



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:04 AM UTC

PDB ID : 1SCB / pdb_00001scb
Title : ENZYME CRYSTAL STRUCTURE IN A NEAT ORGANIC SOLVENT
Authors : Fitzpatrick, P.A.; Steinmetz, A.C.U.; Ringe, D.; Klibanov, A.M.
Deposited on : 1993-07-13
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

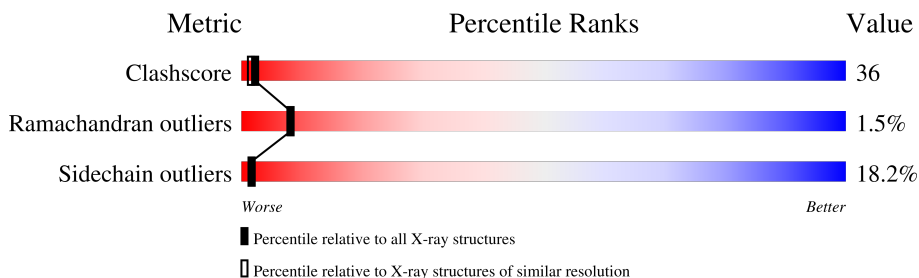
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	274	49% 33% 12% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CCN	A	404	-	-	X	-
3	CCN	A	406	-	-	X	-
3	CCN	A	408	-	-	X	-
3	CCN	A	409	-	-	X	-
3	CCN	A	413	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2056 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			

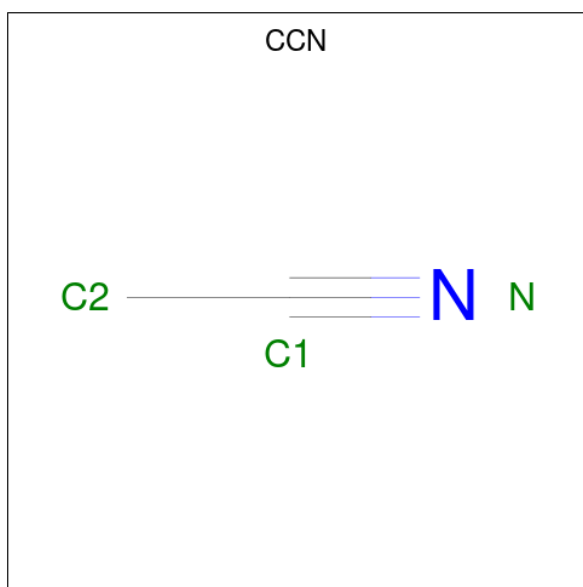
There are 5 discrepancies between the modelled and reference sequences:

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		

- Molecule 3 is ACETONITRILE (CCD ID: CCN) (formula: C₂H₃N).



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

- Molecule 4 is water.

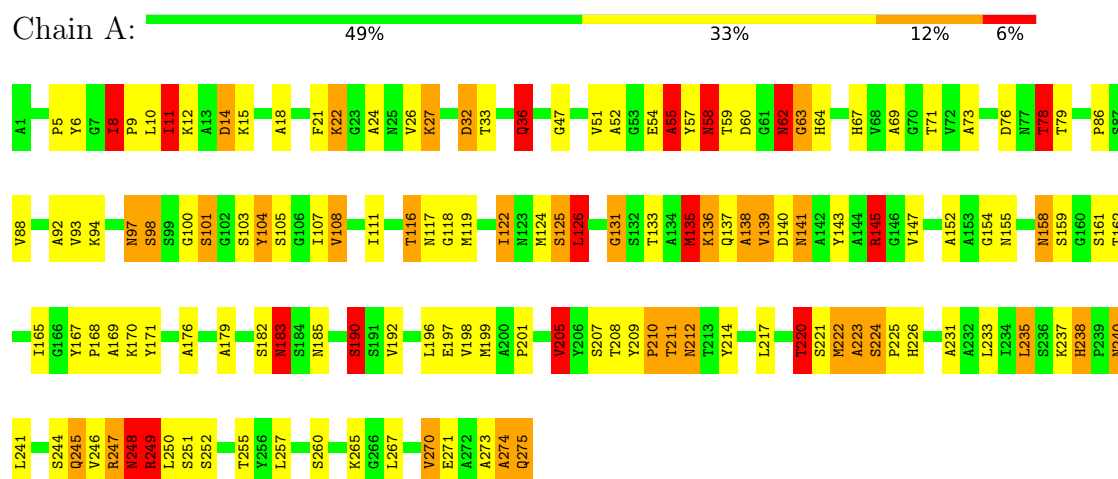
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	99	Total 99	O 99	0	0

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	77.10Å 55.40Å 53.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2056	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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, CCN

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	1.38	3/1952 (0.2%)	2.32	79/2662 (3.0%)

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	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	ALA	C-N	27.26	1.73	1.33
1	A	211	THR	N-CA	-7.67	1.36	1.46
1	A	101	SER	N-CA	5.00	1.51	1.45

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	PRO	CA-C-N	22.71	164.91	121.54
1	A	210	PRO	C-N-CA	22.71	164.91	121.54
1	A	55	ALA	O-C-N	-15.78	101.61	122.59
1	A	125	SER	O-C-N	-15.71	102.73	122.68
1	A	55	ALA	CA-C-N	-11.68	102.06	122.26
1	A	55	ALA	C-N-CA	-11.68	102.06	122.26
1	A	126	LEU	N-CA-CB	10.76	128.67	110.49
1	A	62	ASN	CA-C-O	-9.40	110.24	121.34
1	A	138	ALA	CA-C-N	8.86	131.90	120.56
1	A	138	ALA	C-N-CA	8.86	131.90	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	PRO	CA-C-O	8.81	130.92	121.32
1	A	97	ASN	CA-C-N	8.62	132.96	120.38
1	A	97	ASN	C-N-CA	8.62	132.96	120.38
1	A	131	GLY	N-CA-C	-8.27	100.78	112.60
1	A	248	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	A	190	SER	N-CA-CB	7.45	121.09	109.69
1	A	101	SER	CB-CA-C	7.35	122.94	109.71
1	A	79	THR	CA-CB-OG1	-7.25	98.72	109.60
1	A	60	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	58	ASN	N-CA-C	6.88	120.56	112.72
1	A	210	PRO	O-C-N	-6.82	114.53	122.85
1	A	8	ILE	CA-C-N	6.78	126.24	118.85
1	A	8	ILE	C-N-CA	6.78	126.24	118.85
1	A	73	ALA	N-CA-C	6.68	122.63	112.54
1	A	139	VAL	CB-CA-C	6.66	120.75	112.02
1	A	220	THR	N-CA-CB	-6.55	100.13	110.28
1	A	145	ARG	CD-NE-CZ	6.54	133.56	124.40
1	A	59	THR	O-C-N	6.43	131.14	123.24
1	A	211	THR	CA-CB-OG1	-6.39	100.02	109.60
1	A	224	SER	CA-C-N	6.31	125.88	119.19
1	A	224	SER	C-N-CA	6.31	125.88	119.19
1	A	223	ALA	CA-C-N	6.30	127.97	120.09
1	A	223	ALA	C-N-CA	6.30	127.97	120.09
1	A	18	ALA	CA-C-N	6.28	132.12	121.14
1	A	18	ALA	C-N-CA	6.28	132.12	121.14
1	A	220	THR	CB-CA-C	6.20	122.58	110.67
1	A	211	THR	N-CA-CB	6.13	120.86	110.49
1	A	14	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	244	SER	N-CA-CB	6.08	119.71	110.28
1	A	231	ALA	CA-C-O	-6.05	114.47	120.82
1	A	76	ASP	CA-C-O	-6.00	114.36	120.84
1	A	73	ALA	CA-C-O	-5.80	113.48	119.51
1	A	260	SER	CA-C-N	5.77	128.02	120.28
1	A	260	SER	C-N-CA	5.77	128.02	120.28
1	A	205	VAL	CB-CA-C	5.75	117.92	110.96
1	A	71	THR	CA-CB-OG1	-5.69	101.07	109.60
1	A	248	ASN	CA-CB-CG	5.67	118.27	112.60
1	A	32	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	245	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	A	5	PRO	CB-CA-C	5.56	118.62	111.56
1	A	247	ARG	CA-C-N	5.54	128.26	120.28
1	A	247	ARG	C-N-CA	5.54	128.26	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ARG	NE-CZ-NH1	5.50	127.00	121.50
1	A	93	VAL	CB-CA-C	5.48	118.12	110.99
1	A	26	VAL	CB-CA-C	5.48	118.29	110.84
1	A	78	THR	CB-CA-C	5.46	119.61	110.44
1	A	247	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	A	222	MET	CA-C-O	5.40	125.92	119.60
1	A	185	ASN	CA-C-O	-5.39	114.90	121.36
1	A	274	ALA	CA-C-N	5.37	131.36	121.70
1	A	274	ALA	C-N-CA	5.37	131.36	121.70
1	A	275	GLN	CB-CG-CD	5.36	121.72	112.60
1	A	24	ALA	CB-CA-C	5.35	118.25	109.90
1	A	122	ILE	O-C-N	5.33	128.72	123.18
1	A	11	ILE	N-CA-C	-5.32	107.56	112.83
1	A	54	GLU	CB-CG-CD	5.23	121.49	112.60
1	A	238	HIS	CA-C-N	5.18	124.79	119.56
1	A	238	HIS	C-N-CA	5.18	124.79	119.56
1	A	135	MET	O-C-N	5.16	127.38	122.07
1	A	104	TYR	N-CA-C	-5.16	105.55	111.07
1	A	220	THR	CA-CB-CG2	5.15	119.25	110.50
1	A	247	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A	183	ASN	O-C-N	5.12	128.55	122.26
1	A	101	SER	CA-C-O	5.11	127.75	121.56
1	A	69	ALA	CA-C-N	5.11	125.51	119.94
1	A	69	ALA	C-N-CA	5.11	125.51	119.94
1	A	275	GLN	N-CA-CB	5.08	119.14	110.50
1	A	179	ALA	N-CA-C	5.07	117.67	109.40
1	A	139	VAL	N-CA-CB	-5.05	104.11	110.57

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	SER	Mainchain,Peptide
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	1879	140	0
2	A	1	0	0	0	0
3	A	36	0	36	14	0
4	A	99	0	0	8	0
All	All	2056	0	1915	141	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 36.

All (141) 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:55:ALA:C	1:A:57:TYR:N	1.73	1.45
1:A:152:ALA:HB1	1:A:220:THR:HG23	1.33	1.08
1:A:8:ILE:HG13	1:A:9:PRO:HD3	1.35	1.07
1:A:111:ILE:HG23	4:A:362:HOH:O	1.56	1.02
1:A:27:LYS:HB2	1:A:27:LYS:HZ2	1.21	1.01
1:A:62:ASN:O	1:A:62:ASN:ND2	1.94	1.00
1:A:143:TYR:O	3:A:409:CCN:H23	1.66	0.95
1:A:116:THR:HG22	1:A:117:ASN:ND2	1.84	0.93
1:A:136:LYS:HE3	1:A:140:ASP:OD2	1.71	0.89
1:A:15:LYS:HD3	1:A:271:GLU:OE1	1.73	0.89
1:A:249:ARG:NH1	4:A:400:HOH:O	1.93	0.88
1:A:154:GLY:HA2	3:A:405:CCN:H21	1.55	0.88
1:A:154:GLY:H	1:A:220:THR:HG21	1.40	0.87
1:A:27:LYS:HB2	1:A:27:LYS:NZ	1.92	0.84
1:A:55:ALA:C	1:A:57:TYR:CA	2.50	0.84
1:A:255:THR:O	1:A:257:LEU:HD12	1.77	0.84
1:A:133:THR:O	1:A:137:GLN:HG3	1.79	0.83
1:A:152:ALA:HB1	1:A:220:THR:CG2	2.08	0.82
1:A:63:GLY:HA2	1:A:210:PRO:HG3	1.61	0.82
1:A:249:ARG:HH21	1:A:275:GLN:HB2	1.44	0.82
1:A:63:GLY:HA2	1:A:210:PRO:CG	2.10	0.81
1:A:62:ASN:O	1:A:64:HIS:N	2.12	0.80
1:A:116:THR:HG22	1:A:117:ASN:HD22	1.50	0.77
1:A:63:GLY:HA2	1:A:210:PRO:CD	2.17	0.75
1:A:196:LEU:HD21	1:A:199:MET:HE1	1.69	0.75
1:A:27:LYS:HZ1	1:A:118:GLY:C	1.94	0.75
1:A:122:ILE:HD13	4:A:362:HOH:O	1.85	0.75
1:A:209:TYR:CE2	3:A:408:CCN:H23	2.23	0.74
1:A:221:SER:HB2	3:A:406:CCN:N	2.04	0.73
1:A:36:GLN:HE22	1:A:212:ASN:H	1.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:HG13	1:A:9:PRO:CD	2.17	0.72
1:A:198:VAL:O	1:A:199:MET:HE2	1.92	0.70
1:A:145:ARG:O	1:A:145:ARG:HG3	1.92	0.70
1:A:137:GLN:O	1:A:141:ASN:HB2	1.91	0.69
1:A:27:LYS:NZ	1:A:27:LYS:CB	2.56	0.68
1:A:78:THR:HG22	4:A:293:HOH:O	1.93	0.68
1:A:51:VAL:HA	3:A:413:CCN:C1	2.24	0.68
1:A:55:ALA:CA	1:A:57:TYR:N	2.57	0.68
1:A:63:GLY:CA	1:A:210:PRO:HG3	2.23	0.68
1:A:143:TYR:O	3:A:409:CCN:C2	2.43	0.65
1:A:238:HIS:HE1	1:A:274:ALA:O	1.79	0.64
1:A:103:SER:O	1:A:107:ILE:HG13	1.98	0.64
1:A:190:SER:HB2	4:A:355:HOH:O	1.97	0.63
1:A:155:ASN:OD1	1:A:220:THR:HB	1.99	0.63
1:A:248:ASN:O	1:A:252:SER:HB2	2.01	0.61
1:A:27:LYS:NZ	1:A:118:GLY:O	2.20	0.60
1:A:248:ASN:C	1:A:248:ASN:HD22	2.10	0.59
1:A:10:LEU:HD23	1:A:201:PRO:HG3	1.85	0.59
1:A:63:GLY:H	1:A:210:PRO:HG3	1.68	0.58
1:A:131:GLY:HA3	1:A:171:TYR:OH	2.03	0.58
1:A:108:VAL:HG12	1:A:135:MET:HG2	1.86	0.57
1:A:237:LYS:HZ3	1:A:274:ALA:C	2.11	0.57
1:A:21:PHE:C	1:A:22:LYS:HG3	2.30	0.56
1:A:55:ALA:O	1:A:57:TYR:CA	2.54	0.56
1:A:275:GLN:HG2	1:A:275:GLN:O	2.05	0.56
1:A:136:LYS:HG3	1:A:171:TYR:CD1	2.41	0.56
1:A:158:ASN:C	1:A:158:ASN:HD22	2.14	0.56
1:A:197:GLU:OE2	1:A:247:ARG:NH2	2.26	0.56
1:A:63:GLY:CA	1:A:210:PRO:CG	2.83	0.55
1:A:122:ILE:HD12	1:A:147:VAL:HG11	1.88	0.55
1:A:63:GLY:N	1:A:210:PRO:HG3	2.21	0.54
1:A:154:GLY:N	1:A:220:THR:HG21	2.16	0.54
1:A:249:ARG:NH2	1:A:275:GLN:HB2	2.19	0.54
1:A:165:ILE:O	1:A:170:LYS:NZ	2.41	0.54
1:A:55:ALA:O	1:A:57:TYR:N	2.32	0.53
1:A:197:GLU:HG3	4:A:356:HOH:O	2.08	0.53
1:A:238:HIS:CE1	1:A:274:ALA:O	2.60	0.53
1:A:167:TYR:CZ	1:A:170:LYS:HD2	2.42	0.53
1:A:209:TYR:HE2	3:A:408:CCN:H23	1.70	0.53
1:A:63:GLY:HA3	1:A:209:TYR:CE1	2.43	0.52
1:A:141:ASN:O	1:A:145:ARG:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLY:HA3	1:A:92:ALA:O	2.09	0.52
1:A:12:LYS:HG2	3:A:411:CCN:N	2.25	0.52
1:A:111:ILE:HG21	1:A:138:ALA:HB1	1.91	0.52
1:A:124:MET:HE3	1:A:168:PRO:HG2	1.91	0.52
1:A:22:LYS:NZ	1:A:86:PRO:HG2	2.25	0.51
1:A:8:ILE:HD12	1:A:14:ASP:HB3	1.92	0.51
1:A:100:GLY:O	3:A:404:CCN:H23	2.10	0.51
1:A:136:LYS:HG3	1:A:171:TYR:CE1	2.45	0.51
1:A:27:LYS:NZ	1:A:119:MET:HA	2.25	0.51
1:A:251:SER:HB2	1:A:265:LYS:HG3	1.92	0.50
1:A:104:TYR:O	1:A:108:VAL:HG13	2.12	0.50
1:A:36:GLN:HE21	1:A:210:PRO:HA	1.75	0.50
1:A:55:ALA:CB	1:A:57:TYR:N	2.75	0.49
1:A:207:SER:O	1:A:214:TYR:HA	2.13	0.49
1:A:158:ASN:CB	1:A:192:VAL:HG21	2.43	0.49
3:A:404:CCN:H22	4:A:383:HOH:O	2.13	0.48
1:A:62:ASN:HD22	1:A:64:HIS:H	1.61	0.48
1:A:158:ASN:C	1:A:158:ASN:ND2	2.70	0.48
1:A:27:LYS:NZ	1:A:118:GLY:C	2.67	0.48
1:A:111:ILE:CG2	1:A:138:ALA:HB1	2.44	0.48
1:A:152:ALA:CB	1:A:220:THR:HG23	2.23	0.48
1:A:196:LEU:HD21	1:A:199:MET:CE	2.40	0.48
1:A:221:SER:HB2	3:A:406:CCN:C1	2.43	0.47
1:A:6:TYR:CE1	1:A:182:SER:HA	2.49	0.47
1:A:11:ILE:O	1:A:270:VAL:HG23	2.15	0.46
1:A:55:ALA:C	1:A:57:TYR:HA	2.37	0.46
1:A:205:VAL:HG11	1:A:222:MET:HB3	1.97	0.46
1:A:223:ALA:O	1:A:226:HIS:HB2	2.15	0.46
1:A:235:LEU:CD1	1:A:246:VAL:HG21	2.46	0.46
1:A:116:THR:HA	3:A:410:CCN:H22	1.98	0.46
1:A:183:ASN:ND2	1:A:183:ASN:N	2.63	0.46
1:A:58:ASN:ND2	1:A:58:ASN:H	2.14	0.45
1:A:257:LEU:HD11	1:A:267:LEU:HB3	1.98	0.45
1:A:33:THR:O	1:A:94:LYS:HE2	2.17	0.45
1:A:124:MET:CE	1:A:168:PRO:HG3	2.47	0.45
1:A:159:SER:O	1:A:162:THR:OG1	2.26	0.45
1:A:21:PHE:CD2	1:A:237:LYS:HD2	2.52	0.44
1:A:55:ALA:HB1	1:A:57:TYR:N	2.32	0.44
1:A:124:MET:CE	1:A:168:PRO:CG	2.95	0.44
1:A:205:VAL:CG1	1:A:222:MET:HB3	2.47	0.44
1:A:255:THR:O	1:A:257:LEU:CD1	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASN:OD1	1:A:97:ASN:C	2.60	0.44
1:A:158:ASN:ND2	1:A:158:ASN:O	2.50	0.44
1:A:249:ARG:HH22	1:A:275:GLN:CD	2.25	0.43
1:A:67:HIS:HA	1:A:208:THR:O	2.18	0.43
1:A:209:TYR:CD1	1:A:210:PRO:HD2	2.54	0.43
1:A:116:THR:CG2	1:A:117:ASN:ND2	2.70	0.43
1:A:58:ASN:H	1:A:58:ASN:HD22	1.67	0.43
1:A:126:LEU:HA	3:A:404:CCN:N	2.33	0.43
1:A:237:LYS:NZ	1:A:274:ALA:O	2.36	0.43
1:A:241:LEU:HA	1:A:245:GLN:HE22	1.83	0.43
1:A:248:ASN:C	1:A:248:ASN:ND2	2.76	0.43
1:A:183:ASN:N	1:A:183:ASN:HD22	2.17	0.42
1:A:224:SER:N	1:A:225:PRO:HD2	2.33	0.42
1:A:124:MET:HE3	1:A:168:PRO:CG	2.49	0.42
1:A:235:LEU:HD13	1:A:246:VAL:HG21	2.02	0.42
1:A:58:ASN:HD22	1:A:58:ASN:N	2.17	0.42
1:A:237:LYS:HG2	1:A:238:HIS:CE1	2.54	0.42
1:A:249:ARG:HG2	1:A:273:ALA:O	2.20	0.42
1:A:240:ASN:H	1:A:240:ASN:HD22	1.68	0.41
1:A:241:LEU:HA	1:A:245:GLN:NE2	2.34	0.41
1:A:62:ASN:HB2	1:A:98:SER:O	2.20	0.41
1:A:122:ILE:CD1	4:A:362:HOH:O	2.58	0.41
1:A:8:ILE:N	1:A:9:PRO:CD	2.83	0.41
1:A:52:ALA:N	3:A:413:CCN:N	2.49	0.41
1:A:169:ALA:HB1	1:A:176:ALA:CB	2.51	0.41
1:A:183:ASN:HD22	1:A:183:ASN:H	1.68	0.40
1:A:248:ASN:O	1:A:248:ASN:ND2	2.53	0.40
1:A:196:LEU:HD11	1:A:199:MET:HE1	2.02	0.40
1:A:209:TYR:CG	1:A:210:PRO:HD2	2.56	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%)	258 (95%)	10 (4%)	4 (2%)	8 8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLY
1	A	126	LEU
1	A	55	ALA
1	A	36	GLN

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%)	162 (82%)	36 (18%)	2 2

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	11	ILE
1	A	22	LYS
1	A	27	LYS
1	A	32	ASP
1	A	36	GLN
1	A	58	ASN
1	A	62	ASN
1	A	78	THR
1	A	88	VAL
1	A	98	SER
1	A	101	SER
1	A	105	SER
1	A	108	VAL
1	A	116	THR
1	A	135	MET
1	A	136	LYS

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Mol	Chain	Res	Type
1	A	139	VAL
1	A	141	ASN
1	A	145	ARG
1	A	158	ASN
1	A	161	SER
1	A	183	ASN
1	A	190	SER
1	A	205	VAL
1	A	211	THR
1	A	212	ASN
1	A	217	LEU
1	A	220	THR
1	A	233	LEU
1	A	235	LEU
1	A	240	ASN
1	A	248	ASN
1	A	249	ARG
1	A	250	LEU
1	A	270	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	43	ASN
1	A	58	ASN
1	A	117	ASN
1	A	137	GLN
1	A	141	ASN
1	A	158	ASN
1	A	183	ASN
1	A	238	HIS
1	A	240	ASN
1	A	245	GLN
1	A	248	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CCN	A	414	-	2,2,2	0.16	0	1,1,1	0.49	0
3	CCN	A	406	-	2,2,2	0.28	0	1,1,1	0.49	0
3	CCN	A	410	-	2,2,2	0.35	0	1,1,1	0.43	0
3	CCN	A	408	-	2,2,2	0.38	0	1,1,1	0.25	0
3	CCN	A	411	-	2,2,2	0.32	0	1,1,1	0.14	0
3	CCN	A	413	-	2,2,2	0.30	0	1,1,1	0.22	0
3	CCN	A	416	-	2,2,2	0.17	0	1,1,1	0.29	0
3	CCN	A	409	-	2,2,2	0.62	0	1,1,1	0.00	0
3	CCN	A	405	-	2,2,2	0.71	0	1,1,1	0.23	0
3	CCN	A	415	-	2,2,2	0.13	0	1,1,1	0.09	0
3	CCN	A	407	-	2,2,2	0.39	0	1,1,1	0.27	0
3	CCN	A	404	-	2,2,2	0.43	0	1,1,1	0.27	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.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	406	CCN	2	0
3	A	410	CCN	1	0
3	A	408	CCN	2	0
3	A	411	CCN	1	0
3	A	413	CCN	2	0
3	A	409	CCN	2	0
3	A	405	CCN	1	0
3	A	404	CCN	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	55:ALA	C	57:TYR	N	1.73

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.