



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:49 pm GMT

PDB ID : 3B8H
Title : Structure of the eEF2-ExoA(E546A)-NAD⁺ complex
Authors : Jorgensen, R.; Merrill, A.R.
Deposited on : 2007-11-01
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : trunk28620

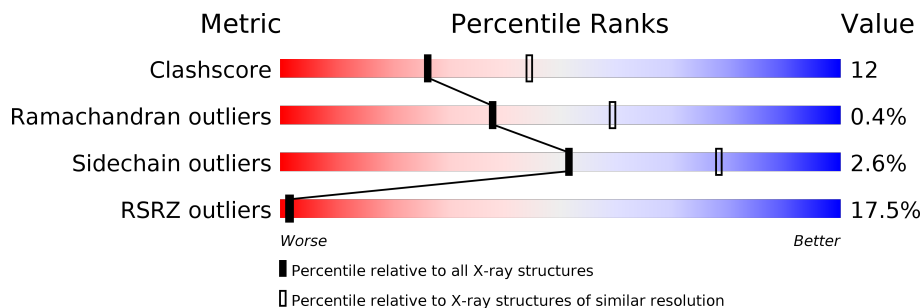
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	842	<div> <div>5%</div> <div>72%</div> <div>25%</div> <div>..</div> </div>
1	C	842	<div> <div>14%</div> <div>71%</div> <div>26%</div> <div>..</div> </div>
1	E	842	<div> <div>44%</div> <div>61%</div> <div>37%</div> <div>.</div> </div>
2	B	207	<div> <div>%</div> <div>86%</div> <div>14%</div> </div>
2	D	207	<div> <div>%</div> <div>86%</div> <div>14%</div> <div>.</div> </div>
2	F	207	<div> <div>%</div> <div>86%</div> <div>13%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24719 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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	C	823	Total	C	N	O	S	0	0	0
			6415	4082	1095	1208	30			
1	E	823	Total	C	N	O	S	0	0	0
			6415	4082	1095	1208	30			

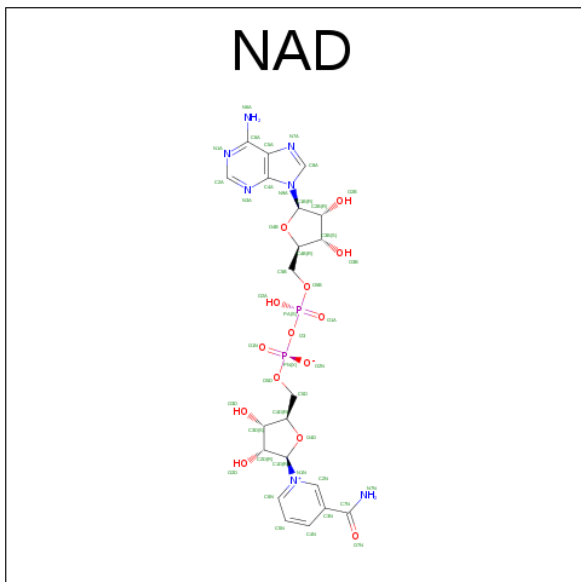
- Molecule 2 is a protein called Exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	1	0
			1592	1004	286	302			
2	D	207	Total	C	N	O	0	0	0
			1584	999	283	302			
2	F	207	Total	C	N	O	0	0	0
			1584	999	283	302			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	399	ALA	-	EXPRESSION TAG	UNP P11439
B	407	VAL	ILE	SEE REMARK 999	UNP P11439
B	515	SER	GLY	SEE REMARK 999	UNP P11439
B	546	ALA	GLU	ENGINEERED	UNP P11439
D	399	ALA	-	EXPRESSION TAG	UNP P11439
D	407	VAL	ILE	SEE REMARK 999	UNP P11439
D	515	SER	GLY	SEE REMARK 999	UNP P11439
D	546	ALA	GLU	ENGINEERED	UNP P11439
F	399	ALA	-	EXPRESSION TAG	UNP P11439
F	407	VAL	ILE	SEE REMARK 999	UNP P11439
F	515	SER	GLY	SEE REMARK 999	UNP P11439
F	546	ALA	GLU	ENGINEERED	UNP P11439

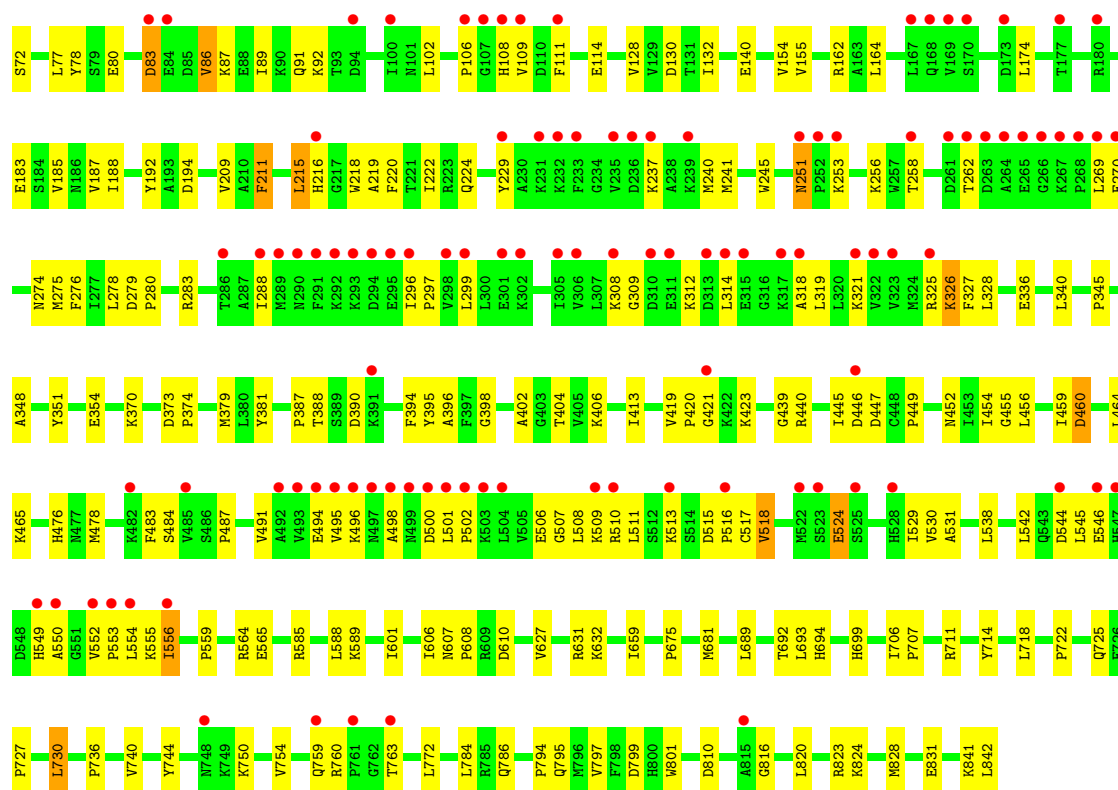
- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

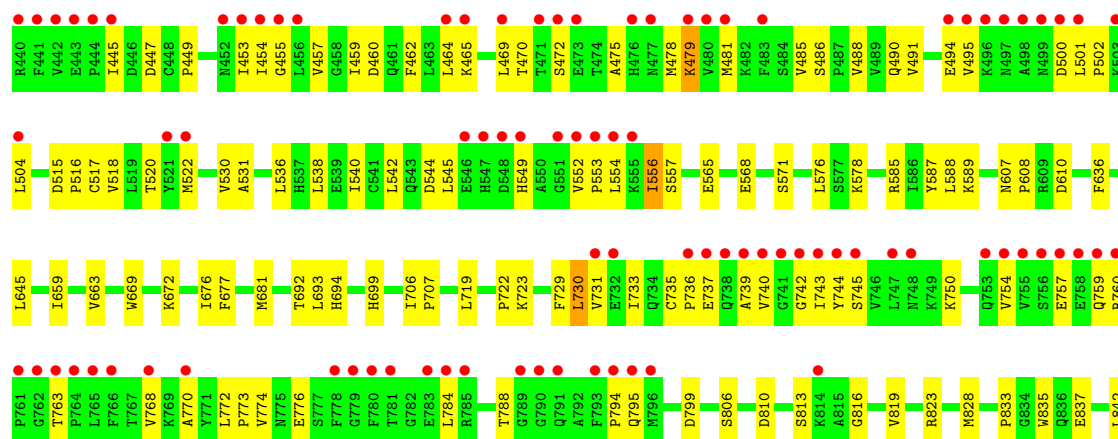


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

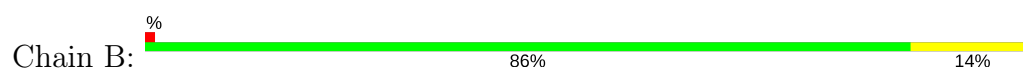
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	116	Total	O	0	0
			116	116		
4	C	77	Total	O	0	0
			77	77		
4	D	142	Total	O	0	0
			142	142		
4	E	60	Total	O	0	0
			60	60		
4	F	88	Total	O	0	0
			88	88		

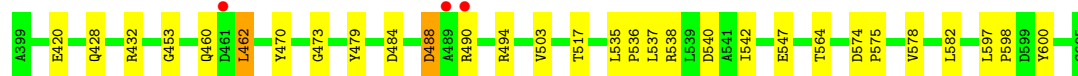
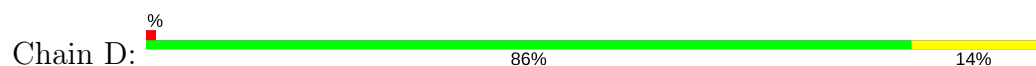




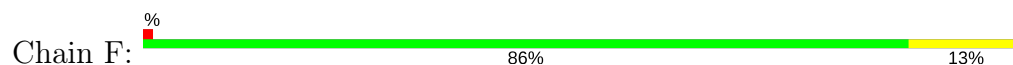
- Molecule 2: Exotoxin A



- Molecule 2: Exotoxin A



- Molecule 2: Exotoxin A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	329.44Å 68.16Å 191.63Å 90.00° 103.28° 90.00°	Depositor
Resolution (Å)	24.99 – 2.50 24.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.99-2.50) 99.0 (24.99-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.256 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24719	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.86 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.9175e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.21	0/6517	0.40	1/8823 (0.0%)
1	C	0.21	0/6517	0.40	0/8823
1	E	0.21	0/6517	0.38	0/8823
2	B	0.21	0/1634	0.40	0/2225
2	D	0.21	0/1623	0.41	0/2211
2	F	0.21	0/1623	0.39	0/2211
All	All	0.21	0/24431	0.39	1/33116 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	GLY	N-CA-C	-5.72	98.79	113.10

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	6405	0	6472	145	0
1	C	6415	0	6488	148	0
1	E	6415	0	6488	226	0
2	B	1592	0	1554	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1584	0	1541	16	0
2	F	1584	0	1541	19	0
3	B	44	0	26	1	0
3	D	44	0	26	1	0
3	F	44	0	26	2	0
4	A	109	0	0	2	0
4	B	116	0	0	1	0
4	C	77	0	0	0	0
4	D	142	0	0	2	0
4	E	60	0	0	1	0
4	F	88	0	0	0	0
All	All	24719	0	24162	567	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 12.

The worst 5 of 567 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:785:ARG:HG2	1:A:785:ARG:HH11	1.18	1.02
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.44	0.98
1:C:404:THR:HG22	1:C:449:PRO:HA	1.48	0.95
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.54	0.89
1:C:694:HIS:CE1	1:C:699:DDE:HD2	2.09	0.88

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	818/842 (97%)	780 (95%)	34 (4%)	4 (0%)	32 53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	818/842 (97%)	776 (95%)	39 (5%)	3 (0%)	38	59
1	E	818/842 (97%)	750 (92%)	65 (8%)	3 (0%)	38	59
2	B	206/207 (100%)	200 (97%)	6 (3%)	0	100	100
2	D	205/207 (99%)	199 (97%)	5 (2%)	1 (0%)	32	53
2	F	205/207 (99%)	201 (98%)	3 (2%)	1 (0%)	32	53
All	All	3070/3147 (98%)	2906 (95%)	152 (5%)	12 (0%)	38	59

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	C	309	GLY
1	E	479	LYS
1	A	479	LYS
1	A	761	PRO

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	699/714 (98%)	678 (97%)	21 (3%)	46	74
1	C	699/714 (98%)	674 (96%)	25 (4%)	40	67
1	E	699/714 (98%)	689 (99%)	10 (1%)	71	90
2	B	161/160 (101%)	158 (98%)	3 (2%)	62	85
2	D	160/160 (100%)	156 (98%)	4 (2%)	53	79
2	F	160/160 (100%)	155 (97%)	5 (3%)	45	73
All	All	2578/2622 (98%)	2510 (97%)	68 (3%)	51	78

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	154	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	326	LYS
1	E	842	LEU
1	C	194	ASP
1	C	251	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	428	GLN
2	F	428	GLN
1	E	30	HIS
1	C	30	HIS
1	E	414	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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$
1	DDE	A	699	1	6,10,21	1.08	1 (16%)	5,12,30	1.27	1 (20%)
1	DDE	C	699	1	15,20,21	1.32	2 (13%)	15,28,30	0.90	0
1	DDE	E	699	1	15,20,21	1.41	2 (13%)	15,28,30	0.98	0

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
1	DDE	A	699	1	-	0/4/6/23	0/1/1/1
1	DDE	C	699	1	-	0/19/21/23	0/1/1/1
1	DDE	E	699	1	-	0/19/21/23	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	699	DDE	CA-C	2.32	1.53	1.50
1	C	699	DDE	CA-C	2.71	1.53	1.50
1	E	699	DDE	CA-C	2.84	1.54	1.50
1	C	699	DDE	CAT-CE1	3.04	1.53	1.50
1	E	699	DDE	CAT-CE1	3.44	1.54	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	DDE	CD2-NE2-CE1	2.04	108.96	105.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	699	DDE	4	0
1	E	699	DDE	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	NAD	B	700	-	41,48,48	0.63	0	43,73,73	1.77	2 (4%)
3	NAD	D	701	-	41,48,48	0.63	0	43,73,73	1.73	2 (4%)
3	NAD	F	702	-	41,48,48	0.65	0	43,73,73	1.82	2 (4%)

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	NAD	B	700	-	-	0/22/62/62	0/5/5/5
3	NAD	D	701	-	-	0/22/62/62	0/5/5/5
3	NAD	F	702	-	-	0/22/62/62	0/5/5/5

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	NAD	N3A-C2A-N1A	-8.72	121.26	128.86
3	F	702	NAD	N3A-C2A-N1A	-8.60	121.36	128.86
3	D	701	NAD	N3A-C2A-N1A	-8.50	121.46	128.86
3	F	702	NAD	C4B-O4B-C1B	-6.29	103.08	109.77
3	B	700	NAD	C4B-O4B-C1B	-5.46	103.95	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	700	NAD	1	0
3	D	701	NAD	1	0
3	F	702	NAD	2	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

6.1 Protein, DNA and RNA chains

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	822/842 (97%)	0.24	45 (5%) 26 27	12, 51, 91, 113	0
1	C	822/842 (97%)	0.75	117 (14%) 3 2	13, 60, 136, 178	0
1	E	822/842 (97%)	2.12	370 (45%) 0 0	10, 124, 182, 229	0
2	B	207/207 (100%)	-0.15	3 (1%) 75 76	10, 22, 54, 89	0
2	D	207/207 (100%)	-0.15	3 (1%) 75 76	9, 21, 52, 95	0
2	F	207/207 (100%)	-0.17	3 (1%) 75 76	12, 27, 62, 91	0
All	All	3087/3147 (98%)	0.80	541 (17%) 2 1	9, 53, 159, 229	0

The worst 5 of 541 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	314	LEU	15.0
1	E	67	GLY	11.0
1	E	315	GLU	10.4
1	E	163	ALA	10.4
1	E	108	HIS	10.2

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	DDE	C	699	20/21	0.92	0.20	-	14,61,107,114	0
1	DDE	A	699	10/21	0.95	0.19	-	40,49,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	DDE	E	699	20/21	0.91	0.24	-	30,62,75,79	0

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(\AA^2)	Q<0.9
3	NAD	B	700	44/44	0.96	0.15	-0.50	4,20,39,42	0
3	NAD	F	702	44/44	0.96	0.14	-0.64	11,24,38,48	0
3	NAD	D	701	44/44	0.96	0.15	-0.67	7,22,38,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.