



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:51 PM UTC

PDB ID : 1LEL / pdb_00001lel
Title : The avidin BCAP complex
Authors : Pazy, Y.; Kulik, T.; Bayer, E.A.; Wilchek, M.; Livnah, O.
Deposited on : 2002-04-10
Resolution : 2.90 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**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

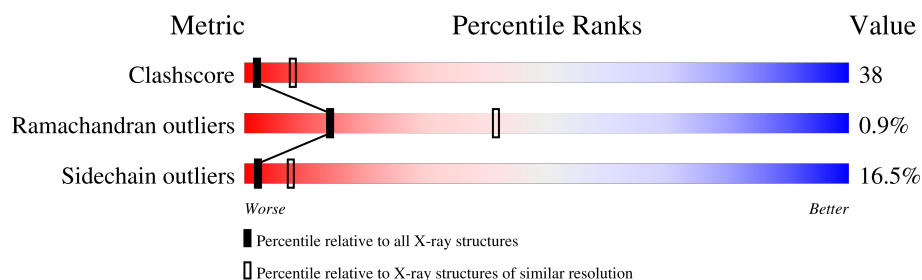
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	128	
1	B	128	

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
2	NAG	A	401	X	-	-	-
2	NAG	B	402	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1871 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.

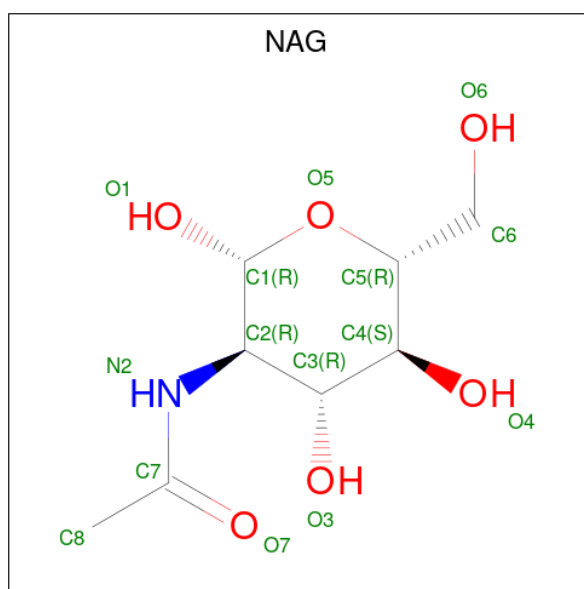
- Molecule 1 is a protein called Avidin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	0	0	0
			889	558	156	171	4			
1	B	115	Total	C	N	O	S	0	0	0
			906	569	158	175	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	THR	ILE	conflict	UNP P02701
B	234	THR	ILE	conflict	UNP P02701

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



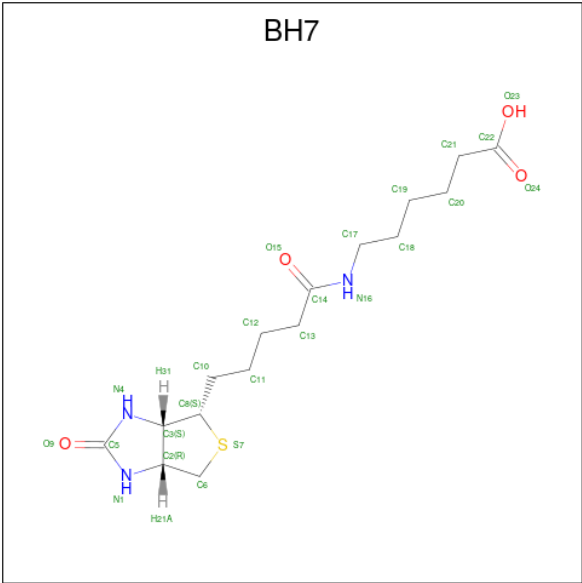
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is E-AMINO BIOTINYL CAPROIC ACID (CCD ID: BH7) (formula: C₁₆H₂₇N₃O₄S).



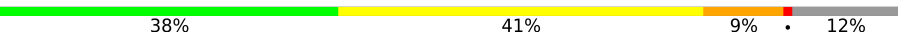
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	16	3	4	1		
3	B	1	Total	C	N	O	S	0	0
			24	16	3	4	1		

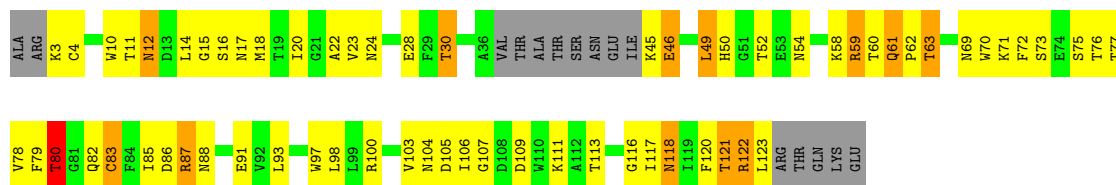
3 Residue-property plots [i](#)

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.

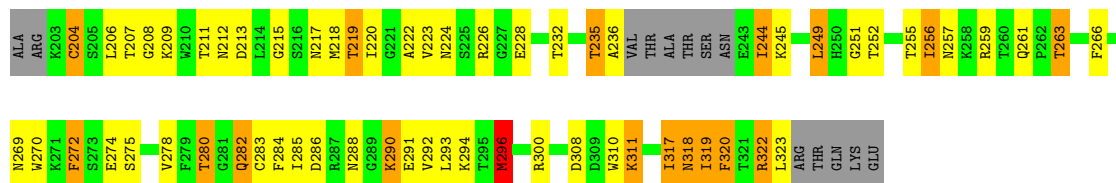
• Molecule 1: Avidin

Chain A: 



• Molecule 1: Avidin

Chain B: 



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 2	Depositor
Cell constants a, b, c, α , β , γ	70.96Å 80.69Å 43.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1871	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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: BH7, NAG

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	0.76	1/906 (0.1%)	1.13	6/1224 (0.5%)
1	B	0.76	1/923 (0.1%)	1.16	5/1247 (0.4%)
All	All	0.76	2/1829 (0.1%)	1.15	11/2471 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	ASN	N-CA	6.19	1.54	1.45
1	B	319	ILE	N-CA	-5.10	1.40	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	THR	N-CA-C	-8.64	96.13	109.52
1	A	85	ILE	N-CA-C	-8.12	95.42	107.51
1	B	212	ASN	N-CA-C	7.43	117.81	108.45
1	B	235	THR	N-CA-C	6.96	120.38	110.14
1	A	61	GLN	CA-C-N	6.24	126.60	119.92
1	A	61	GLN	C-N-CA	6.24	126.60	119.92
1	B	320	PHE	N-CA-C	6.12	119.62	110.14
1	A	12	ASN	N-CA-C	6.05	118.40	109.69
1	A	113	THR	N-CA-C	5.99	119.00	109.24
1	B	296	MET	N-CA-C	-5.10	101.44	109.50
1	B	244	ILE	N-CA-C	-5.03	100.88	108.12

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	889	0	871	77	0
1	B	906	0	887	87	0
2	A	14	0	13	4	0
2	B	14	0	13	2	0
3	A	24	0	26	6	0
3	B	24	0	26	3	0
All	All	1871	0	1836	138	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 38.

All (138) 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:B:288:ASN:HD21	1:B:290:LYS:HE2	1.19	1.07
1:A:103:VAL:H	1:B:282:GLN:HE22	1.11	0.99
1:B:218:MET:HE3	1:B:220:ILE:HD11	1.45	0.96
1:A:45:LYS:HD3	1:A:72:PHE:HB3	1.45	0.95
1:B:211:THR:HB	1:B:323:LEU:HD13	1.57	0.84
1:A:122:ARG:HG3	1:A:122:ARG:HH11	1.42	0.84
1:B:296:MET:HE2	1:B:317:ILE:HG13	1.59	0.83
1:B:288:ASN:ND2	1:B:290:LYS:HE2	1.92	0.83
1:A:103:VAL:H	1:B:282:GLN:NE2	1.78	0.80
1:B:209:LYS:HG3	1:B:219:THR:HG22	1.66	0.76
1:A:11:THR:HB	1:A:123:LEU:HD13	1.70	0.73
1:B:204:CYS:HG	1:B:283:CYS:HG	0.70	0.68
1:B:272:PHE:HD1	1:B:272:PHE:H	1.41	0.67
1:B:256:ILE:HG22	1:B:257:ASN:N	2.09	0.67
1:A:86:ASP:HB3	1:A:88:ASN:OD1	1.93	0.67
1:A:97:TRP:CE2	3:A:402:BH7:H61	2.29	0.67
1:B:224:ASN:ND2	1:B:228:GLU:HG2	2.10	0.66
1:A:15:GLY:O	2:A:401:NAG:H83	1.95	0.66
1:A:106:ILE:HD11	1:B:292:VAL:HG11	1.78	0.65
1:B:218:MET:CE	1:B:220:ILE:HD11	2.25	0.65
1:A:103:VAL:N	1:B:282:GLN:HE22	1.89	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLN:HG2	1:B:284:PHE:CE1	2.32	0.65
1:B:288:ASN:HD21	1:B:290:LYS:CE	2.03	0.64
1:B:290:LYS:NZ	1:B:290:LYS:HB3	2.12	0.64
1:B:211:THR:HB	1:B:323:LEU:CD1	2.27	0.64
1:A:104:ASN:HA	1:B:259:ARG:HH22	1.63	0.63
1:A:106:ILE:CD1	1:B:292:VAL:HG11	2.29	0.63
1:B:296:MET:CE	1:B:317:ILE:HG13	2.27	0.62
1:B:275:SER:HB2	1:B:300:ARG:O	2.01	0.61
1:B:217:ASN:ND2	2:B:402:NAG:C7	2.64	0.60
1:A:45:LYS:CD	1:A:72:PHE:HB3	2.26	0.60
1:B:204:CYS:CB	1:B:283:CYS:SG	2.91	0.59
1:B:251:GLY:HA3	1:B:266:PHE:HB3	1.85	0.59
1:A:16:SER:HA	2:A:401:NAG:H82	1.84	0.59
1:B:204:CYS:CB	1:B:283:CYS:HG	2.15	0.58
1:B:272:PHE:HZ	3:B:2:BH7:H15	1.68	0.58
1:A:76:THR:OG1	1:B:263:THR:CG2	2.51	0.58
1:B:288:ASN:OD1	1:B:290:LYS:HG2	2.02	0.58
1:B:256:ILE:HG22	1:B:257:ASN:OD1	2.04	0.58
1:A:11:THR:CB	1:A:123:LEU:HD13	2.34	0.57
1:A:3:LYS:HG3	1:A:60:THR:HG22	1.87	0.56
1:A:122:ARG:HG3	1:A:122:ARG:NH1	2.15	0.56
1:A:59:ARG:HH11	1:A:59:ARG:CB	2.19	0.55
1:B:204:CYS:HB3	1:B:283:CYS:SG	2.46	0.55
1:A:12:ASN:HD21	1:A:16:SER:HB2	1.71	0.54
1:A:24:ASN:OD1	1:A:28:GLU:N	2.40	0.54
1:A:11:THR:CG2	1:A:123:LEU:HD13	2.37	0.54
1:A:97:TRP:CE2	3:A:402:BH7:C6	2.90	0.53
1:A:54:ASN:HB2	1:A:63:THR:HG22	1.91	0.53
1:A:59:ARG:HH11	1:A:59:ARG:CG	2.21	0.53
1:B:215:GLY:O	2:B:402:NAG:H82	2.09	0.53
1:A:14:LEU:O	1:A:14:LEU:HG	2.08	0.53
1:A:30:THR:HG22	1:A:49:LEU:O	2.09	0.53
1:A:50:HIS:NE2	1:B:226:ARG:NH2	2.57	0.52
1:B:318:ASN:C	1:B:319:ILE:HG13	2.34	0.52
1:A:78:VAL:HG13	1:B:280:THR:HG23	1.89	0.52
1:B:207:THR:OG1	1:B:222:ALA:HA	2.09	0.52
1:B:249:LEU:C	1:B:249:LEU:HD23	2.35	0.52
1:B:249:LEU:C	1:B:249:LEU:CD2	2.83	0.51
1:B:286:ASP:HB3	1:B:290:LYS:HG3	1.92	0.51
1:A:77:THR:HG22	1:A:79:PHE:CE1	2.46	0.51
1:B:244:ILE:O	1:B:245:LYS:HD2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:THR:HG21	1:B:300:ARG:CB	2.41	0.51
1:A:18:MET:HE3	1:A:20:ILE:HD11	1.92	0.50
2:A:401:NAG:O6	2:A:401:NAG:C1	2.59	0.50
1:B:261:GLN:HB3	1:B:283:CYS:O	2.11	0.50
1:B:285:ILE:HG22	1:B:285:ILE:O	2.12	0.50
1:B:224:ASN:HD21	1:B:228:GLU:HG2	1.76	0.50
1:B:291:GLU:OE1	1:B:322:ARG:NH1	2.45	0.50
1:A:62:PRO:O	1:A:82:GLN:HG3	2.10	0.49
1:B:208:GLY:O	1:B:219:THR:HA	2.12	0.49
1:B:272:PHE:CZ	3:B:2:BH7:H15	2.46	0.49
1:B:218:MET:HE3	1:B:220:ILE:CD1	2.32	0.49
1:B:235:THR:OG1	1:B:236:ALA:N	2.44	0.49
1:A:97:TRP:CZ2	3:A:402:BH7:C6	2.95	0.49
1:A:105:ASP:C	1:A:107:GLY:H	2.19	0.49
1:B:286:ASP:HB3	1:B:290:LYS:CG	2.42	0.49
1:B:270:TRP:CZ2	3:B:2:BH7:H12	2.48	0.49
1:A:61:GLN:HB3	1:A:83:CYS:O	2.13	0.48
1:A:76:THR:OG1	1:B:263:THR:HG22	2.12	0.48
1:A:118:ASN:OD1	3:A:402:BH7:N1	2.47	0.48
1:A:100:ARG:NH2	1:A:109:ASP:OD1	2.43	0.48
1:A:104:ASN:OD1	1:B:259:ARG:NH2	2.46	0.48
1:A:73:SER:O	1:B:256:ILE:HG13	2.13	0.48
1:A:78:VAL:HG22	1:A:98:LEU:HB2	1.95	0.48
1:B:224:ASN:C	1:B:224:ASN:OD1	2.57	0.47
1:A:77:THR:CG2	1:A:79:PHE:CE1	2.98	0.47
1:A:52:THR:HG22	1:B:269:ASN:ND2	2.30	0.47
1:B:270:TRP:HE3	1:B:272:PHE:HE1	1.61	0.47
1:A:105:ASP:C	1:A:107:GLY:N	2.71	0.46
1:B:294:LYS:HD2	1:B:319:ILE:HG12	1.97	0.46
1:A:103:VAL:HG22	1:B:282:GLN:NE2	2.30	0.46
1:B:235:THR:O	1:B:236:ALA:HB2	2.16	0.46
1:A:80:THR:CG2	1:B:300:ARG:CB	2.94	0.45
1:A:97:TRP:CZ2	1:A:116:GLY:HA3	2.51	0.45
1:B:286:ASP:OD1	1:B:288:ASN:OD1	2.34	0.45
1:A:54:ASN:HA	1:B:269:ASN:OD1	2.17	0.45
1:A:79:PHE:O	1:B:278:VAL:HG11	2.17	0.45
1:A:97:TRP:CD2	3:A:402:BH7:H61	2.52	0.45
1:A:63:THR:HG21	1:B:275:SER:HA	1.97	0.45
1:B:320:PHE:CD1	1:B:320:PHE:N	2.84	0.45
1:B:310:TRP:CZ3	1:B:311:LYS:HB3	2.52	0.45
1:A:70:TRP:HD1	1:A:75:SER:O	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:THR:HG21	1:B:300:ARG:HB2	1.99	0.44
1:B:290:LYS:HB3	1:B:290:LYS:HZ3	1.79	0.44
1:B:282:GLN:HG2	1:B:284:PHE:CZ	2.53	0.44
1:B:288:ASN:CG	1:B:290:LYS:HE2	2.43	0.43
1:A:45:LYS:HB3	1:A:46:GLU:H	1.56	0.43
1:B:293:LEU:O	1:B:319:ILE:HA	2.18	0.43
1:B:270:TRP:HD1	1:B:275:SER:O	2.02	0.43
1:A:4:CYS:HA	1:A:91:GLU:OE2	2.18	0.43
1:A:80:THR:HG21	1:B:300:ARG:HB3	2.01	0.43
1:A:93:LEU:HB2	1:A:120:PHE:HB2	2.01	0.42
1:A:103:VAL:CG2	1:B:284:PHE:CZ	3.02	0.42
1:A:78:VAL:CG2	1:A:98:LEU:HB2	2.49	0.42
1:A:103:VAL:HG23	1:B:284:PHE:HE1	1.84	0.42
1:B:293:LEU:HB2	1:B:320:PHE:HB2	2.01	0.42
1:A:22:ALA:O	1:A:23:VAL:C	2.62	0.42
1:A:69:ASN:OD1	1:A:69:ASN:N	2.52	0.42
1:B:228:GLU:HB3	1:B:252:THR:HG22	2.01	0.42
1:A:3:LYS:NZ	1:A:59:ARG:O	2.51	0.42
1:A:80:THR:CG2	1:B:300:ARG:HB3	2.50	0.42
1:A:80:THR:CG2	1:B:300:ARG:HB2	2.49	0.42
1:A:15:GLY:O	2:A:401:NAG:C8	2.67	0.42
1:A:87:ARG:HH11	1:A:87:ARG:HG2	1.84	0.42
1:A:59:ARG:NH1	1:A:59:ARG:HG2	2.35	0.41
1:A:105:ASP:CG	1:A:107:GLY:H	2.28	0.41
1:A:79:PHE:CD1	1:A:79:PHE:N	2.87	0.41
1:A:49:LEU:C	1:A:49:LEU:HD23	2.45	0.41
1:A:54:ASN:OD1	1:B:274:GLU:HA	2.21	0.41
1:A:59:ARG:CG	1:A:59:ARG:NH1	2.80	0.41
1:A:103:VAL:HG23	1:B:284:PHE:CE1	2.55	0.41
1:B:272:PHE:CD1	1:B:272:PHE:N	2.72	0.41
1:A:10:TRP:HA	1:A:121:THR:O	2.20	0.41
1:B:256:ILE:HG22	1:B:257:ASN:CG	2.47	0.40
1:A:97:TRP:CZ2	3:A:402:BH7:H62	2.56	0.40
1:B:259:ARG:HG2	1:B:259:ARG:HH11	1.86	0.40
1:B:286:ASP:N	1:B:290:LYS:O	2.50	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	109/128 (85%)	98 (90%)	10 (9%)	1 (1%)	14	41
1	B	111/128 (87%)	108 (97%)	2 (2%)	1 (1%)	14	41
All	All	220/256 (86%)	206 (94%)	12 (6%)	2 (1%)	14	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	256	ILE
1	A	58	LYS

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	99/112 (88%)	85 (86%)	14 (14%)	3	11
1	B	101/112 (90%)	82 (81%)	19 (19%)	1	5
All	All	200/224 (89%)	167 (84%)	33 (16%)	2	8

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	46	GLU
1	A	49	LEU
1	A	59	ARG

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Mol	Chain	Res	Type
1	A	63	THR
1	A	71	LYS
1	A	80	THR
1	A	83	CYS
1	A	87	ARG
1	A	111	LYS
1	A	117	ILE
1	A	118	ASN
1	A	121	THR
1	A	122	ARG
1	B	204	CYS
1	B	206	LEU
1	B	213	ASP
1	B	219	THR
1	B	223	VAL
1	B	232	THR
1	B	249	LEU
1	B	255	THR
1	B	263	THR
1	B	272	PHE
1	B	280	THR
1	B	282	GLN
1	B	290	LYS
1	B	296	MET
1	B	308	ASP
1	B	311	LYS
1	B	317	ILE
1	B	318	ASN
1	B	322	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	82	GLN
1	B	282	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](#)

4 ligands are 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	NAG	B	402	1	14,14,15	0.55	0	17,19,21	0.88	1 (5%)
3	BH7	B	2	-	25,25,25	3.07	11 (44%)	32,32,32	1.59	6 (18%)
2	NAG	A	401	1	14,14,15	0.85	0	17,19,21	1.00	1 (5%)
3	BH7	A	402	-	25,25,25	3.06	11 (44%)	32,32,32	1.59	6 (18%)

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	NAG	B	402	1	1/1/5/7	2/6/23/26	0/1/1/1
3	BH7	B	2	-	-	6/16/37/37	0/2/2/2
2	NAG	A	401	1	1/1/5/7	2/6/23/26	0/1/1/1
3	BH7	A	402	-	-	6/16/37/37	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	BH7	C5-N1	8.52	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	BH7	C5-N1	8.48	1.50	1.35
3	A	402	BH7	O24-C22	6.56	1.43	1.22
3	B	2	BH7	O24-C22	6.56	1.43	1.22
3	B	2	BH7	C14-N16	4.58	1.44	1.33
3	A	402	BH7	C14-N16	4.53	1.44	1.33
3	B	2	BH7	C17-N16	4.26	1.55	1.46
3	A	402	BH7	C17-N16	4.24	1.55	1.46
3	B	2	BH7	C13-C14	3.59	1.58	1.51
3	A	402	BH7	C13-C14	3.56	1.58	1.51
3	A	402	BH7	C5-N4	3.33	1.41	1.35
3	B	2	BH7	C5-N4	3.29	1.41	1.35
3	A	402	BH7	C21-C22	3.25	1.58	1.50
3	B	2	BH7	C21-C22	3.21	1.58	1.50
3	A	402	BH7	C6-C2	3.10	1.59	1.53
3	B	2	BH7	C6-C2	3.08	1.59	1.53
3	A	402	BH7	C2-C3	2.57	1.63	1.55
3	B	2	BH7	C2-C3	2.55	1.63	1.55
3	A	402	BH7	C3-N4	2.39	1.50	1.45
3	B	2	BH7	C3-N4	2.38	1.50	1.45
3	A	402	BH7	C20-C21	2.18	1.60	1.52
3	B	2	BH7	C20-C21	2.17	1.60	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	BH7	O23-C22-C21	3.82	126.08	114.00
3	A	402	BH7	O23-C22-C21	3.81	126.03	114.00
3	A	402	BH7	O24-C22-C21	-3.38	112.36	123.09
3	B	2	BH7	O24-C22-C21	-3.38	112.38	123.09
3	A	402	BH7	C17-N16-C14	2.88	128.18	122.82
3	B	2	BH7	C17-N16-C14	2.83	128.10	122.82
2	A	401	NAG	C2-N2-C7	-2.79	119.17	122.90
3	A	402	BH7	C2-C6-S7	-2.49	102.64	106.06
3	B	2	BH7	C2-C6-S7	-2.48	102.65	106.06
2	B	402	NAG	C2-N2-C7	-2.25	119.88	122.90
3	B	2	BH7	C3-C8-S7	-2.22	102.51	105.03
3	A	402	BH7	C3-C8-S7	-2.15	102.59	105.03
3	B	2	BH7	C12-C13-C14	2.11	119.05	113.19
3	A	402	BH7	C12-C13-C14	2.09	119.00	113.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	NAG	C1
2	B	402	NAG	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	BH7	C11-C12-C13-C14
3	B	2	BH7	C11-C12-C13-C14
2	B	402	NAG	C4-C5-C6-O6
2	A	401	NAG	O5-C5-C6-O6
2	B	402	NAG	O5-C5-C6-O6
2	A	401	NAG	C4-C5-C6-O6
3	A	402	BH7	C12-C13-C14-O15
3	B	2	BH7	C12-C13-C14-O15
3	A	402	BH7	C12-C13-C14-N16
3	B	2	BH7	C12-C13-C14-N16
3	A	402	BH7	C17-C18-C19-C20
3	B	2	BH7	C17-C18-C19-C20
3	A	402	BH7	N16-C17-C18-C19
3	B	2	BH7	N16-C17-C18-C19
3	B	2	BH7	C18-C19-C20-C21
3	A	402	BH7	C18-C19-C20-C21

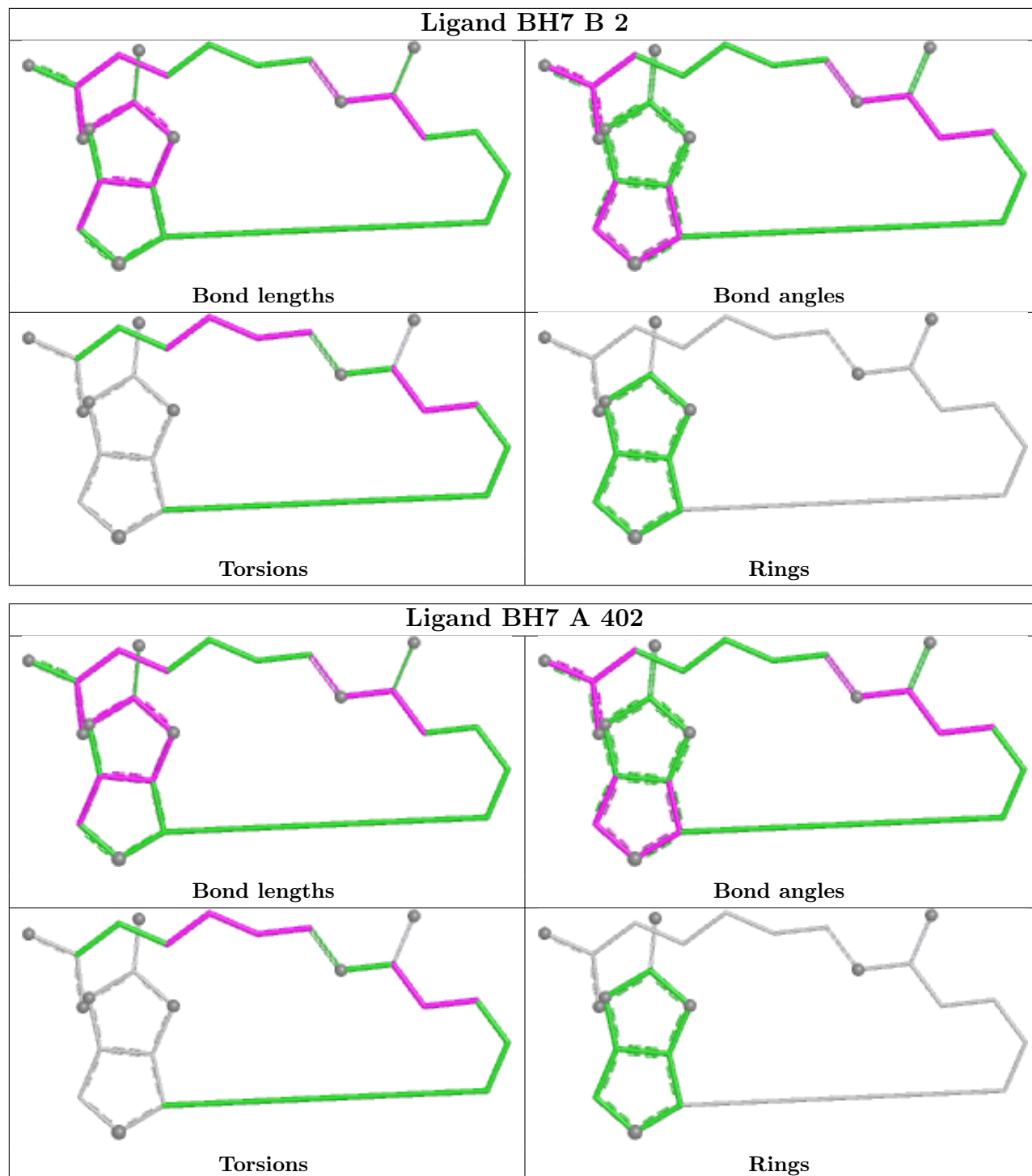
There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	NAG	2	0
3	B	2	BH7	3	0
2	A	401	NAG	4	0
3	A	402	BH7	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



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.