



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:52 AM UTC

PDB ID : 1BIB / pdb_00001bib
Title : THE E. COLI BIOTIN HOLOENZYME SYNTHETASE(SLASH)BIO RE-PRESSOR CRYSTAL STRUCTURE DELINEATES THE BIOTIN AND DNA-BINDING DOMAINS
Authors : Wilson, K.P.; Shewchuk, L.M.; Matthews, B.W.
Deposited on : 1992-07-06
Resolution : 2.80 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

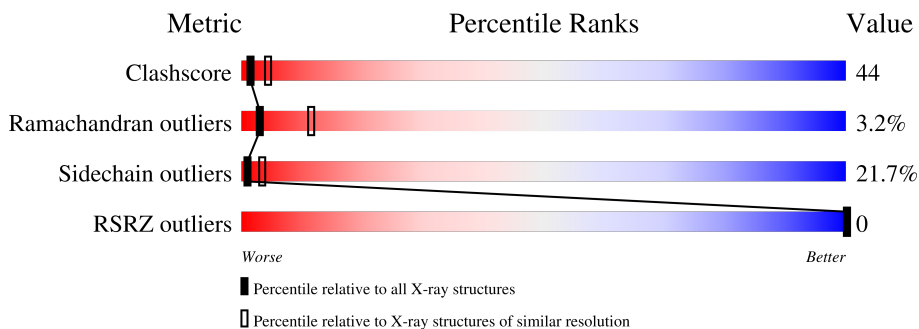
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	321	

2 Entry composition [i](#)

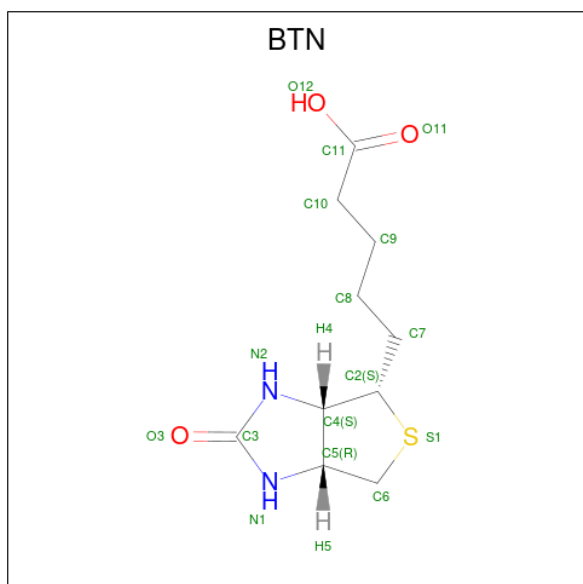
There are 3 unique types of molecules in this entry. The entry contains 2236 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BIR A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2201	1408	383	403	7			

- Molecule 2 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

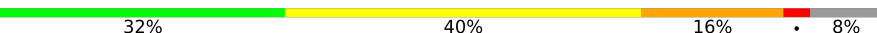
- Molecule 3 is water.

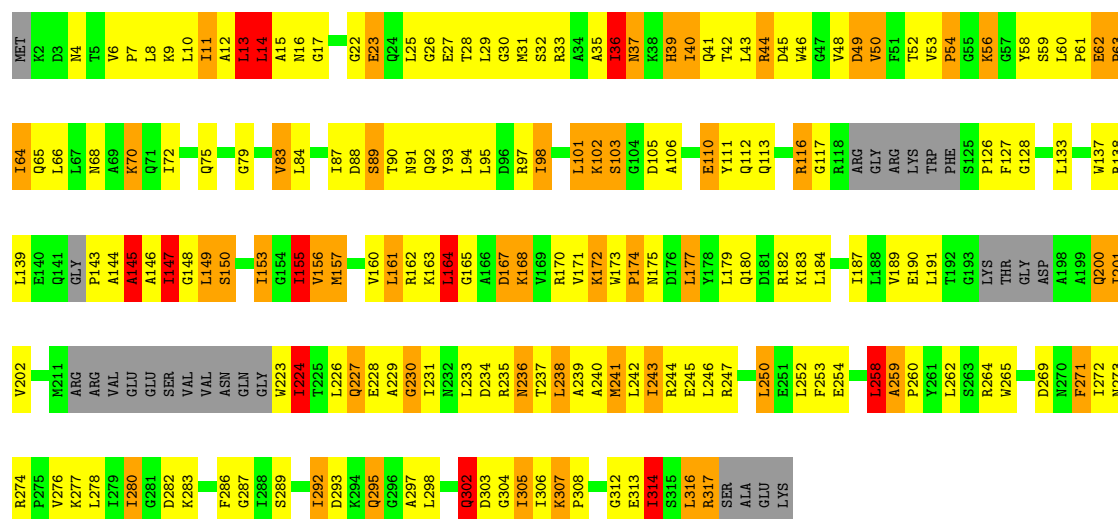
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total 19 O 19	0	0

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 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: BIR A

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.10Å 114.10Å 60.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80 80.68 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80) 89.0 (80.68-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.79Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.173 , (Not available) 0.161 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 191.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2236	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BTN

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	3/2231 (0.1%)	1.91	54/3020 (1.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	VAL	CA-CB	-7.52	1.46	1.54
1	A	156	VAL	N-CA	-6.26	1.39	1.46
1	A	155	ILE	C-N	-5.83	1.27	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ILE	CA-C-N	-9.79	111.05	123.19
1	A	305	ILE	C-N-CA	-9.79	111.05	123.19
1	A	156	VAL	N-CA-CB	-9.32	100.84	110.62
1	A	147	ILE	CA-C-N	-8.82	104.13	121.41
1	A	147	ILE	C-N-CA	-8.82	104.13	121.41
1	A	56	LYS	N-CA-C	7.93	119.83	111.03
1	A	50	VAL	CB-CA-C	7.40	120.61	110.99
1	A	175	ASN	N-CA-C	7.29	121.57	112.03
1	A	258	LEU	N-CA-C	7.08	118.64	111.07
1	A	304	GLY	CA-C-N	-6.94	113.49	123.06
1	A	304	GLY	C-N-CA	-6.94	113.49	123.06
1	A	271	PHE	CA-CB-CG	-6.87	106.93	113.80
1	A	145	ALA	O-C-N	6.78	131.61	122.59
1	A	117	GLY	N-CA-C	6.65	124.81	115.43
1	A	177	LEU	CA-C-O	-6.58	113.73	121.16
1	A	36	ILE	CA-C-N	-6.51	111.06	120.82
1	A	36	ILE	C-N-CA	-6.51	111.06	120.82
1	A	110	GLU	N-CA-CB	6.46	121.65	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	PRO	N-CA-CB	6.46	110.11	103.00
1	A	63	PRO	N-CA-CB	6.36	109.93	103.25
1	A	305	ILE	CB-CA-C	-6.24	101.32	110.62
1	A	98	ILE	N-CA-C	6.16	122.15	109.34
1	A	230	GLY	CA-C-N	-6.11	115.24	122.93
1	A	230	GLY	C-N-CA	-6.11	115.24	122.93
1	A	13	LEU	N-CA-CB	6.09	118.83	110.01
1	A	224	ILE	N-CA-C	6.03	121.88	109.34
1	A	164	LEU	CA-C-N	-5.99	113.16	122.69
1	A	164	LEU	C-N-CA	-5.99	113.16	122.69
1	A	282	ASP	CA-C-N	-5.97	114.58	122.99
1	A	282	ASP	C-N-CA	-5.97	114.58	122.99
1	A	201	ILE	CB-CA-C	-5.82	102.52	110.90
1	A	240	ALA	N-CA-C	5.80	118.06	111.11
1	A	314	ILE	CB-CA-C	5.71	119.50	111.63
1	A	64	ILE	N-CA-CB	-5.71	101.81	112.36
1	A	50	VAL	N-CA-CB	5.56	118.91	111.90
1	A	145	ALA	N-CA-CB	-5.56	101.10	110.49
1	A	145	ALA	CA-C-N	5.55	132.15	121.54
1	A	145	ALA	C-N-CA	5.55	132.15	121.54
1	A	144	ALA	N-CA-C	-5.50	99.08	110.80
1	A	236	ASN	N-CA-CB	5.46	118.63	110.22
1	A	33	ARG	N-CA-C	-5.42	105.48	111.71
1	A	250	LEU	CA-C-N	-5.41	111.49	120.68
1	A	250	LEU	C-N-CA	-5.41	111.49	120.68
1	A	283	LYS	N-CA-C	5.35	117.62	108.90
1	A	227	GLN	O-C-N	5.33	127.79	122.08
1	A	39	HIS	CA-CB-CG	-5.32	108.48	113.80
1	A	106	ALA	N-CA-C	5.30	116.05	108.74
1	A	167	ASP	CA-CB-CG	-5.29	107.31	112.60
1	A	161	LEU	CA-C-O	5.23	126.28	120.63
1	A	165	GLY	N-CA-C	5.21	121.93	114.64
1	A	174	PRO	CB-CA-C	-5.06	99.36	112.00
1	A	14	LEU	CA-C-N	5.05	128.40	120.82
1	A	14	LEU	C-N-CA	5.05	128.40	120.82
1	A	302	GLN	N-CA-CB	5.04	119.14	110.68

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	2201	0	2230	194	0
2	A	16	0	11	0	0
3	A	19	0	0	3	0
All	All	2236	0	2241	194	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 44.

All (194) 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:276:VAL:HG11	1:A:314:ILE:HD11	1.37	1.02
1:A:259:ALA:HA	1:A:262:LEU:HD12	1.49	0.93
1:A:286:PHE:HD2	1:A:317:ARG:HD3	1.32	0.92
1:A:70:LYS:HA	1:A:70:LYS:NZ	1.85	0.92
1:A:316:LEU:HD12	1:A:317:ARG:H	1.33	0.89
1:A:259:ALA:HB3	1:A:260:PRO:HD3	1.56	0.88
1:A:36:ILE:O	1:A:37:ASN:C	2.15	0.87
1:A:147:ILE:O	1:A:148:GLY:C	2.09	0.86
1:A:286:PHE:CD2	1:A:317:ARG:HD3	2.12	0.84
1:A:110:GLU:HB2	1:A:128:GLY:HA2	1.58	0.84
1:A:182:ARG:NH1	1:A:224:ILE:H	1.78	0.82
1:A:182:ARG:NH1	1:A:224:ILE:N	2.29	0.80
1:A:65:GLN:O	1:A:66:LEU:HD23	1.82	0.78
1:A:13:LEU:HD12	1:A:25:LEU:HD22	1.65	0.78
1:A:162:ARG:NH2	1:A:170:ARG:HH12	1.81	0.77
1:A:116:ARG:HH11	1:A:116:ARG:HB3	1.49	0.76
1:A:243:ILE:O	1:A:247:ARG:HG3	1.85	0.76
1:A:160:VAL:HG13	1:A:241:MET:HE2	1.68	0.75
1:A:13:LEU:HD12	1:A:25:LEU:CD2	2.19	0.72
1:A:316:LEU:HD12	1:A:317:ARG:N	2.02	0.72
1:A:70:LYS:HA	1:A:70:LYS:CE	2.20	0.72
1:A:26:GLY:HA2	1:A:36:ILE:HD11	1.71	0.70
1:A:29:LEU:HB3	1:A:31:MET:HE3	1.73	0.69
1:A:65:GLN:HE21	1:A:236:ASN:ND2	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:HG23	1:A:59:SER:O	1.93	0.69
1:A:259:ALA:HA	1:A:262:LEU:CD1	2.24	0.67
1:A:313:GLU:HA	3:A:335:HOH:O	1.93	0.67
1:A:116:ARG:HH11	1:A:116:ARG:CB	2.07	0.67
1:A:170:ARG:HH11	1:A:170:ARG:HG2	1.60	0.67
1:A:97:ARG:HB3	1:A:101:LEU:HD21	1.77	0.66
1:A:88:ASP:OD1	1:A:89:SER:N	2.28	0.66
1:A:49:ASP:HB3	1:A:61:PRO:CG	2.25	0.66
1:A:227:GLN:O	1:A:230:GLY:N	2.30	0.65
1:A:65:GLN:NE2	1:A:234:ASP:OD1	2.29	0.65
1:A:42:THR:O	1:A:45:ASP:N	2.30	0.65
1:A:70:LYS:HA	1:A:70:LYS:HZ3	1.58	0.65
1:A:201:ILE:H	1:A:201:ILE:HD12	1.62	0.65
1:A:68:ASN:OD1	1:A:70:LYS:HB2	1.97	0.64
1:A:10:LEU:HD21	1:A:40:ILE:CD1	2.28	0.64
1:A:37:ASN:ND2	1:A:58:TYR:OH	2.29	0.63
1:A:90:THR:N	1:A:112:GLN:OE1	2.28	0.63
1:A:116:ARG:HH11	1:A:116:ARG:CG	2.12	0.62
1:A:182:ARG:CB	1:A:224:ILE:HB	2.28	0.62
1:A:8:LEU:HA	1:A:11:ILE:HG22	1.80	0.62
1:A:10:LEU:HD21	1:A:40:ILE:HD13	1.80	0.62
1:A:65:GLN:C	1:A:66:LEU:HD23	2.24	0.62
1:A:88:ASP:OD1	1:A:88:ASP:N	2.31	0.62
1:A:241:MET:HG3	1:A:244:ARG:NH2	2.14	0.62
1:A:265:TRP:NE1	1:A:269:ASP:OD2	2.33	0.61
1:A:276:VAL:HG11	1:A:314:ILE:CD1	2.22	0.61
1:A:31:MET:HG3	1:A:35:ALA:HB3	1.83	0.60
1:A:171:VAL:HG12	1:A:172:LYS:N	2.14	0.60
1:A:164:LEU:HD21	1:A:241:MET:SD	2.41	0.60
1:A:182:ARG:HH12	1:A:224:ILE:H	1.49	0.60
1:A:92:GLN:HA	1:A:95:LEU:HD12	1.85	0.59
1:A:278:LEU:HD11	1:A:312:GLY:HA3	1.85	0.59
1:A:293:ASP:OD1	1:A:297:ALA:N	2.33	0.59
1:A:182:ARG:HH11	1:A:224:ILE:N	2.00	0.59
1:A:201:ILE:HD12	1:A:201:ILE:N	2.17	0.59
1:A:9:LYS:O	1:A:12:ALA:HB3	2.02	0.58
1:A:62:GLU:HG2	1:A:63:PRO:O	2.02	0.58
1:A:87:ILE:HG12	1:A:88:ASP:OD1	2.01	0.58
1:A:53:VAL:HB	1:A:56:LYS:CB	2.33	0.58
1:A:182:ARG:HB3	1:A:224:ILE:HB	1.86	0.58
1:A:39:HIS:O	1:A:40:ILE:C	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:O	1:A:239:ALA:C	2.46	0.58
1:A:162:ARG:NH2	1:A:170:ARG:NH1	2.52	0.57
1:A:139:LEU:CD1	1:A:145:ALA:HB2	2.34	0.57
1:A:137:TRP:O	1:A:201:ILE:HD12	2.05	0.57
1:A:155:ILE:HG22	1:A:156:VAL:N	2.19	0.57
1:A:271:PHE:HA	1:A:274:ARG:HD3	1.87	0.57
1:A:273:ASN:N	1:A:289:SER:O	2.38	0.57
1:A:287:GLY:H	1:A:317:ARG:HH12	1.51	0.57
1:A:167:ASP:OD1	1:A:167:ASP:N	2.36	0.56
1:A:88:ASP:CG	1:A:89:SER:H	2.12	0.56
1:A:157:MET:HB3	1:A:177:LEU:HD11	1.88	0.55
1:A:271:PHE:O	1:A:272:ILE:C	2.49	0.55
1:A:89:SER:HA	1:A:112:GLN:OE1	2.05	0.55
1:A:253:PHE:HE1	1:A:258:LEU:HD12	1.70	0.55
1:A:276:VAL:CG1	1:A:314:ILE:HD11	2.26	0.54
1:A:32:SER:HB3	1:A:35:ALA:H	1.72	0.54
1:A:97:ARG:CB	1:A:101:LEU:HD21	2.37	0.54
1:A:103:SER:HB3	1:A:137:TRP:HA	1.89	0.54
1:A:298:LEU:O	1:A:308:PRO:HA	2.07	0.54
1:A:92:GLN:O	1:A:93:TYR:C	2.48	0.54
1:A:162:ARG:HH22	1:A:170:ARG:HH12	1.56	0.53
1:A:126:PRO:O	1:A:127:PHE:C	2.50	0.53
1:A:8:LEU:O	1:A:11:ILE:HG22	2.08	0.53
1:A:128:GLY:O	1:A:235:ARG:NH2	2.42	0.53
1:A:153:ILE:HG22	1:A:187:ILE:HG12	1.90	0.53
1:A:116:ARG:HB3	1:A:116:ARG:NH1	2.19	0.53
1:A:46:TRP:HB2	1:A:48:VAL:HG23	1.91	0.53
1:A:53:VAL:O	1:A:54:PRO:C	2.51	0.53
1:A:259:ALA:CB	1:A:260:PRO:HD3	2.34	0.52
1:A:102:LYS:HA	3:A:349:HOH:O	2.09	0.52
1:A:53:VAL:O	1:A:56:LYS:N	2.43	0.52
1:A:156:VAL:HG12	1:A:157:MET:N	2.18	0.52
1:A:150:SER:OG	1:A:174:PRO:O	2.28	0.52
1:A:201:ILE:HG22	1:A:202:VAL:N	2.25	0.52
1:A:26:GLY:CA	1:A:36:ILE:HD11	2.39	0.51
1:A:91:ASN:O	1:A:95:LEU:HG	2.10	0.51
1:A:183:LYS:O	1:A:223:TRP:O	2.28	0.51
1:A:231:ILE:HG22	1:A:233:LEU:HG	1.92	0.51
1:A:147:ILE:O	1:A:148:GLY:O	2.28	0.51
1:A:111:TYR:HE2	1:A:113:GLN:HG2	1.76	0.51
1:A:42:THR:O	1:A:43:LEU:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASP:C	1:A:295:GLN:H	2.19	0.50
1:A:65:GLN:NE2	1:A:236:ASN:ND2	2.58	0.50
1:A:49:ASP:HB3	1:A:61:PRO:HG3	1.93	0.50
1:A:111:TYR:CE2	1:A:113:GLN:HG2	2.46	0.50
1:A:15:ALA:C	1:A:17:GLY:H	2.18	0.50
1:A:139:LEU:HD12	1:A:145:ALA:HB2	1.93	0.49
1:A:133:LEU:HD23	1:A:133:LEU:C	2.38	0.49
1:A:49:ASP:HB3	1:A:61:PRO:CD	2.43	0.49
1:A:229:ALA:O	1:A:231:ILE:HD12	2.13	0.48
1:A:271:PHE:O	1:A:274:ARG:N	2.39	0.48
1:A:89:SER:OG	1:A:92:GLN:HB2	2.14	0.48
1:A:241:MET:HG3	1:A:244:ARG:HH22	1.78	0.48
1:A:162:ARG:HH21	1:A:170:ARG:NH1	2.12	0.48
1:A:252:LEU:HD12	1:A:252:LEU:O	2.14	0.47
1:A:162:ARG:HG2	1:A:167:ASP:HA	1.94	0.47
1:A:246:LEU:HA	1:A:246:LEU:HD23	1.52	0.47
1:A:286:PHE:HD2	1:A:317:ARG:CD	2.16	0.47
1:A:238:LEU:O	1:A:242:LEU:HG	2.14	0.47
1:A:4:ASN:O	1:A:7:PRO:HD2	2.14	0.47
1:A:116:ARG:HH11	1:A:116:ARG:HG2	1.78	0.47
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.72	0.47
1:A:72:ILE:HG13	1:A:236:ASN:HB3	1.97	0.47
1:A:269:ASP:HB3	1:A:272:ILE:HB	1.97	0.47
1:A:160:VAL:O	1:A:161:LEU:C	2.56	0.46
1:A:182:ARG:HB2	1:A:224:ILE:HB	1.95	0.46
1:A:226:LEU:HD13	1:A:233:LEU:HD12	1.98	0.46
1:A:49:ASP:O	1:A:60:LEU:HD23	2.16	0.46
1:A:149:LEU:C	1:A:149:LEU:HD12	2.41	0.46
1:A:305:ILE:HG22	1:A:306:ILE:N	2.30	0.46
1:A:22:GLY:O	1:A:23:GLU:C	2.58	0.46
1:A:111:TYR:CE2	1:A:113:GLN:CG	2.98	0.46
1:A:49:ASP:O	1:A:61:PRO:HD3	2.16	0.46
1:A:153:ILE:CG2	1:A:187:ILE:HG12	2.46	0.46
1:A:14:LEU:O	1:A:60:LEU:HD12	2.16	0.46
1:A:163:LYS:NZ	1:A:245:GLU:OE2	2.46	0.45
1:A:168:LYS:HE3	1:A:168:LYS:HB2	1.59	0.45
1:A:17:GLY:HA3	1:A:63:PRO:HD3	1.98	0.45
1:A:111:TYR:HE2	1:A:113:GLN:CG	2.30	0.45
1:A:180:GLN:N	3:A:354:HOH:O	2.49	0.45
1:A:264:ARG:O	1:A:265:TRP:C	2.57	0.45
1:A:41:GLN:HA	1:A:41:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLN:NE2	1:A:236:ASN:HD22	2.16	0.44
1:A:94:LEU:O	1:A:95:LEU:C	2.59	0.44
1:A:103:SER:HB3	1:A:138:ARG:H	1.83	0.44
1:A:170:ARG:NH1	1:A:170:ARG:CG	2.80	0.44
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.62	0.44
1:A:26:GLY:O	1:A:30:GLY:N	2.43	0.44
1:A:280:ILE:HG23	1:A:312:GLY:HA3	2.00	0.44
1:A:64:ILE:CG2	1:A:66:LEU:HD21	2.48	0.44
1:A:170:ARG:HG2	1:A:170:ARG:NH1	2.30	0.44
1:A:64:ILE:HG22	1:A:66:LEU:HD21	1.99	0.44
1:A:10:LEU:CD2	1:A:39:HIS:HB2	2.48	0.43
1:A:171:VAL:CG1	1:A:172:LYS:N	2.81	0.43
1:A:43:LEU:O	1:A:48:VAL:HG23	2.19	0.43
1:A:173:TRP:HA	1:A:174:PRO:HA	1.58	0.43
1:A:31:MET:HE2	1:A:31:MET:HB3	1.90	0.43
1:A:46:TRP:N	1:A:46:TRP:CD1	2.81	0.43
1:A:179:LEU:HB3	1:A:224:ILE:HD12	2.00	0.43
1:A:10:LEU:HD12	1:A:10:LEU:HA	1.79	0.42
1:A:234:ASP:OD2	1:A:237:THR:N	2.52	0.42
1:A:259:ALA:CB	1:A:260:PRO:CD	2.98	0.42
1:A:43:LEU:O	1:A:44:ARG:C	2.57	0.42
1:A:254:GLU:O	1:A:254:GLU:HG2	2.19	0.42
1:A:286:PHE:HB3	1:A:317:ARG:NH1	2.34	0.42
1:A:302:GLN:O	1:A:303:ASP:C	2.61	0.42
1:A:64:ILE:HG22	1:A:66:LEU:CD2	2.49	0.42
1:A:70:LYS:HA	1:A:70:LYS:HZ2	1.78	0.42
1:A:102:LYS:N	1:A:105:ASP:OD2	2.46	0.42
1:A:149:LEU:O	1:A:150:SER:C	2.62	0.42
1:A:241:MET:CG	1:A:244:ARG:NH2	2.83	0.42
1:A:10:LEU:HD22	1:A:39:HIS:HB2	2.02	0.41
1:A:155:ILE:CG2	1:A:156:VAL:N	2.83	0.41
1:A:201:ILE:N	1:A:201:ILE:CD1	2.80	0.41
1:A:110:GLU:O	1:A:128:GLY:N	2.46	0.41
1:A:258:LEU:O	1:A:259:ALA:C	2.64	0.41
1:A:156:VAL:O	1:A:157:MET:C	2.58	0.41
1:A:171:VAL:HG12	1:A:172:LYS:H	1.84	0.41
1:A:6:VAL:O	1:A:7:PRO:C	2.63	0.41
1:A:307:LYS:HB2	1:A:308:PRO:CD	2.51	0.41
1:A:40:ILE:HA	1:A:40:ILE:HD12	1.72	0.41
1:A:103:SER:HB2	1:A:137:TRP:CE3	2.56	0.41
1:A:83:VAL:C	1:A:84:LEU:HG	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:VAL:HG12	1:A:190:GLU:N	2.35	0.41
1:A:11:ILE:O	1:A:12:ALA:C	2.64	0.41
1:A:149:LEU:HD13	1:A:149:LEU:HA	1.70	0.40
1:A:48:VAL:HG12	1:A:49:ASP:N	2.36	0.40
1:A:200:GLN:HE21	1:A:200:GLN:HB2	1.44	0.40
1:A:292:ILE:HD12	1:A:293:ASP:O	2.22	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	284/321 (88%)	243 (86%)	32 (11%)	9 (3%)	3	11

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	79	GLY
1	A	146	ALA
1	A	224	ILE
1	A	145	ALA
1	A	228	GLU
1	A	27	GLU
1	A	54	PRO
1	A	259	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	221/258 (86%)	173 (78%)	48 (22%)	1 3

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	13	LEU
1	A	14	LEU
1	A	23	GLU
1	A	28	THR
1	A	36	ILE
1	A	37	ASN
1	A	40	ILE
1	A	44	ARG
1	A	49	ASP
1	A	52	THR
1	A	62	GLU
1	A	70	LYS
1	A	75	GLN
1	A	83	VAL
1	A	89	SER
1	A	98	ILE
1	A	101	LEU
1	A	102	LYS
1	A	103	SER
1	A	116	ARG
1	A	147	ILE
1	A	149	LEU
1	A	150	SER
1	A	153	ILE
1	A	155	ILE
1	A	157	MET
1	A	164	LEU
1	A	168	LYS
1	A	172	LYS
1	A	184	LEU
1	A	191	LEU
1	A	200	GLN
1	A	224	ILE

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Mol	Chain	Res	Type
1	A	238	LEU
1	A	241	MET
1	A	243	ILE
1	A	250	LEU
1	A	258	LEU
1	A	277	LYS
1	A	280	ILE
1	A	292	ILE
1	A	295	GLN
1	A	302	GLN
1	A	307	LYS
1	A	314	ILE
1	A	316	LEU
1	A	317	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	71	GLN
1	A	200	GLN
1	A	236	ASN
1	A	295	GLN
1	A	302	GLN

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

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	BTN	A	500	-	17,17,17	3.49	9 (52%)	23,23,23	2.61	8 (34%)

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
2	BTN	A	500	-	-	3/7/28/28	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	BTN	C9-C10	-9.60	1.17	1.52
2	A	500	BTN	C4-N2	-5.37	1.35	1.45
2	A	500	BTN	O12-C11	-4.47	1.16	1.30
2	A	500	BTN	C2-S1	-4.43	1.75	1.82
2	A	500	BTN	C8-C9	3.30	1.68	1.51
2	A	500	BTN	C7-C2	3.19	1.61	1.52
2	A	500	BTN	C6-S1	2.53	1.88	1.81
2	A	500	BTN	O11-C11	2.53	1.30	1.22
2	A	500	BTN	C3-N1	2.14	1.39	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	BTN	C2-C4-N2	6.56	120.29	113.34
2	A	500	BTN	C6-C5-N1	-5.44	106.17	113.18
2	A	500	BTN	O3-C3-N2	4.50	132.37	125.89
2	A	500	BTN	O3-C3-N1	-3.89	120.30	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	BTN	C4-C2-S1	-3.58	100.97	105.03
2	A	500	BTN	C8-C9-C10	-3.23	101.25	113.13
2	A	500	BTN	C8-C7-C2	-2.42	108.47	114.04
2	A	500	BTN	C9-C8-C7	-2.08	105.76	113.62

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	BTN	S1-C2-C7-C8
2	A	500	BTN	C4-C2-C7-C8
2	A	500	BTN	C7-C8-C9-C10

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	294/321 (91%)	-0.67	0 100 100	17, 46, 91, 100	0

There are no RSRZ outliers to report.

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

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

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	BTN	A	500	16/16	0.98	0.07	25,34,83,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.