



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:33 AM GMT

PDB ID : 3B82
Title : Structure of the eEF2-ExoA(E546H)-NAD⁺ complex
Authors : Jorgensen, R.; Merrill, A.R.
Deposited on : 2007-10-31
Resolution : 2.35 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 (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

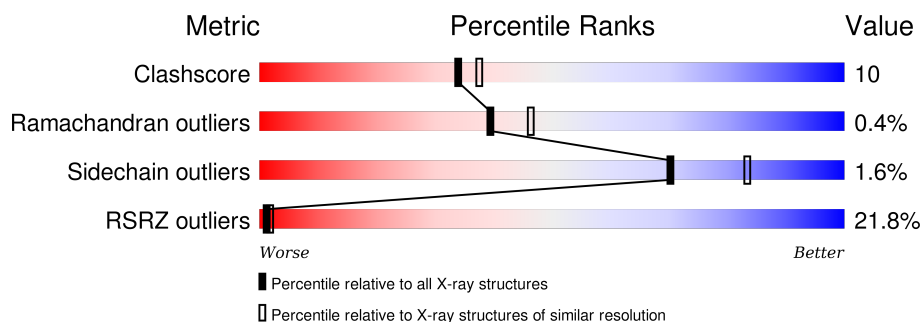
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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>9%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	C	842	<div> <div>16%</div> <div>72%</div> <div>25%</div> <div>..</div> </div>
1	E	842	<div> <div>52%</div> <div>65%</div> <div>32%</div> <div>..</div> </div>
2	B	207	<div> <div>4%</div> <div>85%</div> <div>15%</div> </div>
2	D	207	<div> <div>4%</div> <div>86%</div> <div>14%</div> <div>.</div> </div>
2	F	207	<div> <div>4%</div> <div>87%</div> <div>13%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24682 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			

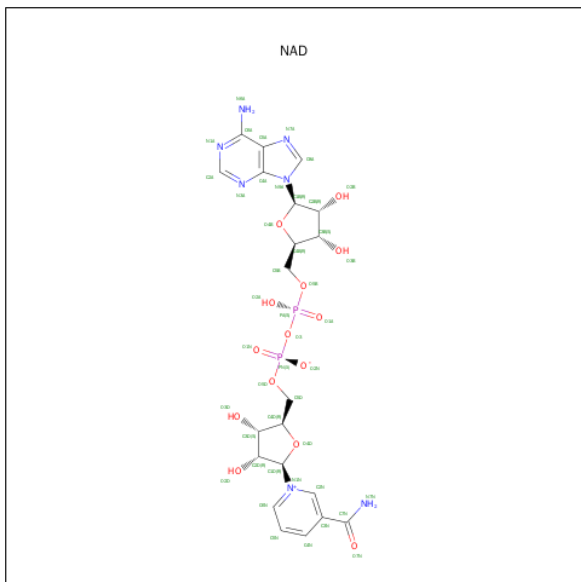
- Molecule 2 is a protein called Exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	0	0
			1589	1002	285	302			
2	D	207	Total	C	N	O	0	0	0
			1589	1002	285	302			
2	F	207	Total	C	N	O	0	0	0
			1589	1002	285	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	HIS	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	HIS	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	HIS	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		

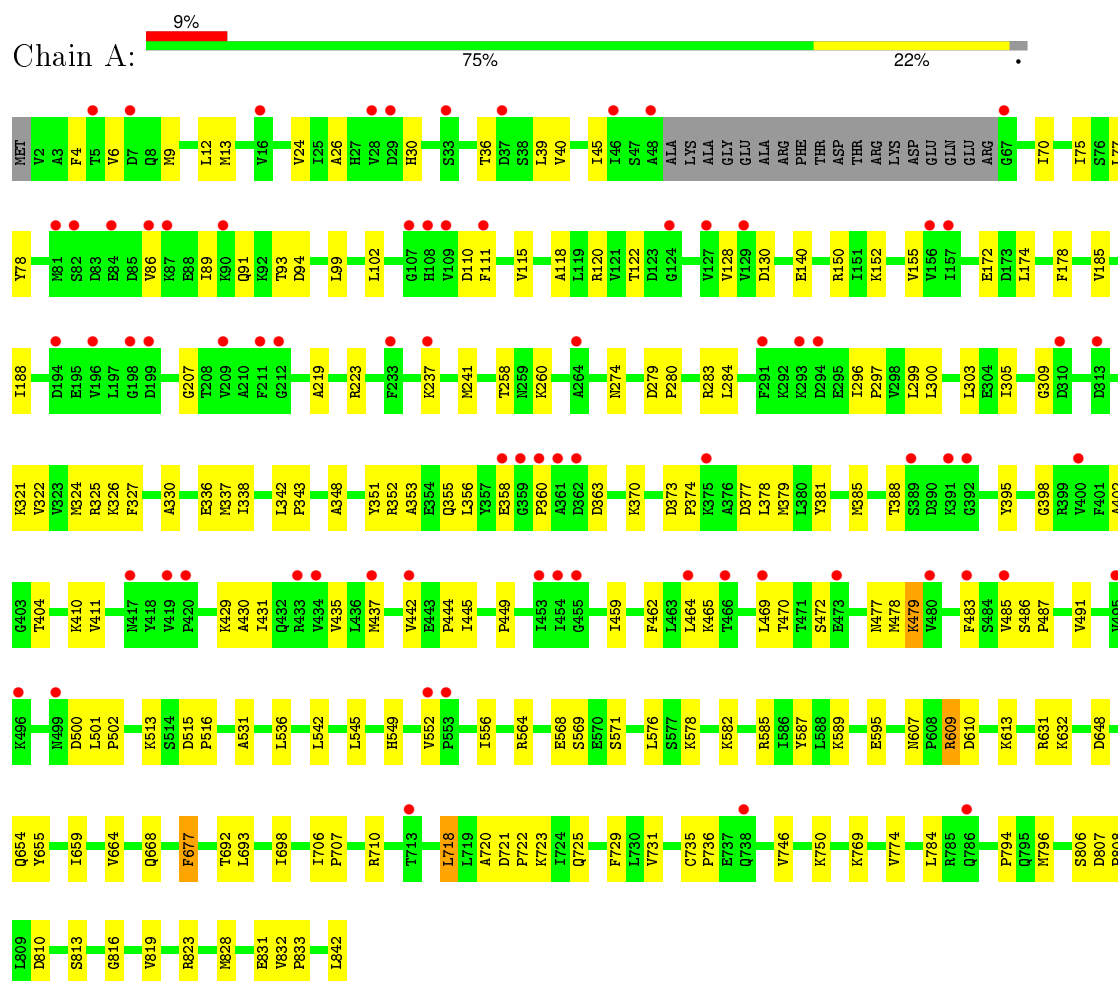
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total	O	0	0
			83	83		
4	B	117	Total	O	0	0
			117	117		
4	C	85	Total	O	0	0
			85	85		
4	D	124	Total	O	0	0
			124	124		
4	E	45	Total	O	0	0
			45	45		
4	F	94	Total	O	0	0
			94	94		

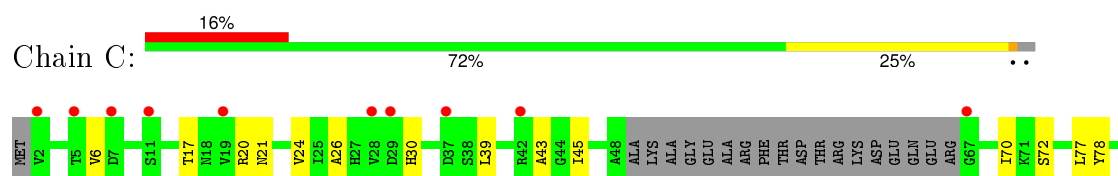
3 Residue-property plots

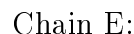
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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.

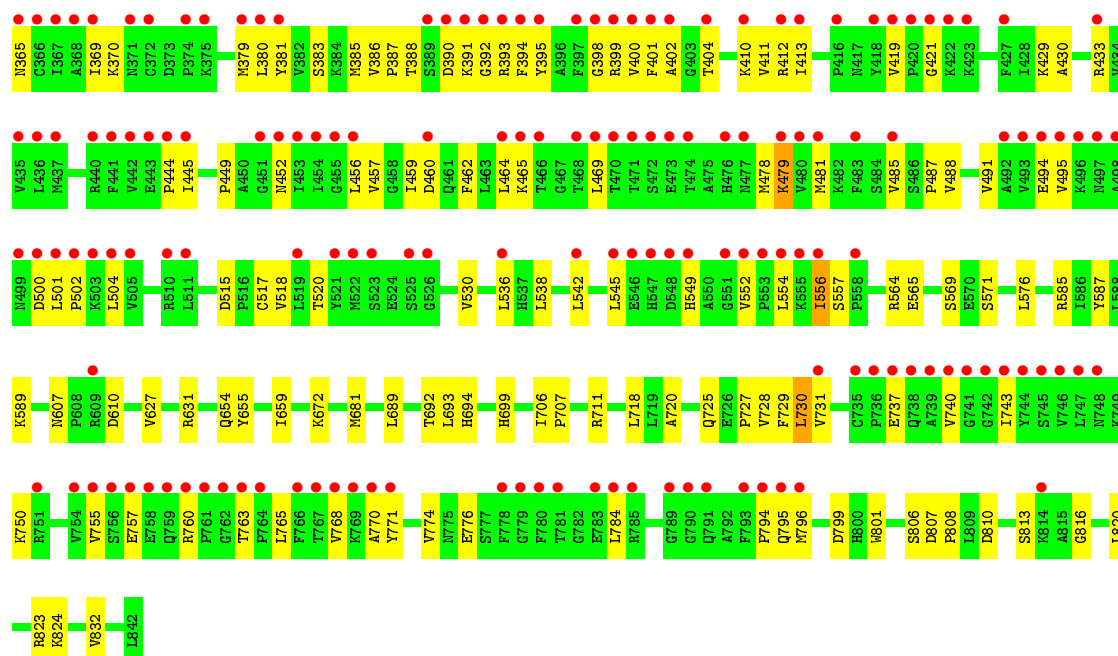
• Molecule 1: Elongation factor 2



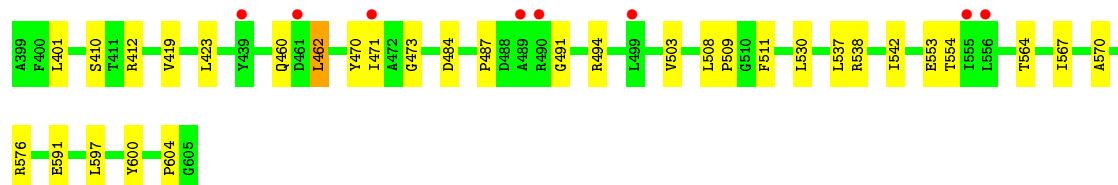
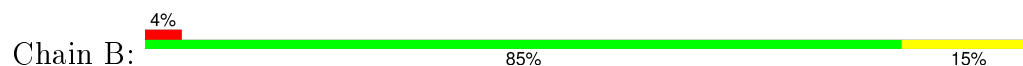
• Molecule 1: Elongation factor 2



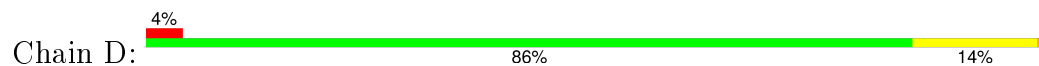




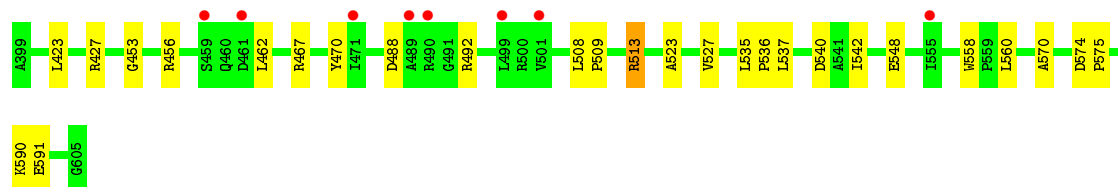
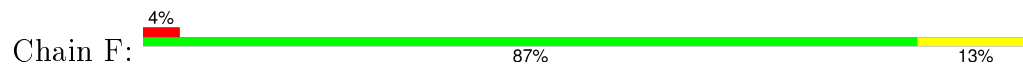
• Molecule 2: Exotoxin A



• 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	327.57Å 68.46Å 189.99Å 90.00° 103.04° 90.00°	Depositor
Resolution (Å)	25.00 – 2.35 25.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (25.00-2.35) 98.5 (25.00-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.36Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.257 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 169195 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24682	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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 40.05 % 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 2.8973e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.20	0/6517	0.37	0/8823
1	C	0.20	0/6517	0.37	0/8823
1	E	0.20	0/6517	0.37	0/8823
2	B	0.20	0/1629	0.38	0/2219
2	D	0.20	0/1629	0.40	0/2219
2	F	0.20	0/1629	0.38	0/2219
All	All	0.20	0/24438	0.37	0/33126

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	121	0
1	C	6415	0	6488	132	0
1	E	6415	0	6488	189	0
2	B	1589	0	1543	18	0
2	D	1589	0	1543	15	0
2	F	1589	0	1543	13	0
3	B	44	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	44	0	26	3	0
3	F	44	0	26	1	0
4	A	83	0	0	1	0
4	B	117	0	0	1	0
4	C	85	0	0	0	0
4	D	124	0	0	1	0
4	E	45	0	0	0	0
4	F	94	0	0	1	0
All	All	24682	0	24155	488	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 10.

The worst 5 of 488 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:759:GLN:HG2	1:C:760:ARG:H	1.38	0.86
1:E:488:VAL:HG11	1:E:774:VAL:HG21	1.57	0.85
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.57	0.84
1:C:404:THR:HG22	1:C:449:PRO:HA	1.58	0.83
1:E:391:LYS:HG3	1:E:392:GLY:H	1.43	0.82

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	818/842 (97%)	779 (95%)	36 (4%)	3 (0%)	39	46
1	C	818/842 (97%)	778 (95%)	35 (4%)	5 (1%)	30	34
1	E	818/842 (97%)	762 (93%)	53 (6%)	3 (0%)	39	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	205/207 (99%)	201 (98%)	4 (2%)	0	100	100
2	D	205/207 (99%)	200 (98%)	5 (2%)	0	100	100
2	F	205/207 (99%)	199 (97%)	5 (2%)	1 (0%)	34	39
All	All	3069/3147 (98%)	2919 (95%)	138 (4%)	12 (0%)	39	46

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	C	168	GLN
1	E	479	LYS
1	A	479	LYS
1	C	795	GLN

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%)	692 (99%)	7 (1%)	82	91
1	C	699/714 (98%)	688 (98%)	11 (2%)	70	83
1	E	699/714 (98%)	690 (99%)	9 (1%)	76	87
2	B	161/161 (100%)	160 (99%)	1 (1%)	90	96
2	D	161/161 (100%)	154 (96%)	7 (4%)	35	45
2	F	161/161 (100%)	155 (96%)	6 (4%)	41	53
All	All	2580/2625 (98%)	2539 (98%)	41 (2%)	70	83

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	842	LEU
2	D	498	LEU
2	F	513	ARG
2	D	422	LEU

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Mol	Chain	Res	Type
2	D	458	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	485	GLN
1	E	753	GLN
1	C	753	GLN
2	B	428	GLN
1	C	528	HIS

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	5,10,21	0.55	0	3,12,30	1.69	1 (33%)
1	DDE	C	699	1	13,20,21	0.84	0	16,28,30	0.65	0
1	DDE	E	699	1	13,20,21	0.85	1 (7%)	16,28,30	0.71	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	699	DDE	CD2-NE2	-2.01	1.33	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	DDE	CD2-NE2-CE1	2.05	108.95	105.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	699	DDE	4	0
1	E	699	DDE	3	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	-	38,48,48	0.65	1 (2%)	47,73,73	1.84	4 (8%)
3	NAD	D	701	-	38,48,48	0.65	1 (2%)	47,73,73	1.92	4 (8%)
3	NAD	F	702	-	38,48,48	0.66	0	47,73,73	1.89	4 (8%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	NAD	O4B-C1B	2.01	1.43	1.41
3	D	701	NAD	O4B-C1B	2.04	1.43	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	701	NAD	N3A-C2A-N1A	-9.40	121.69	128.89
3	F	702	NAD	N3A-C2A-N1A	-9.35	121.74	128.89
3	B	700	NAD	N3A-C2A-N1A	-9.02	121.98	128.89
3	D	701	NAD	PN-O3-PA	-4.80	119.26	132.73
3	F	702	NAD	PN-O3-PA	-4.50	120.09	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	700	NAD	2	0
3	D	701	NAD	3	0
3	F	702	NAD	1	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	822/842 (97%)	0.48	75 (9%) 11 18	14, 55, 97, 118	0
1	C	822/842 (97%)	0.89	134 (16%) 2 4	16, 61, 135, 187	0
1	E	822/842 (97%)	2.66	440 (53%) 0 0	16, 136, 189, 262	0
2	B	207/207 (100%)	0.15	8 (3%) 43 57	14, 27, 61, 94	0
2	D	207/207 (100%)	0.14	8 (3%) 43 57	12, 25, 57, 89	0
2	F	207/207 (100%)	0.14	8 (3%) 43 57	17, 29, 62, 108	0
All	All	3087/3147 (98%)	1.10	673 (21%) 1 2	12, 57, 169, 262	0

The worst 5 of 673 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	108	HIS	13.8
1	E	314	LEU	13.2
1	E	195	GLU	13.1
1	E	67	GLY	13.0
1	E	157	ILE	11.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	DDE	A	699	10/21	0.95	0.14	-	45,60,66,70	0
1	DDE	C	699	20/21	0.93	0.21	-	29,64,106,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	DDE	E	699	20/21	0.92	0.21	-	38,73,107,109	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	-0.34	17,28,45,62	0
3	NAD	F	702	44/44	0.95	0.15	-0.42	11,32,48,56	0
3	NAD	D	701	44/44	0.96	0.15	-0.55	7,24,49,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.