248:ASN:HD22	2.21	0.48
1:A:125:SER:HB3	1:A:221:SER:OG	2.12	0.48
1:A:51:VAL:HG12	1:A:54:GLU:HG2	1.95	0.48
1:A:4:VAL:O	1:A:5:PRO:C	2.55	0.48
1:A:59:THR:O	1:A:94:LYS:NZ	2.47	0.48
1:A:70:GLY:O	1:A:74:ALA:HB2	2.13	0.48
1:A:124:MET:HG2	1:A:126:LEU:HD21	1.96	0.48
1:A:36:GLN:HE22	1:A:211:THR:H	1.54	0.47
1:A:13:ALA:HA	1:A:270:VAL:HG11	1.97	0.47
1:A:171:TYR:C	1:A:173:SER:N	2.73	0.47
1:A:165:ILE:HD12	1:A:169:ALA:CB	2.43	0.47
1:A:5:PRO:C	1:A:7:GLY:N	2.72	0.46
1:A:36:GLN:OE1	1:A:38:SER:OG	2.33	0.46
1:A:32:ASP:OD2	1:A:33:THR:HG23	2.16	0.46
1:A:115:THR:HG22	1:A:145:ARG:NE	2.27	0.46
1:A:12:LYS:HG2	1:A:15:LYS:HD2	1.98	0.45
1:A:48:ALA:O	1:A:93:VAL:HA	2.16	0.45
1:A:66:THR:O	1:A:208:THR:OG1	2.34	0.45
1:A:198:VAL:C	1:A:199:MET:HE2	2.41	0.45
1:A:241:LEU:CD2	1:A:245:GLN:NE2	2.79	0.45
1:A:257:LEU:CD1	1:A:267:LEU:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:HD13	1:A:14:ASP:HB3	1.95	0.45
1:A:24:ALA:O	1:A:25:ASN:HB2	2.16	0.45
1:A:124:MET:O	1:A:151:ALA:HA	2.16	0.45
1:A:84:VAL:HG11	1:A:229:GLY:HA3	1.98	0.45
1:A:209:TYR:CD1	1:A:210:PRO:HD2	2.52	0.45
1:A:111:ILE:O	1:A:114:ALA:HB3	2.17	0.45
1:A:26:VAL:HG11	1:A:232:ALA:HA	2.00	0.44
1:A:141:ASN:HD22	1:A:141:ASN:HA	1.54	0.44
1:A:113:TRP:CE3	1:A:113:TRP:C	2.96	0.44
1:A:230:ALA:CB	1:A:270:VAL:HG22	2.46	0.44
1:A:43:ASN:ND2	1:A:43:ASN:C	2.74	0.43
1:A:242:SER:O	1:A:243:ALA:C	2.60	0.43
1:A:5:PRO:O	1:A:7:GLY:N	2.52	0.43
1:A:57:TYR:O	1:A:58:ASN:CB	2.59	0.43
1:A:247:ARG:O	1:A:251:SER:HB3	2.18	0.43
1:A:201:PRO:O	1:A:226:HIS:CE1	2.72	0.43
1:A:115:THR:CG2	1:A:145:ARG:HE	2.30	0.43
1:A:124:MET:HG2	1:A:126:LEU:CG	2.48	0.43
1:A:240:ASN:OD1	1:A:241:LEU:HD23	2.19	0.43
1:A:224:SER:N	1:A:225:PRO:CD	2.81	0.42
1:A:62:ASN:OD1	1:A:98:SER:O	2.37	0.42
1:A:12:LYS:HG2	1:A:15:LYS:CD	2.50	0.42
1:A:23:GLY:O	1:A:24:ALA:C	2.61	0.42
1:A:197:GLU:O	1:A:198:VAL:HG12	2.20	0.42
1:A:255:THR:O	1:A:257:LEU:CD1	2.62	0.42
1:A:70:GLY:O	1:A:74:ALA:CB	2.68	0.42
1:A:50:PHE:CE1	1:A:110:GLY:HA2	2.55	0.41
1:A:124:MET:HB2	1:A:124:MET:HE3	1.79	0.41
1:A:11:ILE:HD12	1:A:270:VAL:CG2	2.50	0.41
1:A:184:SER:O	1:A:257:LEU:CD2	2.69	0.41
1:A:98:SER:C	1:A:100:GLY:N	2.77	0.41
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.71	0.41
1:A:197:GLU:C	1:A:198:VAL:CG1	2.94	0.40
1:A:84:VAL:C	1:A:86:PRO:HD3	2.46	0.40
1:A:242:SER:O	1:A:243:ALA:O	2.38	0.40
1:A:1:ALA:HB1	1:A:78:THR:O	2.20	0.40
1:A:197:GLU:O	1:A:198:VAL:CG1	2.69	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	272/274 (99%)	237 (87%)	25 (9%)	10 (4%)	2 3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLY
1	A	98	SER
1	A	251	SER
1	A	253	THR
1	A	211	THR
1	A	6	TYR
1	A	172	ASP
1	A	259	SER
1	A	243	ALA
1	A	274	ALA

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	198/198 (100%)	147 (74%)	51 (26%)	0 1

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS

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Mol	Chain	Res	Type
1	A	25	ASN
1	A	27	LYS
1	A	28	VAL
1	A	32	ASP
1	A	33	THR
1	A	41	ASP
1	A	43	ASN
1	A	62	ASN
1	A	79	THR
1	A	88	VAL
1	A	97	ASN
1	A	99	SER
1	A	101	SER
1	A	108	VAL
1	A	111	ILE
1	A	116	THR
1	A	124	MET
1	A	126	LEU
1	A	130	SER
1	A	135	MET
1	A	139	VAL
1	A	141	ASN
1	A	145	ARG
1	A	150	VAL
1	A	156	SER
1	A	158	ASN
1	A	165	ILE
1	A	170	LYS
1	A	180	VAL
1	A	183	ASN
1	A	188	SER
1	A	191	SER
1	A	197	GLU
1	A	198	VAL
1	A	205	VAL
1	A	212	ASN
1	A	213	THR
1	A	220	THR
1	A	221	SER
1	A	233	LEU
1	A	234	ILE
1	A	235	LEU

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Mol	Chain	Res	Type
1	A	244	SER
1	A	245	GLN
1	A	248	ASN
1	A	249	ARG
1	A	250	LEU
1	A	251	SER
1	A	252	SER
1	A	253	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	43	ASN
1	A	137	GLN
1	A	141	ASN
1	A	158	ASN
1	A	183	ASN
1	A	245	GLN
1	A	248	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

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.