



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:03 PM GMT

PDB ID : 1RXJ
Title : Crystal structure of streptavidin mutant (M2) where the L3,4 loop was replaced by that of avidin
Authors : Eisenberg-Domovich, Y.; Pazy, Y.; Nir, O.; Raboy, B.; Bayer, E.A.; Wilchek, M.; Livnah, O.
Deposited on : 2003-12-18
Resolution : 1.14 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

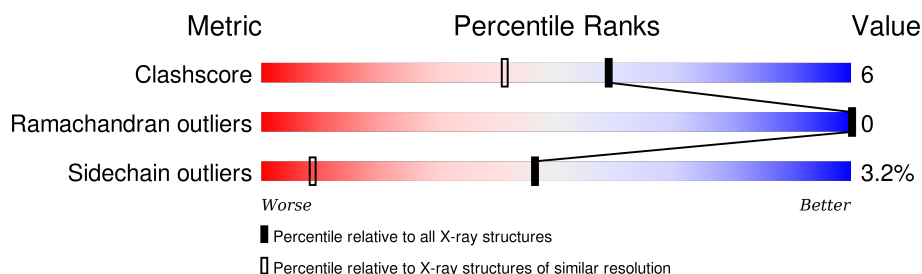
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.14 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	1593 (1.20-1.08)
Ramachandran outliers	100387	1521 (1.20-1.08)
Sidechain outliers	100360	1518 (1.20-1.08)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	121	 90% • • 5%
1	B	121	 80% 14% • 5%
1	C	121	 86% 6% • 7%
1	D	121	 85% 8% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4257 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 Streptavidin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	3	4	0
			898	564	156	178			
1	B	115	Total	C	N	O	4	6	0
			908	571	157	180			
1	C	112	Total	C	N	O	3	4	0
			876	550	151	175			
1	D	114	Total	C	N	O	4	2	0
			877	551	152	174			

There are 32 discrepancies between the modelled and reference sequences:

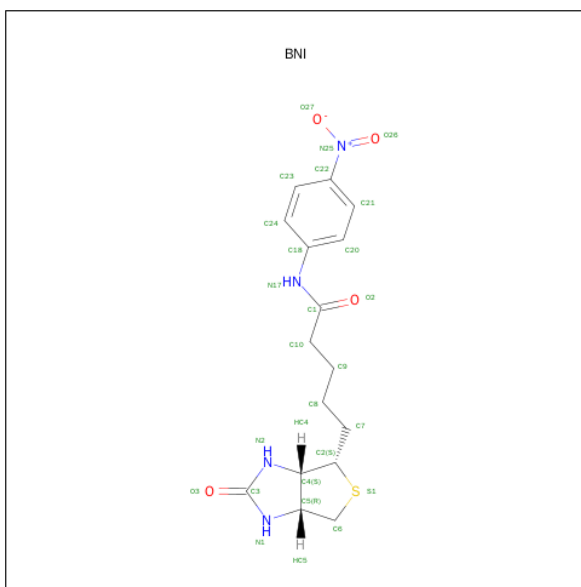
Chain	Residue	Modelled	Actual	Comment	Reference
A	48	SER	-	SEE REMARK 999	UNP P22629
A	46	ALA	-	SEE REMARK 999	UNP P22629
A	47	THR	-	SEE REMARK 999	UNP P22629
A	48	SER	GLY	SEE REMARK 999	UNP P22629
A	49	ASN	ASN	SEE REMARK 999	UNP P22629
A	50	GLU	ALA	SEE REMARK 999	UNP P22629
A	51	ILE	GLU	SEE REMARK 999	UNP P22629
A	52	LYS	SER	SEE REMARK 999	UNP P22629
B	48	SER	-	SEE REMARK 999	UNP P22629
B	46	ALA	-	SEE REMARK 999	UNP P22629
B	47	THR	-	SEE REMARK 999	UNP P22629
B	48	SER	GLY	SEE REMARK 999	UNP P22629
B	49	ASN	ASN	SEE REMARK 999	UNP P22629
B	50	GLU	ALA	SEE REMARK 999	UNP P22629
B	51	ILE	GLU	SEE REMARK 999	UNP P22629
B	52	LYS	SER	SEE REMARK 999	UNP P22629
C	48	SER	-	SEE REMARK 999	UNP P22629
C	46	ALA	-	SEE REMARK 999	UNP P22629
C	47	THR	-	SEE REMARK 999	UNP P22629
C	48	SER	GLY	SEE REMARK 999	UNP P22629
C	49	ASN	ASN	SEE REMARK 999	UNP P22629

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Chain	Residue	Modelled	Actual	Comment	Reference
C	50	GLU	ALA	SEE REMARK 999	UNP P22629
C	51	ILE	GLU	SEE REMARK 999	UNP P22629
C	52	LYS	SER	SEE REMARK 999	UNP P22629
D	48	SER	-	SEE REMARK 999	UNP P22629
D	46	ALA	-	SEE REMARK 999	UNP P22629
D	47	THR	-	SEE REMARK 999	UNP P22629
D	48	SER	GLY	SEE REMARK 999	UNP P22629
D	49	ASN	ASN	SEE REMARK 999	UNP P22629
D	50	GLU	ALA	SEE REMARK 999	UNP P22629
D	51	ILE	GLU	SEE REMARK 999	UNP P22629
D	52	LYS	SER	SEE REMARK 999	UNP P22629

- Molecule 2 is 5-(2-OXO-HEXAHYDRO-THIENO[3,4-D]IMIDAZOL-6-YL)-PENTANOIC ACID (4-NITRO-PHENYL)-AMIDE (three-letter code: BNI) (formula: C₁₆H₂₀N₄O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			25	16	4	4	1		
2	B	1	Total	C	N	O	S	0	0
			25	16	4	4	1		
2	C	1	Total	C	N	O	S	0	0
			25	16	4	4	1		
2	D	1	Total	C	N	O	S	0	0
			25	16	4	4	1		

- Molecule 3 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	184	Total 184	O 184	0	0
3	B	131	Total 131	O 131	0	0
3	C	139	Total 139	O 139	0	0
3	D	144	Total 144	O 144	0	0

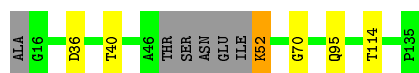
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.


Note EDS was not executed.

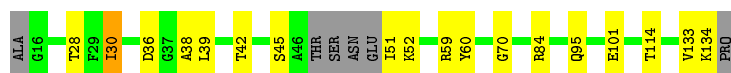
• Molecule 1: Streptavidin

Chain A:  90% • • 5%



• Molecule 1: Streptavidin

Chain B:  80% 14% • 5%




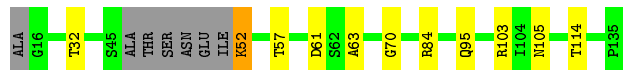
• Molecule 1: Streptavidin

Chain C:  86% 6% • 7%



• Molecule 1: Streptavidin

Chain D:  85% 8% • 6%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.35Å 85.08Å 57.69Å 90.00° 98.17° 90.00°	Depositor
Resolution (Å)	56.80 – 1.14	Depositor
% Data completeness (in resolution range)	97.0 (56.80-1.14)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.179 , 0.200	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4257	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: BNI

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	0.65	2/920 (0.2%)	0.76	2/1257 (0.2%)
1	B	0.41	0/935	0.73	1/1277 (0.1%)
1	C	0.45	1/897 (0.1%)	0.78	1/1227 (0.1%)
1	D	0.38	0/899	0.74	1/1229 (0.1%)
All	All	0.48	3/3651 (0.1%)	0.75	5/4990 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	LYS	CG-CD	14.67	2.02	1.52
1	C	52	LYS	CG-CD	-7.36	1.27	1.52
1	A	52	LYS	CE-NZ	7.11	1.66	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	LYS	CB-CG-CD	10.57	139.09	111.60
1	A	36	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	52	LYS	CB-CG-CD	-6.67	94.25	111.60
1	D	52	LYS	CA-CB-CG	-5.80	100.63	113.40
1	B	36	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	133[B]	VAL	Mainchain

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	898	0	851	6	0
1	B	908	0	857	23	0
1	C	876	0	824	11	0
1	D	877	0	828	11	0
2	A	25	0	20	0	0
2	B	25	0	20	0	0
2	C	25	0	20	0	0
2	D	25	0	20	0	0
3	A	184	0	0	1	0
3	B	131	0	0	2	0
3	C	139	0	0	1	0
3	D	144	0	0	2	0
All	All	4257	0	3440	41	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 6.

All (41) 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:C:80:LYS:NZ	1:D:61:ASP:OD1	1.97	0.96
1:A:114:THR:H	1:B:95:GLN:HE22	1.20	0.88
1:C:95:GLN:HE22	1:D:114:THR:H	1.22	0.85
1:A:95:GLN:HE22	1:B:114:THR:H	1.24	0.83
1:C:114:THR:H	1:D:95:GLN:HE22	1.27	0.82
1:C:40[A]:THR:HG22	3:C:817:HOH:O	1.80	0.82
1:D:103:ARG:NE	1:D:105:ASN:HD21	1.94	0.66
1:B:28[A]:THR:HG21	3:B:840:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ILE:HG23	1:B:42:THR:OG1	2.07	0.55
1:B:30:ILE:CG2	1:B:42:THR:OG1	2.54	0.55
1:A:114:THR:H	1:B:95:GLN:NE2	1.99	0.55
1:B:39[A]:LEU:HD12	1:B:39[A]:LEU:N	2.23	0.54
1:C:95:GLN:NE2	1:D:114:THR:H	2.01	0.54
1:B:39[B]:LEU:HD12	1:B:39[B]:LEU:N	2.23	0.54
1:B:39[A]:LEU:HD13	1:B:59:ARG:CA	2.39	0.51
1:C:80:LYS:HZ1	1:D:63:ALA:H	1.58	0.50
1:C:70:GLY:HA3	1:C:95:GLN:HE21	1.76	0.50
1:D:57[B]:THR:CG2	3:D:869:HOH:O	2.60	0.50
1:A:40[B]:THR:HG23	3:A:852:HOH:O	2.10	0.49
1:C:114:THR:H	1:D:95:GLN:NE2	2.04	0.49
1:B:39[B]:LEU:HD13	1:B:59:ARG:CA	2.41	0.49
1:B:39[A]:LEU:HD11	1:B:60:TYR:HB3	1.94	0.49
1:B:38:ALA:C	1:B:39[B]:LEU:HD12	2.34	0.48
1:B:39[B]:LEU:HD11	1:B:60:TYR:HB3	1.97	0.47
1:B:38:ALA:C	1:B:39[A]:LEU:HD12	2.36	0.46
1:A:95:GLN:NE2	1:B:114:THR:H	2.04	0.46
1:C:80:LYS:HZ2	1:C:80:LYS:HB2	1.80	0.45
1:B:39[B]:LEU:CD1	1:B:39[B]:LEU:N	2.80	0.44
1:D:70:GLY:HA3	1:D:95:GLN:HE21	1.82	0.44
1:B:39[A]:LEU:CD1	1:B:39[A]:LEU:N	2.81	0.44
1:C:103:ARG:HH11	1:C:129[B]:THR:HG21	1.82	0.44
1:B:70:GLY:HA3	1:B:95:GLN:HE21	1.83	0.44
1:A:70:GLY:HA3	1:A:95:GLN:HE21	1.84	0.42
1:B:39[A]:LEU:HD11	1:B:60:TYR:CD1	2.55	0.42
1:B:39[A]:LEU:CD1	1:B:60:TYR:HD1	2.32	0.41
1:C:80:LYS:HE3	1:D:63:ALA:HB3	2.00	0.41
1:D:32[A]:THR:HG23	3:D:859:HOH:O	2.19	0.41
1:B:39[B]:LEU:HD11	1:B:60:TYR:CD1	2.55	0.41
1:B:39[B]:LEU:CD1	1:B:60:TYR:HD1	2.33	0.40
1:B:39[A]:LEU:HD11	1:B:60:TYR:HD1	1.86	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	115/121 (95%)	113 (98%)	2 (2%)	0	100	100
1	B	117/121 (97%)	113 (97%)	4 (3%)	0	100	100
1	C	112/121 (93%)	108 (96%)	4 (4%)	0	100	100
1	D	112/121 (93%)	110 (98%)	2 (2%)	0	100	100
All	All	456/484 (94%)	444 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	90/91 (99%)	89 (99%)	1 (1%)	80	47
1	B	92/91 (101%)	85 (92%)	7 (8%)	16	1
1	C	88/91 (97%)	87 (99%)	1 (1%)	80	47
1	D	88/91 (97%)	86 (98%)	2 (2%)	58	17
All	All	358/364 (98%)	347 (97%)	11 (3%)	46	9

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	B	30	ILE
1	B	45	SER
1	B	51	ILE
1	B	52	LYS
1	B	84	ARG
1	B	101	GLU
1	B	134	LYS

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Mol	Chain	Res	Type
1	C	52	LYS
1	D	52	LYS
1	D	84	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	95	GLN
1	B	95	GLN
1	B	107	GLN
1	C	82	ASN
1	C	95	GLN
1	D	82	ASN
1	D	95	GLN
1	D	107	GLN

5.3.3 RNA [i](#)

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 carbohydrates 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	BNI	A	801	-	23,27,27	1.97	7 (30%)	28,37,37	1.40	4 (14%)
2	BNI	B	802	-	23,27,27	1.97	7 (30%)	28,37,37	1.42	5 (17%)
2	BNI	C	803	-	23,27,27	1.98	7 (30%)	28,37,37	1.32	3 (10%)
2	BNI	D	804	-	23,27,27	1.97	7 (30%)	28,37,37	1.34	4 (14%)

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	BNI	A	801	-	-	0/15/36/36	0/3/3/3
2	BNI	B	802	-	-	0/15/36/36	0/3/3/3
2	BNI	C	803	-	-	0/15/36/36	0/3/3/3
2	BNI	D	804	-	-	0/15/36/36	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	804	BNI	C18-N17	-2.50	1.36	1.41
2	C	803	BNI	C18-N17	-2.38	1.37	1.41
2	A	801	BNI	C18-N17	-2.29	1.37	1.41
2	B	802	BNI	C18-N17	-2.23	1.37	1.41
2	D	804	BNI	C24-C23	2.00	1.42	1.38
2	A	801	BNI	C7-C2	2.08	1.57	1.52
2	B	802	BNI	C7-C2	2.10	1.57	1.52
2	A	801	BNI	C23-C22	2.17	1.43	1.38
2	D	804	BNI	C23-C22	2.26	1.43	1.38
2	C	803	BNI	C23-C22	2.30	1.43	1.38
2	B	802	BNI	C23-C22	2.33	1.43	1.38
2	C	803	BNI	C7-C2	2.41	1.58	1.52
2	D	804	BNI	C20-C18	2.86	1.43	1.39
2	C	803	BNI	C20-C18	2.87	1.43	1.39
2	B	802	BNI	C20-C18	2.97	1.44	1.39
2	A	801	BNI	C20-C18	3.00	1.44	1.39
2	A	801	BNI	C21-C20	3.26	1.44	1.38
2	D	804	BNI	C21-C20	3.32	1.44	1.38
2	C	803	BNI	C21-C20	3.35	1.44	1.38
2	B	802	BNI	C21-C20	3.50	1.45	1.38
2	C	803	BNI	C21-C22	3.86	1.46	1.38
2	A	801	BNI	C21-C22	3.90	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	BNI	C21-C22	4.03	1.47	1.38
2	D	804	BNI	C21-C22	4.06	1.47	1.38
2	D	804	BNI	C24-C18	4.58	1.46	1.39
2	C	803	BNI	C24-C18	4.68	1.46	1.39
2	B	802	BNI	C24-C18	4.71	1.47	1.39
2	A	801	BNI	C24-C18	4.72	1.47	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	804	BNI	C4-N2-C3	-2.69	110.09	112.66
2	A	801	BNI	O2-C1-N17	-2.63	119.02	123.72
2	D	804	BNI	O2-C1-N17	-2.55	119.17	123.72
2	C	803	BNI	O2-C1-N17	-2.45	119.34	123.72
2	A	801	BNI	C4-N2-C3	-2.43	110.33	112.66
2	B	802	BNI	O2-C1-N17	-2.10	119.97	123.72
2	B	802	BNI	C4-N2-C3	-2.08	110.67	112.66
2	B	802	BNI	O3-C3-N2	-2.08	123.49	125.90
2	C	803	BNI	N2-C3-N1	2.80	110.82	108.88
2	D	804	BNI	C10-C1-N17	2.88	119.39	114.52
2	B	802	BNI	N2-C3-N1	2.92	110.90	108.88
2	D	804	BNI	N2-C3-N1	3.27	111.14	108.88
2	A	801	BNI	C10-C1-N17	3.47	120.38	114.52
2	A	801	BNI	N2-C3-N1	3.50	111.30	108.88
2	B	802	BNI	C10-C1-N17	3.51	120.45	114.52
2	C	803	BNI	C10-C1-N17	3.70	120.78	114.52

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.