



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:09 AM UTC

PDB ID : 1AVD / pdb_00001avd
Title : THREE-DIMENSIONAL STRUCTURE OF THE TETRAGONAL CRYSTAL FORM OF EGG-WHITE AVIDIN IN ITS FUNCTIONAL COMPLEX WITH BIOTIN AT 2.7 ANGSTROMS RESOLUTION
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Deposited on : 1993-03-05
Resolution : 2.70 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

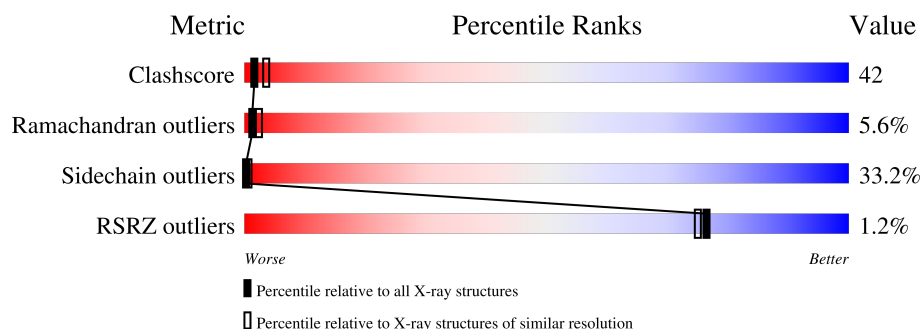
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	128	
1	B	128	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2022 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	123	Total	C	N	O	S	73	0	0
			964	602	170	188	4			
1	B	124	Total	C	N	O	S	67	0	0
			975	608	174	189	4			

There are 2 discrepancies between the modelled and reference sequences:

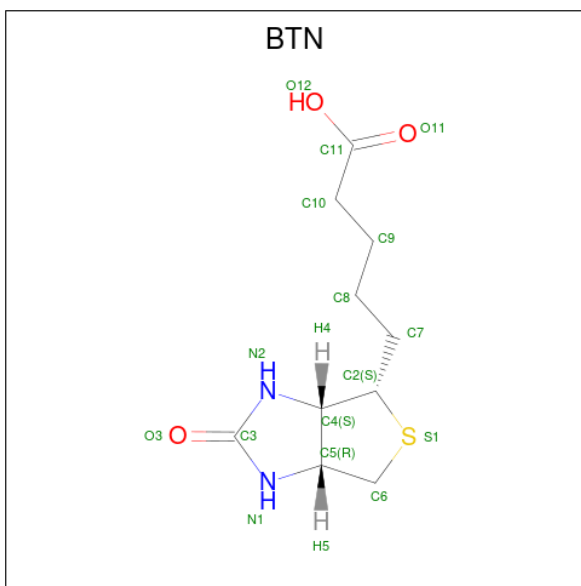
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	THR	ILE	SEE REMARK 999	UNP P02701
B	34	THR	ILE	SEE REMARK 999	UNP P02701

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 3 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$).



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

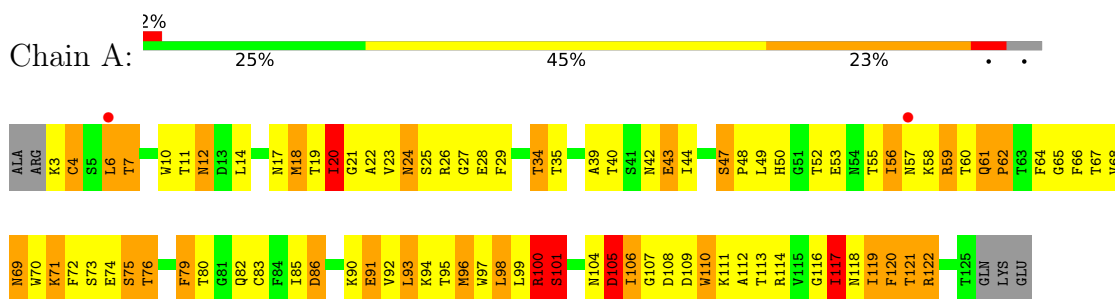
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	18	Total	O	0	0
			18	18		

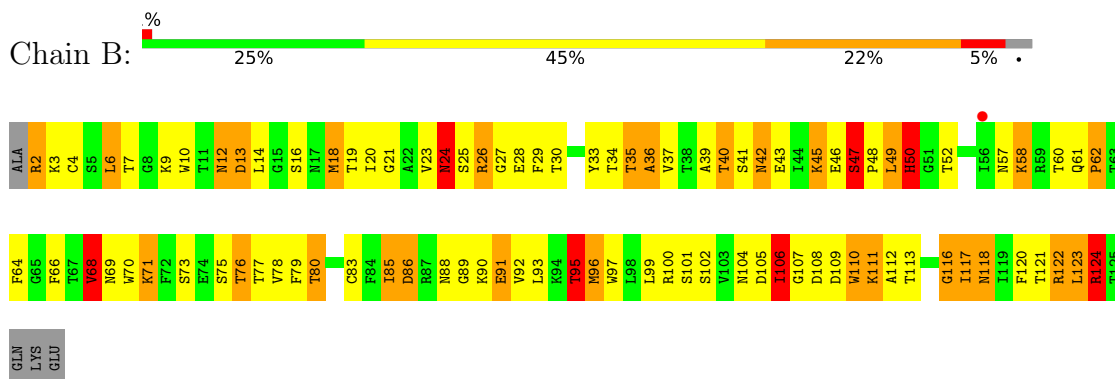
3 Residue-property plots

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: AVIDIN



- Molecule 1: AVIDIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.15Å 80.15Å 85.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.70 58.40 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70) 89.7 (58.40-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.174 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 243.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2022	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BTN, 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	1.50	5/982 (0.5%)	2.00	29/1330 (2.2%)
1	B	1.48	3/993 (0.3%)	1.96	36/1344 (2.7%)
All	All	1.49	8/1975 (0.4%)	1.98	65/2674 (2.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	35	THR	C-N	-6.07	1.24	1.33
1	A	52	THR	N-CA	-5.97	1.38	1.46
1	A	101	SER	CA-C	-5.59	1.45	1.52
1	A	111	LYS	CA-C	-5.46	1.45	1.52
1	B	49	LEU	CA-C	-5.42	1.46	1.52
1	A	100	ARG	N-CA	-5.29	1.39	1.46
1	A	97	TRP	NE1-CE2	-5.14	1.31	1.37
1	B	80	THR	CA-C	-5.05	1.46	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	HIS	CA-CB-CG	13.90	127.70	113.80
1	A	24	ASN	CA-CB-CG	-9.68	102.92	112.60
1	B	62	PRO	CB-CA-C	-9.61	98.36	110.95
1	B	68	VAL	N-CA-CB	9.54	124.04	111.64
1	B	95	THR	N-CA-CB	-8.36	98.08	111.62
1	A	39	ALA	N-CA-C	-7.98	104.02	114.31
1	B	80	THR	CA-CB-OG1	7.86	121.38	109.60
1	A	108	ASP	CA-CB-CG	7.77	120.37	112.60
1	A	12	ASN	CA-CB-CG	-7.61	104.99	112.60
1	B	25	SER	N-CA-C	-7.54	103.96	113.01
1	B	80	THR	CB-CA-C	-7.54	96.46	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	THR	N-CA-CB	7.37	123.19	110.81
1	A	104	ASN	N-CA-CB	7.30	121.63	110.61
1	B	42	ASN	CB-CA-C	7.28	123.49	110.16
1	A	12	ASN	CB-CA-C	-7.22	97.95	110.45
1	A	100	ARG	CB-CA-C	6.80	120.91	109.48
1	B	39	ALA	N-CA-C	-6.76	104.84	113.23
1	B	42	ASN	N-CA-CB	6.76	123.21	111.39
1	A	79	PHE	CA-CB-CG	6.72	120.52	113.80
1	B	24	ASN	CB-CA-C	-6.64	97.20	110.42
1	B	85	ILE	N-CA-CB	6.48	119.51	111.41
1	B	33	TYR	CA-C-O	6.40	127.42	120.32
1	B	68	VAL	CA-CB-CG1	-6.34	99.62	110.40
1	A	98	LEU	N-CA-CB	6.22	121.65	110.83
1	B	118	ASN	CA-CB-CG	-6.14	106.46	112.60
1	B	89	GLY	CA-C-O	6.11	125.91	119.06
1	B	41	SER	CB-CA-C	-6.04	102.36	111.73
1	A	69	ASN	N-CA-CB	6.03	119.34	110.35
1	B	47	SER	CB-CA-C	6.03	117.94	108.84
1	A	113	THR	N-CA-C	5.95	119.23	108.69
1	A	20	ILE	CB-CA-C	-5.90	101.84	110.81
1	A	99	LEU	CA-C-N	-5.82	113.98	122.65
1	A	99	LEU	C-N-CA	-5.82	113.98	122.65
1	B	50	HIS	CA-CB-CG	5.78	119.58	113.80
1	B	96	MET	CB-CA-C	5.73	120.65	110.16
1	B	88	ASN	N-CA-C	-5.73	106.14	113.01
1	A	75	SER	N-CA-C	5.69	118.90	110.48
1	B	112	ALA	N-CA-C	5.66	120.05	113.20
1	A	119	ILE	CA-C-N	-5.63	113.80	122.87
1	A	119	ILE	C-N-CA	-5.63	113.80	122.87
1	B	104	ASN	CB-CA-C	-5.63	98.89	110.38
1	A	25	SER	N-CA-C	-5.46	107.16	113.88
1	A	117	ILE	CB-CA-C	-5.44	102.37	111.29
1	B	42	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	36	ALA	N-CA-CB	-5.35	102.78	110.65
1	B	40	THR	CA-C-N	5.35	131.25	123.12
1	B	40	THR	C-N-CA	5.35	131.25	123.12
1	B	58	LYS	N-CA-CB	5.32	119.48	110.49
1	B	107	GLY	N-CA-C	-5.32	107.27	115.73
1	A	117	ILE	CB-CG1-CD1	-5.30	102.66	113.80
1	A	24	ASN	CB-CA-C	-5.29	99.89	110.42
1	A	66	PHE	O-C-N	5.25	129.04	123.42
1	A	76	THR	N-CA-CB	5.23	119.47	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	THR	CA-C-N	5.22	130.50	122.93
1	B	113	THR	C-N-CA	5.22	130.50	122.93
1	B	80	THR	OG1-CB-CG2	5.19	119.69	109.30
1	A	62	PRO	CB-CA-C	-5.15	104.21	110.95
1	B	14	LEU	CA-C-N	-5.12	115.39	122.86
1	B	14	LEU	C-N-CA	-5.12	115.39	122.86
1	B	116	GLY	N-CA-C	5.10	118.92	110.55
1	A	80	THR	CA-CB-OG1	-5.09	101.96	109.60
1	B	95	THR	N-CA-C	5.07	116.69	109.14
1	A	61	GLN	CA-C-N	5.02	125.00	120.03
1	A	61	GLN	C-N-CA	5.02	125.00	120.03
1	A	105	ASP	N-CA-C	5.01	117.56	108.69

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	964	0	946	74	0
1	B	975	0	960	79	0
2	A	14	0	13	0	0
3	A	16	0	15	4	0
3	B	16	0	15	5	0
4	A	19	0	0	3	1
4	B	18	0	0	1	0
All	All	2022	0	1949	151	1

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 42.

All (151) 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:24:ASN:HB3	1:B:26:ARG:H	1.29	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LYS:HE2	1:B:45:LYS:HA	1.49	0.92
1:B:75:SER:HB2	1:B:100:ARG:O	1.81	0.80
1:A:70:TRP:CZ2	3:A:400:BTN:H81	2.22	0.75
1:B:93:LEU:HB2	1:B:120:PHE:HB2	1.67	0.74
1:B:100:ARG:HD2	1:B:101:SER:O	1.89	0.72
1:A:12:ASN:HB3	1:A:14:LEU:H	1.55	0.71
1:A:29:PHE:HE2	1:A:53:GLU:HB2	1.53	0.71
1:B:2:ARG:HG3	1:B:3:LYS:H	1.57	0.70
1:B:70:TRP:CZ2	3:B:401:BTN:H81	2.29	0.67
1:B:122:ARG:HD2	1:B:124:ARG:CD	2.25	0.65
1:B:10:TRP:CZ3	1:B:93:LEU:HD13	2.33	0.64
1:A:73:SER:C	1:A:75:SER:H	2.05	0.64
1:B:97:TRP:CZ2	1:B:116:GLY:HA3	2.33	0.63
1:A:18:MET:HE3	1:A:20:ILE:HD11	1.81	0.63
1:A:7:THR:HG1	1:A:21:GLY:C	2.07	0.63
1:A:7:THR:OG1	1:A:22:ALA:HA	1.99	0.62
1:B:66:PHE:CE1	1:B:79:PHE:CD1	2.87	0.62
1:B:95:THR:CG2	1:B:118:ASN:HB2	2.29	0.62
1:B:70:TRP:CE2	3:B:401:BTN:H81	2.36	0.61
1:A:49:LEU:HD12	1:A:49:LEU:O	2.01	0.60
1:B:110:TRP:CZ2	1:B:111:LYS:HE3	2.37	0.59
1:A:29:PHE:CE2	1:A:53:GLU:HB2	2.36	0.59
1:B:12:ASN:OD1	1:B:12:ASN:C	2.45	0.59
1:B:24:ASN:CB	1:B:26:ARG:H	2.10	0.59
1:B:122:ARG:CD	1:B:124:ARG:HD2	2.33	0.58
1:B:70:TRP:CH2	3:B:401:BTN:H81	2.39	0.58
1:A:86:ASP:HB2	1:A:90:LYS:O	2.04	0.58
1:B:48:PRO:HD2	1:B:69:ASN:O	2.04	0.58
1:B:61:GLN:HB3	1:B:83:CYS:O	2.04	0.57
1:A:65:GLY:HA2	1:A:79:PHE:O	2.04	0.57
1:A:61:GLN:HB2	4:A:521:HOH:O	2.03	0.57
1:B:122:ARG:HD2	1:B:124:ARG:HD3	1.86	0.57
1:A:49:LEU:HD12	1:A:49:LEU:C	2.30	0.56
1:B:18:MET:HG2	1:B:120:PHE:HE2	1.70	0.56
1:B:18:MET:HE2	1:B:120:PHE:CD2	2.41	0.56
1:A:49:LEU:HA	1:A:67:THR:O	2.06	0.55
1:B:47:SER:HB3	1:B:48:PRO:HD2	1.88	0.55
1:B:4:CYS:SG	1:B:91:GLU:HG2	2.47	0.54
1:A:26:ARG:HB2	1:A:28:GLU:OE2	2.07	0.54
1:A:24:ASN:HB3	1:A:26:ARG:H	1.72	0.54
1:B:47:SER:CB	1:B:48:PRO:HD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:C	1:B:49:LEU:HD12	2.34	0.53
1:B:77:THR:HG22	1:B:78:VAL:N	2.22	0.53
1:B:105:ASP:O	1:B:108:ASP:N	2.34	0.53
1:B:2:ARG:HG3	1:B:3:LYS:N	2.22	0.53
1:A:64:PHE:CZ	1:A:95:THR:HG22	2.44	0.53
1:A:67:THR:HG22	1:A:68:VAL:N	2.24	0.53
1:B:122:ARG:CD	1:B:124:ARG:CD	2.86	0.53
1:B:27:GLY:O	1:B:29:PHE:HD1	1.91	0.53
1:B:47:SER:CB	1:B:48:PRO:CD	2.88	0.52
1:B:86:ASP:HB2	1:B:90:LYS:O	2.10	0.52
1:A:47:SER:HB3	1:A:48:PRO:HD2	1.92	0.51
1:B:18:MET:HG2	1:B:120:PHE:CE2	2.45	0.51
1:A:73:SER:C	1:A:75:SER:N	2.68	0.51
1:B:109:ASP:O	1:B:111:LYS:N	2.44	0.51
1:B:95:THR:HG23	1:B:96:MET:N	2.26	0.51
1:A:35:THR:HG23	1:A:35:THR:O	2.12	0.50
1:B:95:THR:HG22	1:B:118:ASN:O	2.11	0.50
1:A:10:TRP:HB3	1:A:121:THR:O	2.11	0.50
1:A:64:PHE:CZ	1:A:93:LEU:HG	2.46	0.50
1:B:86:ASP:OD1	1:B:92:VAL:HG21	2.12	0.50
1:B:18:MET:HE2	1:B:120:PHE:CE2	2.48	0.49
1:A:91:GLU:CD	1:A:122:ARG:HH11	2.21	0.49
1:A:6:LEU:HD12	1:A:29:PHE:CE2	2.47	0.49
1:A:120:PHE:N	1:A:120:PHE:CD1	2.81	0.49
1:A:91:GLU:CD	1:A:122:ARG:NH1	2.71	0.49
1:B:30:THR:HG22	1:B:50:HIS:CB	2.44	0.48
1:A:70:TRP:HZ2	3:A:400:BTN:S1	2.37	0.48
1:A:70:TRP:CE2	3:A:400:BTN:H81	2.49	0.48
1:A:49:LEU:HB3	1:A:68:VAL:HG22	1.96	0.48
1:A:107:GLY:HA3	4:A:542:HOH:O	2.14	0.48
1:B:2:ARG:CG	1:B:3:LYS:N	2.77	0.47
1:B:68:VAL:O	1:B:76:THR:HG22	2.14	0.47
1:A:64:PHE:CZ	1:A:95:THR:CG2	2.98	0.47
1:A:117:ILE:HD12	1:A:117:ILE:HG21	1.43	0.47
1:B:9:LYS:HB3	1:B:123:LEU:HD12	1.97	0.47
1:B:16:SER:OG	1:B:36:ALA:N	2.47	0.47
1:B:62:PRO:HD2	1:B:83:CYS:HB3	1.96	0.47
1:A:7:THR:O	1:A:122:ARG:NH2	2.48	0.47
1:A:47:SER:HB3	1:A:69:ASN:O	2.15	0.47
1:A:73:SER:OG	1:A:75:SER:HB3	2.15	0.47
1:B:117:ILE:HG23	1:B:118:ASN:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:HB	1:A:118:ASN:H	1.50	0.46
1:B:48:PRO:HG2	1:B:69:ASN:HB3	1.98	0.46
1:B:91:GLU:C	1:B:92:VAL:HG23	2.40	0.46
1:A:48:PRO:HD2	1:A:69:ASN:O	2.15	0.46
1:A:4:CYS:SG	1:A:83:CYS:C	2.98	0.46
1:B:2:ARG:NH2	4:B:545:HOH:O	2.47	0.46
1:B:95:THR:HG22	1:B:118:ASN:HB2	1.97	0.46
1:B:13:ASP:OD1	1:B:13:ASP:N	2.49	0.46
1:B:36:ALA:C	1:B:37:VAL:HG13	2.40	0.46
1:B:106:ILE:C	1:B:108:ASP:H	2.22	0.46
1:B:47:SER:HB3	1:B:48:PRO:CD	2.46	0.45
1:B:71:LYS:HD3	1:B:71:LYS:HA	1.59	0.45
1:A:12:ASN:OD1	1:A:120:PHE:CE2	2.69	0.45
1:B:95:THR:CG2	1:B:118:ASN:CB	2.94	0.45
1:A:24:ASN:HD22	1:A:24:ASN:HA	1.20	0.45
1:A:47:SER:HA	1:A:48:PRO:HD3	1.67	0.45
1:B:109:ASP:O	1:B:110:TRP:C	2.59	0.45
1:B:7:THR:HG23	1:B:21:GLY:O	2.17	0.45
1:B:75:SER:HB2	1:B:101:SER:HA	1.99	0.44
1:A:12:ASN:HA	1:A:119:ILE:O	2.16	0.44
1:B:28:GLU:HG3	1:B:52:THR:CG2	2.48	0.44
1:B:45:LYS:HA	1:B:45:LYS:CE	2.22	0.44
1:A:71:LYS:HA	1:A:71:LYS:HD3	1.36	0.44
1:B:28:GLU:HG3	1:B:52:THR:HG22	1.99	0.43
1:A:10:TRP:CE3	1:A:122:ARG:HG2	2.53	0.43
1:A:64:PHE:HZ	1:A:95:THR:CG2	2.32	0.43
1:A:105:ASP:C	1:A:107:GLY:N	2.74	0.43
1:B:93:LEU:CB	1:B:120:PHE:HB2	2.42	0.43
1:A:70:TRP:HB2	1:A:75:SER:O	2.19	0.43
1:A:110:TRP:O	1:A:110:TRP:HE3	2.02	0.43
1:B:30:THR:HG22	1:B:50:HIS:HB3	2.00	0.43
1:B:95:THR:HG22	1:B:118:ASN:CB	2.49	0.43
1:A:27:GLY:O	1:A:53:GLU:N	2.46	0.43
1:A:100:ARG:CZ	1:A:112:ALA:HB1	2.49	0.42
1:B:68:VAL:O	1:B:76:THR:CG2	2.67	0.42
1:A:100:ARG:CZ	1:A:112:ALA:CB	2.96	0.42
1:A:100:ARG:HD3	1:A:101:SER:O	2.19	0.42
1:A:17:ASN:O	1:A:34:THR:N	2.48	0.42
1:A:100:ARG:NH2	1:A:109:ASP:OD1	2.39	0.42
1:B:6:LEU:HD12	1:B:6:LEU:HA	1.23	0.42
1:B:30:THR:HG22	1:B:50:HIS:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HD12	1:A:20:ILE:HG21	1.67	0.42
1:A:96:MET:HE1	1:B:116:GLY:HA2	2.00	0.42
1:B:64:PHE:CD1	1:B:64:PHE:C	2.98	0.42
1:B:106:ILE:C	1:B:108:ASP:N	2.75	0.42
1:A:62:PRO:O	1:A:82:GLN:HG3	2.20	0.41
1:A:62:PRO:HD2	1:A:83:CYS:HB3	2.02	0.41
1:A:69:ASN:C	1:A:69:ASN:HD22	2.28	0.41
1:A:106:ILE:H	1:A:106:ILE:HG12	1.48	0.41
1:A:20:ILE:HG23	1:A:20:ILE:HD13	1.77	0.41
1:A:118:ASN:HB3	1:A:120:PHE:CE1	2.56	0.41
1:A:107:GLY:CA	4:A:542:HOH:O	2.67	0.41
1:A:59:ARG:C	1:A:61:GLN:H	2.28	0.41
1:A:70:TRP:CZ2	3:A:400:BTN:C8	2.98	0.41
1:A:110:TRP:O	1:A:110:TRP:CE3	2.74	0.41
1:B:30:THR:HA	1:B:49:LEU:O	2.20	0.41
1:B:70:TRP:CZ2	3:B:401:BTN:C8	3.03	0.41
1:B:77:THR:CG2	1:B:78:VAL:N	2.81	0.41
1:A:43:GLU:O	1:A:43:GLU:HG3	2.20	0.41
1:A:91:GLU:OE2	1:A:122:ARG:NH1	2.54	0.40
1:A:18:MET:CE	1:A:20:ILE:HD11	2.50	0.40
1:A:23:VAL:HA	1:A:28:GLU:O	2.21	0.40
1:A:72:PHE:CD1	1:A:72:PHE:N	2.89	0.40
1:B:49:LEU:C	1:B:49:LEU:CD1	2.94	0.40
1:A:116:GLY:HA2	1:B:96:MET:HE1	2.02	0.40
1:B:35:THR:OG1	1:B:36:ALA:N	2.53	0.40
1:A:47:SER:CB	1:A:48:PRO:CD	2.99	0.40
1:B:70:TRP:CH2	3:B:401:BTN:H71	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:505:HOH:O	4:A:505:HOH:O[2_655]	1.61	0.59

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	91/128 (71%)	80 (88%)	7 (8%)	4 (4%)	2	4
1	B	122/128 (95%)	103 (84%)	11 (9%)	8 (7%)	1	1
All	All	213/256 (83%)	183 (86%)	18 (8%)	12 (6%)	1	2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ILE
1	B	24	ASN
1	B	57	ASN
1	A	58	LYS
1	B	23	VAL
1	B	58	LYS
1	B	110	TRP
1	B	124	ARG
1	A	110	TRP
1	B	13	ASP
1	A	86	ASP
1	B	106	ILE

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	108/112 (96%)	70 (65%)	38 (35%)	0	0
1	B	109/112 (97%)	75 (69%)	34 (31%)	0	1
All	All	217/224 (97%)	145 (67%)	72 (33%)	0	1

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	CYS
1	A	6	LEU
1	A	7	THR
1	A	11	THR
1	A	18	MET
1	A	19	THR
1	A	20	ILE
1	A	34	THR
1	A	40	THR
1	A	42	ASN
1	A	43	GLU
1	A	44	ILE
1	A	47	SER
1	A	55	THR
1	A	56	ILE
1	A	57	ASN
1	A	59	ARG
1	A	60	THR
1	A	71	LYS
1	A	74	GLU
1	A	76	THR
1	A	85	ILE
1	A	91	GLU
1	A	92	VAL
1	A	93	LEU
1	A	94	LYS
1	A	96	MET
1	A	98	LEU
1	A	100	ARG
1	A	101	SER
1	A	105	ASP
1	A	106	ILE
1	A	114	ARG
1	A	117	ILE
1	A	120	PHE
1	A	121	THR
1	A	122	ARG
1	B	2	ARG
1	B	6	LEU
1	B	12	ASN
1	B	18	MET
1	B	19	THR

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Mol	Chain	Res	Type
1	B	20	ILE
1	B	26	ARG
1	B	34	THR
1	B	40	THR
1	B	42	ASN
1	B	43	GLU
1	B	45	LYS
1	B	46	GLU
1	B	47	SER
1	B	50	HIS
1	B	60	THR
1	B	68	VAL
1	B	71	LYS
1	B	73	SER
1	B	76	THR
1	B	80	THR
1	B	85	ILE
1	B	86	ASP
1	B	91	GLU
1	B	95	THR
1	B	99	LEU
1	B	102	SER
1	B	106	ILE
1	B	111	LYS
1	B	117	ILE
1	B	121	THR
1	B	122	ARG
1	B	123	LEU
1	B	124	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	69	ASN
1	A	104	ASN
1	B	24	ASN

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](#)

3 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	$\# Z > 2$
3	BTN	A	400	-	17,17,17	0.73	0	23,23,23	3.12	6 (26%)
3	BTN	B	401	-	17,17,17	1.08	0	23,23,23	3.12	7 (30%)
2	NAG	A	600	1	14,14,15	0.97	1 (7%)	17,19,21	1.47	3 (17%)

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
3	BTN	A	400	-	-	2/7/28/28	0/2/2/2
3	BTN	B	401	-	-	5/7/28/28	0/2/2/2
2	NAG	A	600	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	NAG	C8-C7	2.85	1.56	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	BTN	C2-C4-N2	-13.20	99.36	113.34
3	B	401	BTN	C4-C2-S1	-8.86	94.97	105.03
3	B	401	BTN	C2-C4-N2	-6.70	106.24	113.34
3	B	401	BTN	C2-C4-C5	6.04	116.28	108.89
3	B	401	BTN	C7-C2-C4	-4.27	102.42	114.51
3	A	400	BTN	C5-C6-S1	-3.59	101.12	106.06
3	A	400	BTN	C6-C5-N1	-3.56	108.60	113.18
3	B	401	BTN	C8-C7-C2	3.35	121.74	114.04
3	B	401	BTN	C5-C6-S1	-3.21	101.65	106.06
2	A	600	NAG	O5-C5-C4	-2.57	104.57	110.83
3	B	401	BTN	N2-C3-N1	-2.30	106.19	108.85
2	A	600	NAG	O5-C5-C6	-2.28	103.23	107.66
3	A	400	BTN	C7-C2-C4	-2.20	108.28	114.51
2	A	600	NAG	C2-N2-C7	-2.18	119.98	122.90
3	A	400	BTN	C2-C4-C5	-2.15	106.26	108.89
3	A	400	BTN	C5-N1-C3	2.15	115.54	112.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	NAG	C8-C7-N2-C2
2	A	600	NAG	O7-C7-N2-C2
3	B	401	BTN	C2-C7-C8-C9
3	B	401	BTN	S1-C2-C7-C8
2	A	600	NAG	O5-C5-C6-O6
2	A	600	NAG	C4-C5-C6-O6
3	B	401	BTN	C11-C10-C9-C8
3	B	401	BTN	C9-C10-C11-O11
3	B	401	BTN	C9-C10-C11-O12
3	A	400	BTN	C2-C7-C8-C9
3	A	400	BTN	C9-C10-C11-O12

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	BTN	4	0
3	B	401	BTN	5	0

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	122/128 (95%)	-0.25	2 (1%) 70 68	5, 30, 53, 80	23 (18%)
1	B	123/128 (96%)	-0.25	1 (0%) 82 81	9, 31, 51, 67	26 (21%)
All	All	245/256 (95%)	-0.25	3 (1%) 76 75	5, 30, 53, 80	49 (20%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	LEU	2.7
1	B	56	ILE	2.3
1	A	57	ASN	2.1

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	NAG	A	600	14/15	0.83	0.12	27,74,90,90	2
3	BTN	B	401	16/16	0.96	0.08	4,20,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BTN	A	400	16/16	0.97	0.07	4,26,60,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.