



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 10:38 pm GMT

PDB ID : 1SBC  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

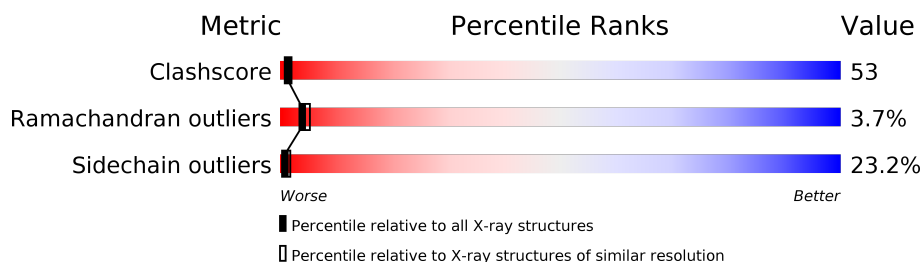
# 1 Overall quality at a glance

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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	274	

## 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 (three-letter code: CA) (formula: Ca).

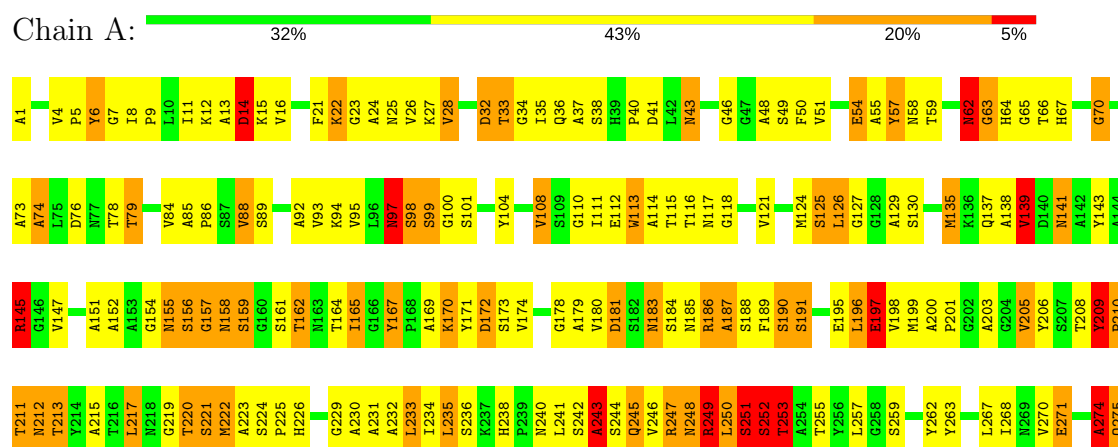
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

### 3 Residue-property plots

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

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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	9.0	wwPDB-VP

## 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: 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	0.90	4/1952 (0.2%)	2.00	58/2662 (2.2%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	GLU	CD-OE2	7.61	1.34	1.25
1	A	271	GLU	CD-OE2	6.69	1.33	1.25
1	A	112	GLU	CD-OE2	6.00	1.32	1.25
1	A	195	GLU	CD-OE2	5.75	1.31	1.25

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ARG	NE-CZ-NH1	17.13	128.86	120.30
1	A	247	ARG	CD-NE-CZ	14.66	144.13	123.60
1	A	249	ARG	NE-CZ-NH2	-13.12	113.74	120.30
1	A	145	ARG	NE-CZ-NH1	11.72	126.16	120.30
1	A	62	ASN	CA-CB-CG	10.47	136.42	113.40
1	A	139	VAL	CB-CA-C	8.50	127.55	111.40
1	A	235	LEU	CA-CB-CG	7.97	133.62	115.30
1	A	186	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	275	GLN	N-CA-CB	7.86	124.74	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ARG	CD-NE-CZ	7.53	134.14	123.60
1	A	167	TYR	CB-CG-CD2	-7.13	116.72	121.00
1	A	157	GLY	N-CA-C	-7.03	95.54	113.10
1	A	181	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	167	TYR	CB-CG-CD1	6.80	125.08	121.00
1	A	145	ARG	CD-NE-CZ	6.70	132.98	123.60
1	A	253	THR	CA-CB-CG2	6.53	121.54	112.40
1	A	129	ALA	CB-CA-C	6.50	119.85	110.10
1	A	263	TYR	CB-CG-CD2	6.44	124.86	121.00
1	A	113	TRP	CB-CA-C	6.35	123.09	110.40
1	A	76	ASP	CA-CB-CG	6.34	127.36	113.40
1	A	161	SER	CB-CA-C	6.27	122.02	110.10
1	A	243	ALA	CB-CA-C	6.25	119.47	110.10
1	A	159	SER	N-CA-CB	6.22	119.83	110.50
1	A	54	GLU	OE1-CD-OE2	6.14	130.67	123.30
1	A	172	ASP	CB-CA-C	6.11	122.62	110.40
1	A	253	THR	N-CA-CB	5.89	121.50	110.30
1	A	97	ASN	CA-CB-CG	5.89	126.36	113.40
1	A	181	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	A	217	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	162	THR	O-C-N	5.79	131.97	122.70
1	A	262	TYR	CB-CG-CD1	5.72	124.43	121.00
1	A	187	ALA	CB-CA-C	5.71	118.67	110.10
1	A	213	THR	CA-CB-CG2	5.55	120.17	112.40
1	A	155	ASN	CB-CA-C	5.52	121.44	110.40
1	A	213	THR	CA-CB-OG1	-5.51	97.43	109.00
1	A	197	GLU	CG-CD-OE2	-5.40	107.50	118.30
1	A	74	ALA	CB-CA-C	5.36	118.14	110.10
1	A	190	SER	CA-CB-OG	-5.34	96.78	111.20
1	A	209	TYR	N-CA-CB	5.33	120.20	110.60
1	A	54	GLU	CB-CA-C	-5.31	99.79	110.40
1	A	172	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	210	PRO	C-N-CA	5.29	134.92	121.70
1	A	196	LEU	CB-CA-C	5.28	120.23	110.20
1	A	195	GLU	CG-CD-OE2	-5.24	107.82	118.30
1	A	253	THR	C-N-CA	5.23	134.77	121.70
1	A	99	SER	N-CA-CB	5.21	118.31	110.50
1	A	274	ALA	C-N-CA	5.21	134.71	121.70
1	A	250	LEU	CB-CA-C	5.15	119.98	110.20
1	A	76	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	125	SER	N-CA-CB	5.10	118.15	110.50
1	A	187	ALA	C-N-CA	5.10	134.45	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ALA	N-CA-CB	5.07	117.20	110.10
1	A	262	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	70	GLY	O-C-N	5.05	130.77	122.70
1	A	14	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	252	SER	CA-C-O	-5.03	109.53	120.10
1	A	21	PHE	CA-C-O	5.03	130.67	120.10
1	A	145	ARG	NH1-CZ-NH2	-5.03	113.87	119.40

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	202	0
2	A	1	0	0	0	0
All	All	1921	0	1881	202	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 53.

All (202) 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:183:ASN:ND2	1:A:183:ASN:N	2.15	0.93
1:A:238:HIS:CE1	1:A:275:GLN:HB2	2.04	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:8:ILE:HG13	1:A:9:PRO:HD3	1.58	0.84
1:A:183:ASN:H	1:A:183:ASN:HD22	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: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:242:SER:O	1:A:246:VAL:HG23	1.93	0.68
1:A:49:SER:HB2	1:A:57:TYR:HB2	1.75	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:217:LEU:HD23	1:A:222:MET:CE	2.25	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:205:VAL:HG11	1:A:222:MET:HB3	1.77	0.66
1:A:63:GLY:CA	1:A:210:PRO:HG3	2.24	0.66
1:A:217:LEU:HD23	1:A:222:MET:HE1	1.77	0.66
1:A:249:ARG:CZ	1:A:253:THR:HG21	2.27	0.65
1:A:15:LYS:HD3	1:A:271:GLU:OE1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:111:ILE:CG2	1:A:138:ALA:HB1	2.28	0.64
1:A:63:GLY:HA2	1:A:210:PRO:CG	2.27	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:165:ILE:HD11	1:A:169:ALA:C	2.20	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: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:8:ILE:N	1:A:9:PRO:CD	2.63	0.61
1:A:224:SER:N	1:A:225:PRO:HD2	2.16	0.60
1:A:64:HIS:CE1	1:A:221:SER:HG	2.20	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: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:135:MET:O	1:A:139:VAL:HB	2.06	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: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: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:57:TYR:H	1:A:94:LYS:HZ2	1.55	0.54
1:A:238:HIS:HB3	1:A:241:LEU:HG	1.87	0.54
1:A:84:VAL:CG1	1:A:229:GLY:HA3	2.37	0.54
1:A:234:ILE:HG21	1:A:246:VAL:HG13	1.90	0.54
1:A:184:SER:O	1:A:257:LEU:HD23	2.07	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: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:37:ALA:HB2	1:A:58:ASN:OD1	2.09	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:223:ALA:C	1:A:225:PRO:HD2	2.31	0.51
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:159:SER:HB3	1:A:164:THR:CG2	2.35	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
1:A:191:SER:O	1:A:196:LEU:HD22	2.10	0.51
1:A:36:GLN:HE21	1:A:210:PRO:HA	1.76	0.51
1:A:111:ILE:HG22	1:A:138:ALA:HB1	1.93	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:238:HIS:NE2	1:A:275:GLN:OE1	2.44	0.50
1:A:51:VAL:HG11	1:A:97:ASN:HA	1.94	0.50
1:A:51:VAL:HG13	1:A:97:ASN:CG	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:SER:H	1:A:245:GLN:CB	2.25	0.50
1:A:23:GLY:HA2	1:A:236:SER:HB3	1.92	0.49
1:A:11:ILE:HD12	1:A:270:VAL:HG21	1.94	0.49
1:A:6:TYR:CD1	1:A:6:TYR:C	2.86	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:26:VAL:O	1:A:89:SER:N	2.39	0.49
1:A:111:ILE:HG21	1:A:138:ALA:CB	2.43	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:171:TYR:C	1:A:173:SER:H	2.16	0.48
1:A:59:THR:O	1:A:94:LYS:NZ	2.47	0.48
1:A:124:MET:HG2	1:A:126:LEU:HD21	1.96	0.48
1:A:70:GLY:O	1:A:74:ALA:HB2	2.13	0.48
1:A:98:SER:C	1:A:100:GLY:H	2.16	0.47
1:A:222:MET:C	1:A:225:PRO:HD2	2.35	0.47
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:165:ILE:HD12	1:A:169:ALA:CB	2.43	0.47
1:A:158:ASN:C	1:A:164:THR:HG21	2.36	0.46
1:A:73:ALA:O	1:A:74:ALA:C	2.52	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:78:THR:C	1:A:79:THR:HG22	2.35	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:46:GLY:C	1:A:57:TYR:OH	2.54	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
1:A:124:MET:O	1:A:151:ALA:HA	2.16	0.45
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:209:TYR:CD1	1:A:210:PRO:HD2	2.52	0.45
1:A:84:VAL:HG11	1:A:229:GLY:HA3	1.98	0.45
1:A:111:ILE:O	1:A:114:ALA:HB3	2.17	0.45
1:A:178:GLY:HA3	1:A:199:MET:HE1	1.99	0.44
1:A:26:VAL:HG11	1:A:232:ALA:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASN:HA	1:A:141:ASN:HD22	1.54	0.44
1:A:157:GLY:C	1:A:158:ASN:HD22	2.21	0.44
1:A:5:PRO:C	1:A:7:GLY:H	2.21	0.44
1:A:248:ASN:C	1:A:248:ASN:HD22	2.21	0.44
1:A:230:ALA:CB	1:A:270:VAL:HG22	2.46	0.44
1:A:4:VAL:O	1:A:5:PRO:C	2.55	0.43
1:A:57:TYR:O	1:A:58:ASN:CB	2.59	0.43
1:A:5:PRO:O	1:A:7:GLY:N	2.52	0.43
1:A:247:ARG:O	1:A:251:SER:HB3	2.18	0.43
1:A:22:LYS:NZ	1:A:86:PRO:HG2	2.33	0.43
1:A:201:PRO:O	1:A:226:HIS:CE1	2.72	0.43
1:A:124:MET:HG2	1:A:126:LEU:CG	2.48	0.43
1:A:115:THR:CG2	1:A:145:ARG:HE	2.30	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:171:TYR:C	1:A:173:SER:N	2.73	0.42
1:A:12:LYS:HG2	1:A:15:LYS:CD	2.50	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:5:PRO:C	1:A:7:GLY:N	2.72	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:43:ASN:ND2	1:A:43:ASN:C	2.74	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:233:LEU:HA	1:A:233:LEU:HD12	1.71	0.41
1:A:217:LEU:CD2	1:A:222:MET:HE2	2.50	0.41
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

### 5.3.1 Protein backbone

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%)	4	5

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 ⓘ

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%)	152 (77%)	46 (23%)	1	1

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	22	LYS
1	A	28	VAL
1	A	32	ASP
1	A	33	THR
1	A	41	ASP
1	A	43	ASN
1	A	57	TYR
1	A	62	ASN

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Mol	Chain	Res	Type
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	116	THR
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	156	SER
1	A	158	ASN
1	A	165	ILE
1	A	170	LYS
1	A	183	ASN
1	A	188	SER
1	A	191	SER
1	A	197	GLU
1	A	205	VAL
1	A	209	TYR
1	A	212	ASN
1	A	213	THR
1	A	220	THR
1	A	221	SER
1	A	222	MET
1	A	233	LEU
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

Some 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

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Mol	Chain	Res	Type
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 carbohydrates 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.