



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:34 PM GMT

PDB ID : 1BIB
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

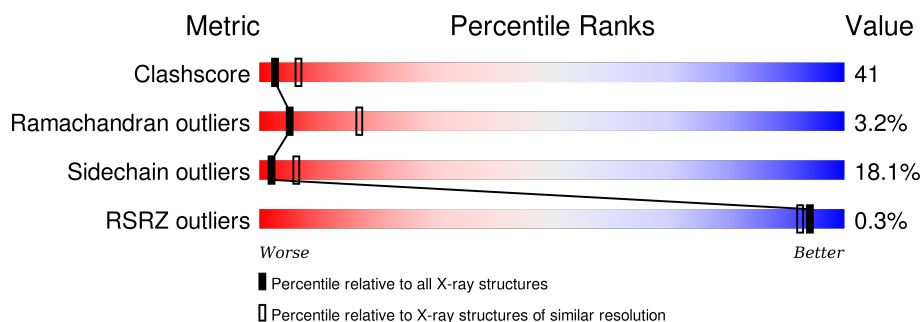
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

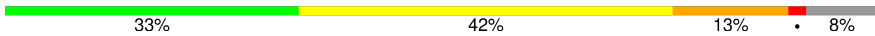
The reported resolution of this entry is 2.80 Å.

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	321	

2 Entry composition [i](#)

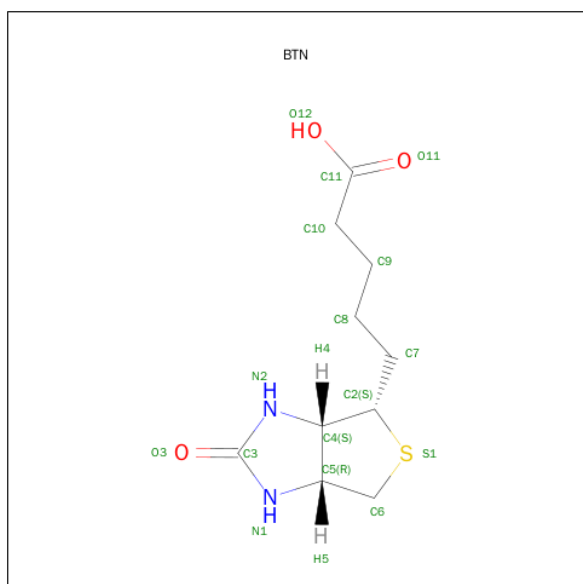
There are 3 unique types of molecules in this entry. The entry contains 2236 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: BTN) (formula: C₁₀H₁₆N₂O₃S).



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

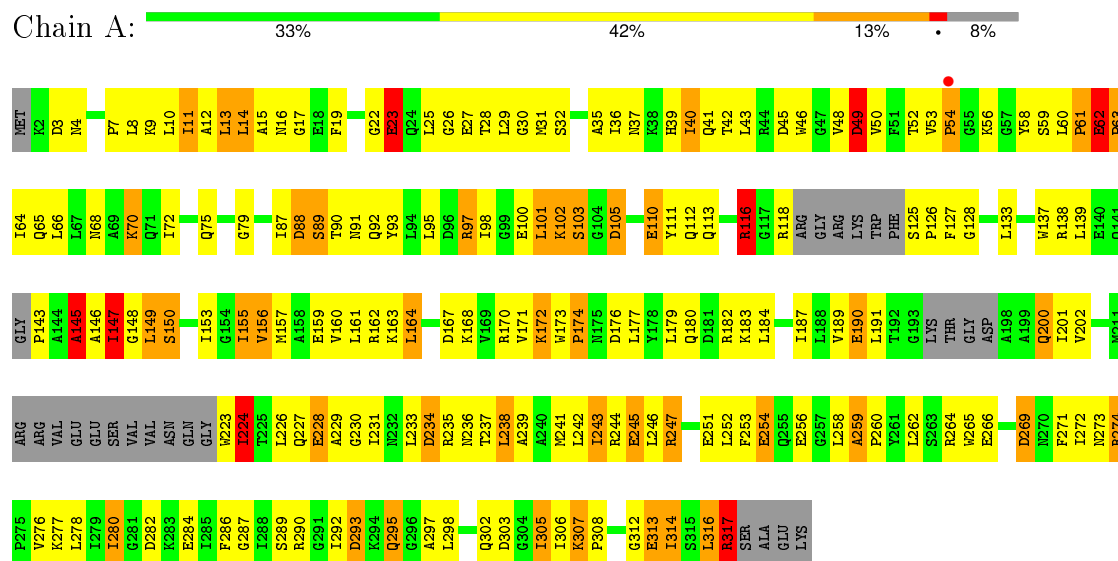
- Molecule 3 is water.

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

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 errors 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 ($\text{RSRZ} > 2$). 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.10 Å 114.10 Å 60.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80) 89.3 (19.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.79 Å)	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.	DCC
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 159.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 9137 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.06	13/2231 (0.6%)	1.58	37/3020 (1.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	GLU	CD-OE2	7.60	1.34	1.25
1	A	266	GLU	CD-OE1	6.99	1.33	1.25
1	A	159	GLU	CD-OE1	6.66	1.32	1.25
1	A	190	GLU	CD-OE2	6.47	1.32	1.25
1	A	284	GLU	CD-OE2	6.35	1.32	1.25
1	A	245	GLU	CD-OE1	6.32	1.32	1.25
1	A	62	GLU	CD-OE2	6.25	1.32	1.25
1	A	313	GLU	CD-OE1	6.19	1.32	1.25
1	A	251	GLU	CD-OE1	6.10	1.32	1.25
1	A	256	GLU	CD-OE2	5.99	1.32	1.25
1	A	100	GLU	CD-OE1	5.86	1.32	1.25
1	A	254	GLU	CD-OE2	5.81	1.32	1.25
1	A	228	GLU	CD-OE2	5.79	1.32	1.25

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ILE	C-N-CA	-8.65	104.13	122.30
1	A	105	ASP	CB-CG-OD1	-8.64	110.52	118.30
1	A	269	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	A	290	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	282	ASP	CB-CG-OD2	7.25	124.82	118.30
1	A	176	ASP	CB-CG-OD1	-7.03	111.97	118.30
1	A	290	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	293	ASP	CB-CG-OD1	6.66	124.30	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	A	145	ALA	N-CA-CB	-6.43	101.10	110.10
1	A	274	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	234	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	145	ALA	CA-C-N	-6.33	103.28	117.20
1	A	269	ASP	CB-CG-OD1	6.29	123.97	118.30
1	A	49	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	293	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	49	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	282	ASP	CB-CG-OD1	-6.18	112.73	118.30
1	A	118	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	110	GLU	N-CA-CB	6.14	121.65	110.60
1	A	88	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	116	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	303	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	A	118	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	88	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	A	143	PRO	N-CA-CB	5.68	110.11	103.30
1	A	145	ALA	O-C-N	5.57	131.61	122.70
1	A	63	PRO	N-CA-CB	5.52	109.93	103.30
1	A	97	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	176	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	156	VAL	CA-CB-CG1	-5.44	102.74	110.90
1	A	247	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	317	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	274	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	305	ILE	CB-CA-C	-5.14	101.32	111.60
1	A	174	PRO	CB-CA-C	-5.06	99.36	112.00
1	A	156	VAL	CG1-CB-CG2	5.03	118.94	110.90

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	182	0
2	A	16	0	11	0	0
3	A	19	0	0	3	0
All	All	2236	0	2241	182	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 41.

All (182) 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: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:36:ILE:O	1:A:37:ASN:C	2.15	0.82
1:A:182:ARG:NH1	1:A:224:ILE:H	1.78	0.82
1:A:147:ILE:O	1:A:148:GLY:C	2.09	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: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:65:GLN:HE21	1:A:236:ASN:ND2	1.90	0.69
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLN:NE2	1:A:234:ASP:OD1	2.29	0.65
1:A:70:LYS:HA	1:A:70:LYS:HZ3	1.58	0.65
1:A:42:THR:O	1:A:45:ASP:N	2.30	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:171:VAL:HG12	1:A:172:LYS:N	2.14	0.62
1:A:10:LEU:HD21	1:A:40:ILE:HD13	1.80	0.62
1:A:8:LEU:HA	1:A:11:ILE:HG22	1.80	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: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:87:ILE:HG12	1:A:88:ASP:OD1	2.01	0.58
1:A:62:GLU:HG2	1:A:63:PRO:O	2.02	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:155:ILE:HG22	1:A:156:VAL:N	2.19	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:65:GLN:C	1:A:66:LEU:HD23	2.24	0.57
1:A:137:TRP:O	1:A:201:ILE:HD12	2.05	0.57
1:A:287:GLY:H	1:A:317:ARG:HH12	1.51	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:167:ASP:OD1	1:A:167:ASP:N	2.36	0.56
1:A:157:MET:HB3	1:A:177:LEU:HD11	1.88	0.55
1:A:89:SER:HA	1:A:112:GLN:OE1	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:32:SER:HB3	1:A:35:ALA:H	1.72	0.54
1:A:298:LEU:O	1:A:308:PRO:HA	2.07	0.54
1:A:162:ARG:HH22	1:A:170:ARG:HH12	1.56	0.53
1:A:39:HIS:O	1:A:40:ILE:C	2.44	0.53
1:A:238:LEU:O	1:A:239:ALA:C	2.46	0.53
1:A:128:GLY:O	1:A:235:ARG:NH2	2.42	0.53
1:A:8:LEU:O	1:A:11:ILE:HG22	2.08	0.53
1:A:153:ILE:HG22	1:A:187:ILE:HG12	1.90	0.53
1:A:116:ARG:NH1	1:A:116:ARG:HB3	2.19	0.53
1:A:46:TRP:HB2	1:A:48:VAL:HG23	1.91	0.53
1:A:156:VAL:HG12	1:A:157:MET:N	2.18	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: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:88:ASP:CG	1:A:89:SER:H	2.12	0.51
1:A:231:ILE:HG22	1:A:233:LEU:HG	1.92	0.51
1:A:183:LYS:O	1:A:223:TRP:O	2.28	0.51
1:A:147:ILE:O	1:A:148:GLY:O	2.28	0.51
1:A:271:PHE:O	1:A:272:ILE:C	2.49	0.51
1:A:111:TYR:HE2	1:A:113:GLN:HG2	1.76	0.51
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:139:LEU:HD12	1:A:145:ALA:HB2	1.93	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:126:PRO:O	1:A:127:PHE:C	2.50	0.48
1:A:92:GLN:O	1:A:93:TYR:C	2.48	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:53:VAL:O	1:A:54:PRO:C	2.51	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:O	1:A:252:LEU:HD12	2.14	0.47
1:A:286:PHE:HD2	1:A:317:ARG:CD	2.16	0.47
1:A:162:ARG:HG2	1:A:167:ASP:HA	1.94	0.47
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.52	0.47
1:A:238:LEU:O	1:A:242:LEU:HG	2.14	0.47
1:A:116:ARG:HH11	1:A:116:ARG:HG2	1.78	0.47
1:A:4:ASN:O	1:A:7:PRO:HD2	2.14	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: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:305:ILE:HG22	1:A:306:ILE:N	2.30	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:42:THR:O	1:A:43:LEU:C	2.50	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:HB2	1:A:168:LYS:HE3	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:15:ALA:C	1:A:17:GLY:H	2.18	0.45
1:A:293:ASP:C	1:A:295:GLN:H	2.19	0.45
1:A:41:GLN:HA	1:A:41:GLN:OE1	2.17	0.44
1:A:65:GLN:NE2	1:A:236:ASN:HD22	2.16	0.44
1:A:133:LEU:HD23	1:A:133:LEU:C	2.38	0.44
1:A:170:ARG:NH1	1:A:170:ARG:CG	2.80	0.44
1:A:103:SER:HB3	1:A:138:ARG:H	1.83	0.44
1:A:226:LEU:HA	1:A:226:LEU:HD23	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:NH1	1:A:170:ARG:HG2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:O	1:A:254:GLU:HG2	2.19	0.43
1:A:46:TRP:CD1	1:A:46:TRP:N	2.81	0.43
1:A:179:LEU:HB3	1:A:224:ILE:HD12	2.00	0.43
1:A:234:ASP:OD2	1:A:237:THR:N	2.52	0.42
1:A:10:LEU:HA	1:A:10:LEU:HD12	1.79	0.42
1:A:259:ALA:CB	1:A:260:PRO:CD	2.98	0.42
1:A:286:PHE:HB3	1:A:317:ARG:NH1	2.34	0.42
1:A:70:LYS:HA	1:A:70:LYS:HZ2	1.78	0.42
1:A:64:ILE:HG22	1:A:66:LEU:CD2	2.49	0.42
1:A:102:LYS:N	1:A:105:ASP:OD2	2.46	0.42
1:A:160:VAL:O	1:A:161:LEU:C	2.56	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:149:LEU:C	1:A:149:LEU:HD12	2.41	0.41
1:A:22:GLY:O	1:A:23:GLU:C	2.58	0.41
1:A:201:ILE:CD1	1:A:201:ILE:N	2.80	0.41
1:A:110:GLU:O	1:A:128:GLY:N	2.46	0.41
1:A:171:VAL:HG12	1:A:172:LYS:H	1.84	0.41
1:A:307:LYS:HB2	1:A:308:PRO:CD	2.51	0.41
1:A:103:SER:HB2	1:A:137:TRP:CE3	2.56	0.41
1:A:40:ILE:HA	1:A:40:ILE:HD12	1.72	0.41
1:A:189:VAL:HG12	1:A:190:GLU:N	2.35	0.41
1:A:149:LEU:HA	1:A:149:LEU:HD13	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:264:ARG:O	1:A:265:TRP:C	2.57	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%)	5	17

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 ⓘ

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%)	181 (82%)	40 (18%)	2	6

All (40) 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	19	PHE
1	A	23	GLU
1	A	28	THR
1	A	40	ILE
1	A	49	ASP
1	A	52	THR
1	A	61	PRO
1	A	62	GLU
1	A	70	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	75	GLN
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	125	SER
1	A	147	ILE
1	A	149	LEU
1	A	150	SER
1	A	155	ILE
1	A	164	LEU
1	A	172	LYS
1	A	184	LEU
1	A	191	LEU
1	A	200	GLN
1	A	224	ILE
1	A	238	LEU
1	A	243	ILE
1	A	277	LYS
1	A	280	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	71	GLN
1	A	200	GLN
1	A	227	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 carbohydrates 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	-	12,17,17	3.39	7 (58%)	13,23,23	2.63	7 (53%)

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	-	-	0/5/28/28	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	BTN	C9-C10	-7.23	1.17	1.52
2	A	500	BTN	C4-N2	-5.25	1.35	1.45
2	A	500	BTN	C2-S1	-4.37	1.75	1.82
2	A	500	BTN	C6-S1	2.34	1.88	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	BTN	C3-N1	2.81	1.39	1.35
2	A	500	BTN	C8-C9	2.88	1.68	1.51
2	A	500	BTN	C7-C2	3.66	1.61	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	BTN	O3-C3-N1	-4.83	120.30	125.90
2	A	500	BTN	C8-C9-C10	-2.99	101.25	113.90
2	A	500	BTN	N2-C3-N1	-2.26	107.32	108.88
2	A	500	BTN	C8-C7-C2	-2.25	108.47	113.70
2	A	500	BTN	C9-C8-C7	-2.22	105.76	113.66
2	A	500	BTN	C5-N1-C3	-2.12	110.90	112.49
2	A	500	BTN	O3-C3-N2	5.57	132.37	125.90

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 [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%)	-0.88	1 (0%) 94 92	17, 46, 91, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	PRO	2.5

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	BTN	A	500	16/16	0.98	0.12	0.16	25,34,83,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.