



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:58 AM GMT

PDB ID : 3B78
Title : Structure of the eEF2-ExoA(R551H)-NAD⁺complex
Authors : Jorgensen, R.; Merrill, A.R.
Deposited on : 2007-10-30
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

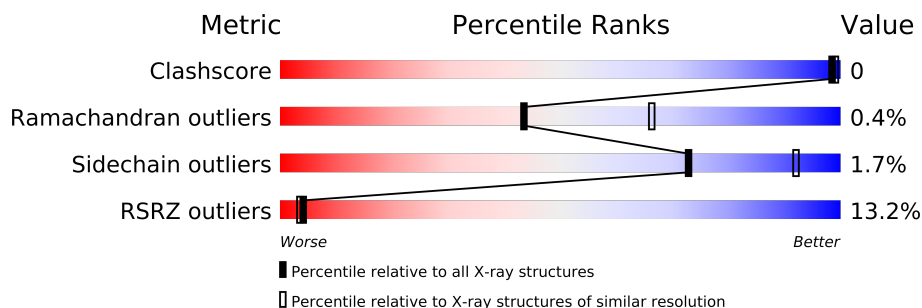
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	842	
1	C	842	
1	E	842	
2	B	207	
2	D	207	
2	F	207	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24616 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			6405	4075	1093	1207	30			

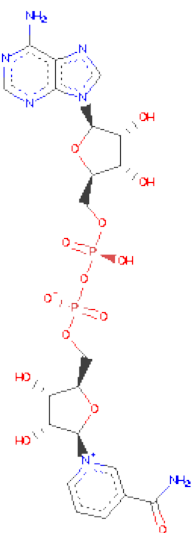
- Molecule 2 is a protein called Exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	0	0
			1587	1001	282	304			
2	D	207	Total	C	N	O	0	0	0
			1587	1001	282	304			
2	F	207	Total	C	N	O	0	0	0
			1587	1001	282	304			

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	551	HIS	ARG	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	551	HIS	ARG	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	551	HIS	ARG	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.

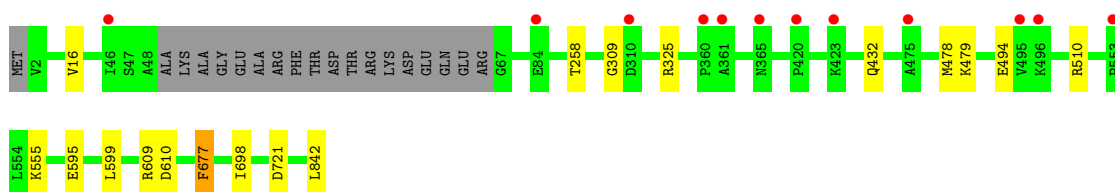
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	103	Total	O	0	0
			103	103		
4	C	84	Total	O	0	0
			84	84		
4	D	106	Total	O	0	0
			106	106		
4	E	35	Total	O	0	0
			35	35		
4	F	76	Total	O	0	0
			76	76		

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.

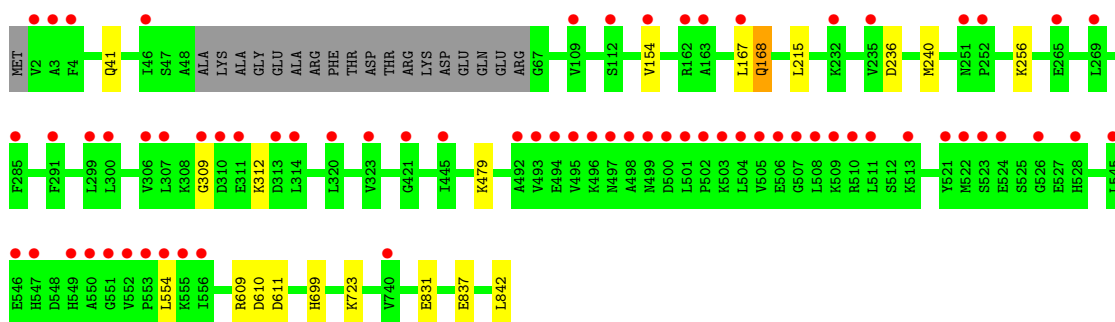
• Molecule 1: Elongation factor 2

Chain A: 



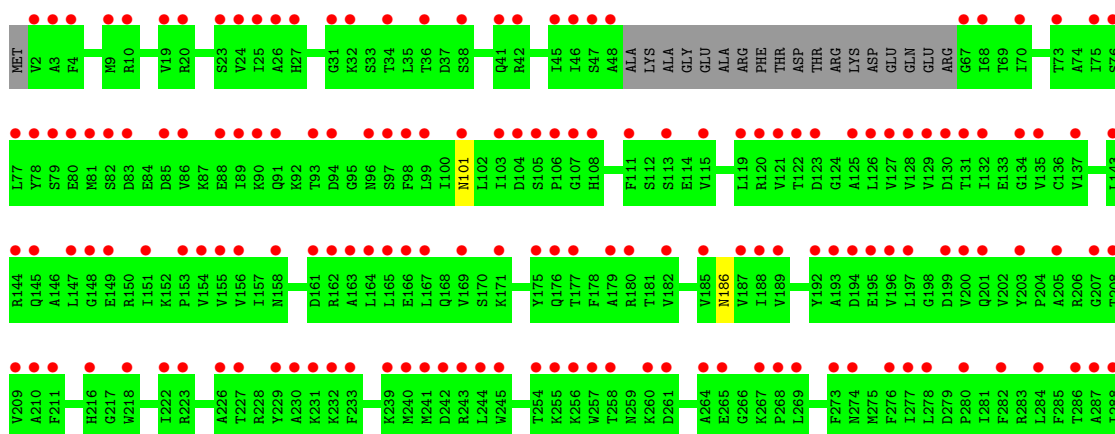
• Molecule 1: Elongation factor 2

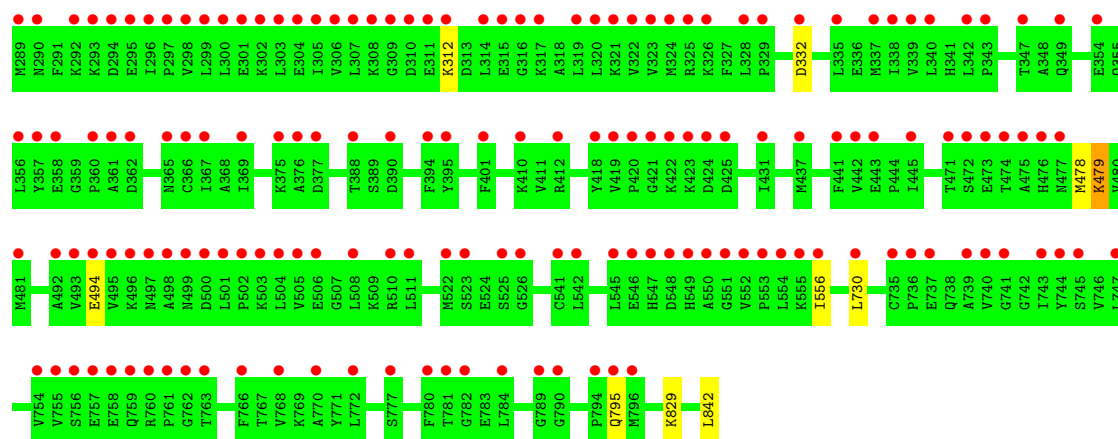
Chain C: 



• Molecule 1: Elongation factor 2

Chain E: 





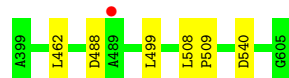
- Molecule 2: Exotoxin A

Chain B:



- Molecule 2: Exotoxin A

Chain D:



- Molecule 2: Exotoxin A

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	327.14Å 68.13Å 190.58Å 90.00° 102.99° 90.00°	Depositor
Resolution (Å)	46.55 – 2.50 46.55 – 2.48	Depositor EDS
% Data completeness (in resolution range)	93.3 (46.55-2.50) 92.0 (46.55-2.48)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.242 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 134421 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24616	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 38.77 % 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 3.5087e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.39	0/8823
1	C	0.21	0/6517	0.38	0/8823
1	E	0.21	0/6517	0.37	0/8823
2	B	0.21	0/1627	0.40	0/2217
2	D	0.21	0/1627	0.40	0/2217
2	F	0.21	0/1627	0.38	0/2217
All	All	0.21	0/24432	0.38	0/33120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6405	0	0	3	0
1	C	6415	0	0	4	0
1	E	6405	0	0	1	0
2	B	1587	0	0	1	0
2	D	1587	0	0	1	0
2	F	1587	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	0	0
3	D	44	0	26	1	0
3	F	44	0	26	0	0
4	A	94	0	0	0	0
4	B	103	0	0	0	0
4	C	84	0	0	0	0
4	D	106	0	0	0	0
4	E	35	0	0	0	0
4	F	76	0	0	0	0
All	All	24616	0	78	11	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 0.

All (11) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:699:DDE:CAA	3:D:701:NAD:H4D	2.33	0.59
1:C:699:DDE:CAB	1:C:699:DDE:CAT	2.86	0.54
1:E:478:MET:O	1:E:479:LYS:C	2.49	0.51
1:A:478:MET:O	1:A:479:LYS:C	2.54	0.46
2:B:508:LEU:N	2:B:509:PRO:CD	2.81	0.43
2:F:508:LEU:N	2:F:509:PRO:CD	2.83	0.41
2:D:508:LEU:N	2:D:509:PRO:CD	2.84	0.41
1:A:677:PHE:N	1:A:677:PHE:CD2	2.88	0.41
1:C:167:LEU:O	1:C:168:GLN:C	2.59	0.40
1:C:610:ASP:OD1	1:C:611:ASP:N	2.55	0.40
1:A:494:GLU:O	1:A:555:LYS:N	2.54	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	818/842 (97%)	781 (96%)	34 (4%)	3 (0%)	43 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	818/842 (97%)	780 (95%)	33 (4%)	5 (1%)	33	55
1	E	818/842 (97%)	763 (93%)	52 (6%)	3 (0%)	43	66
2	B	205/207 (99%)	201 (98%)	4 (2%)	0	100	100
2	D	205/207 (99%)	198 (97%)	6 (3%)	1 (0%)	38	60
2	F	205/207 (99%)	200 (98%)	5 (2%)	0	100	100
All	All	3069/3147 (98%)	2923 (95%)	134 (4%)	12 (0%)	43	66

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	E	479	LYS
1	A	432	GLN
1	C	168	GLN
1	C	479	LYS
2	D	488	ASP
1	E	556	ILE
1	E	795	GLN
1	C	554	LEU
1	C	215	LEU
1	A	721	ASP
1	C	309	GLY

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%)	688 (98%)	11 (2%)	75	93
1	C	699/714 (98%)	688 (98%)	11 (2%)	75	93
1	E	699/714 (98%)	691 (99%)	8 (1%)	84	96
2	B	161/161 (100%)	157 (98%)	4 (2%)	60	85
2	D	161/161 (100%)	158 (98%)	3 (2%)	69	90
2	F	161/161 (100%)	154 (96%)	7 (4%)	40	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2580/2625 (98%)	2536 (98%)	44 (2%)	73	92

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	258	THR
1	A	325	ARG
1	A	510	ARG
1	A	595	GLU
1	A	599	LEU
1	A	609	ARG
1	A	610	ASP
1	A	677	PHE
1	A	698	ILE
1	A	842	LEU
2	B	460	GLN
2	B	462	LEU
2	B	492	ARG
2	B	548	GLU
1	C	41	GLN
1	C	154	VAL
1	C	236	ASP
1	C	240	MET
1	C	256	LYS
1	C	312	LYS
1	C	609	ARG
1	C	723	LYS
1	C	831	GLU
1	C	837	GLU
1	C	842	LEU
2	D	462	LEU
2	D	499	LEU
2	D	540	ASP
1	E	101	ASN
1	E	186	ASN
1	E	312	LYS
1	E	332	ASP
1	E	494	GLU
1	E	730	LEU
1	E	829	LYS
1	E	842	LEU

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Mol	Chain	Res	Type
2	F	462	LEU
2	F	499	LEU
2	F	513	ARG
2	F	540	ASP
2	F	547	GLU
2	F	548	GLU
2	F	560	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	8,10,21	6.28	2 (25%)	7,12,30	0.52	0
1	DDE	C	699	1	20,20,21	4.43	5 (25%)	26,28,30	1.66	5 (19%)
1	DDE	E	699	1	8,10,21	6.37	2 (25%)	7,12,30	0.81	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDE	E	699	1	-	0/4/6/23	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	699	DDE	O-C	18.86	1.24	1.11
1	E	699	DDE	O-C	17.78	1.23	1.11
1	A	699	DDE	O-C	17.55	1.23	1.11
1	C	699	DDE	CD2-CG	-2.99	1.33	1.36
1	C	699	DDE	CA-C	2.84	1.53	1.48
1	E	699	DDE	CA-C	2.60	1.53	1.48
1	A	699	DDE	CA-C	2.47	1.52	1.48
1	C	699	DDE	CD2-NE2	-2.33	1.33	1.36
1	C	699	DDE	CBW-NCB	-2.22	1.49	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	DDE	C-CA-N	-5.43	108.40	113.83
1	C	699	DDE	CAU-CBW-CBI	-2.76	105.41	110.91
1	C	699	DDE	CBI-CBW-NCB	-2.30	107.95	110.58
1	C	699	DDE	NE2-CE1-ND1	-2.26	107.68	111.41
1	C	699	DDE	CAA-NCB-CAB	-2.12	103.96	108.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	48,48,48	0.79	1 (2%)	73,73,73	1.87	9 (12%)
3	NAD	D	701	-	48,48,48	0.80	2 (4%)	73,73,73	1.90	10 (13%)
3	NAD	F	702	-	48,48,48	0.79	1 (2%)	73,73,73	1.90	10 (13%)

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	-	-	0/30/62/62	0/3/5/5
3	NAD	D	701	-	-	0/30/62/62	0/3/5/5
3	NAD	F	702	-	-	0/30/62/62	0/3/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	NAD	C4A-N9A	-2.98	1.33	1.37
3	F	702	NAD	C4A-N9A	-2.89	1.33	1.37
3	D	701	NAD	C4A-N9A	-2.82	1.33	1.37
3	D	701	NAD	C8A-N9A	-2.03	1.33	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	NAD	N3A-C2A-N1A	-9.19	121.03	128.71
3	F	702	NAD	N3A-C2A-N1A	-9.02	121.17	128.71
3	D	701	NAD	N3A-C2A-N1A	-9.00	121.18	128.71
3	D	701	NAD	C4B-O4B-C1B	-6.96	102.19	109.75
3	F	702	NAD	C4B-O4B-C1B	-6.72	102.45	109.75
3	B	700	NAD	C4B-O4B-C1B	-6.70	102.47	109.75
3	D	701	NAD	O4B-C1B-N9A	6.15	114.16	108.44
3	F	702	NAD	O4B-C1B-N9A	6.04	114.06	108.44
3	B	700	NAD	O4B-C1B-N9A	5.14	113.22	108.44
3	D	701	NAD	N3A-C4A-N9A	3.88	132.43	125.43
3	F	702	NAD	N3A-C4A-N9A	3.74	132.18	125.43
3	B	700	NAD	N3A-C4A-N9A	3.69	132.09	125.43
3	D	701	NAD	C3D-C2D-C1D	3.62	106.57	100.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	NAD	C3D-C2D-C1D	3.57	106.49	100.91
3	F	702	NAD	C3D-C2D-C1D	3.51	106.41	100.91
3	F	702	NAD	C4A-C5A-N7A	-2.70	107.21	109.52
3	D	701	NAD	C5A-C4A-N3A	-2.69	119.85	125.70
3	F	702	NAD	C5A-C4A-N3A	-2.66	119.91	125.70
3	D	701	NAD	C4A-C5A-N7A	-2.62	107.28	109.52
3	D	701	NAD	PN-O3-PA	-2.54	122.04	132.95
3	B	700	NAD	C4A-C5A-N7A	-2.54	107.35	109.52
3	B	700	NAD	C5A-C4A-N3A	-2.52	120.21	125.70
3	B	700	NAD	PN-O3-PA	-2.24	123.35	132.95
3	F	702	NAD	PN-O3-PA	-2.17	123.63	132.95
3	D	701	NAD	C2A-N3A-C4A	2.14	120.10	114.01
3	F	702	NAD	C2A-N3A-C4A	2.12	120.06	114.01
3	B	700	NAD	C2A-N3A-C4A	2.09	119.95	114.01
3	F	702	NAD	C2D-C1D-N1N	-2.07	110.36	113.86
3	D	701	NAD	C2D-C1D-N1N	-2.07	110.36	113.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	823/842 (97%)	0.07	12 (1%) 70 72	17, 53, 92, 120	0
1	C	823/842 (97%)	0.45	70 (8%) 11 10	18, 60, 134, 199	0
1	E	823/842 (97%)	1.80	323 (39%) 1 0	19, 131, 186, 266	0
2	B	207/207 (100%)	-0.09	0 100 100	16, 33, 80, 99	0
2	D	207/207 (100%)	-0.16	1 (0%) 88 90	16, 30, 66, 88	0
2	F	207/207 (100%)	-0.09	2 (0%) 79 81	20, 36, 82, 118	0
All	All	3090/3147 (98%)	0.60	408 (13%) 4 3	16, 57, 165, 266	0

All (408) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	195	GLU	9.9
1	E	766	PHE	9.5
1	C	495	VAL	9.3
1	E	179	ALA	8.7
1	E	311	GLU	8.7
1	E	231	LYS	8.6
1	E	78	TYR	8.6
1	C	550	ALA	8.3
1	E	167	LEU	7.8
1	E	307	LEU	7.7
1	E	314	LEU	7.7
1	E	339	VAL	7.7
1	C	493	VAL	7.5
1	E	239	LYS	7.3
1	E	332	ASP	7.2
1	E	81	MET	7.2
1	E	277	ILE	7.1
1	E	210	ALA	7.0
1	E	276	PHE	7.0

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Mol	Chain	Res	Type	RSRZ
1	E	321	LYS	6.9
1	E	420	PRO	6.9
1	E	88	GLU	6.8
1	E	320	LEU	6.8
1	E	107	GLY	6.8
1	E	310	ASP	6.7
1	C	523	SER	6.7
1	E	299	LEU	6.6
1	E	553	PRO	6.6
1	E	315	GLU	6.4
1	E	108	HIS	6.3
1	E	280	PRO	6.3
1	E	26	ALA	6.2
1	E	175	TYR	6.2
1	E	193	ALA	6.2
1	C	506	GLU	6.1
1	E	367	ILE	6.1
1	C	522	MET	6.1
1	E	86	VAL	6.0
1	E	308	LYS	6.0
1	E	761	PRO	5.9
1	E	554	LEU	5.9
1	E	192	TYR	5.9
1	E	303	LEU	5.8
1	E	335	LEU	5.8
1	E	743	ILE	5.7
1	E	194	ASP	5.7
1	E	745	SER	5.6
1	C	494	GLU	5.6
1	E	99	LEU	5.5
1	E	366	CYS	5.5
1	E	245	TRP	5.4
1	E	476	HIS	5.4
1	E	504	LEU	5.4
1	E	273	PHE	5.4
1	E	525	SER	5.4
1	E	789	GLY	5.4
1	C	502	PRO	5.3
1	E	495	VAL	5.3
1	E	278	LEU	5.2
1	C	508	LEU	5.2
1	C	549	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	23	SER	5.1
1	E	442	VAL	5.1
1	C	551	GLY	5.1
1	E	98	PHE	5.1
1	E	498	ALA	5.0
1	E	97	SER	5.0
1	E	132	ILE	5.0
1	E	89	ILE	5.0
1	E	492	ALA	4.9
1	E	240	MET	4.9
1	E	129	VAL	4.9
1	E	163	ALA	4.9
1	E	419	VAL	4.9
1	E	555	LYS	4.9
1	E	289	MET	4.8
1	E	196	VAL	4.8
1	E	316	GLY	4.8
1	C	499	ASN	4.8
1	E	233	PHE	4.8
1	E	338	ILE	4.8
1	E	323	VAL	4.8
1	E	269	LEU	4.7
1	E	770	ALA	4.7
1	E	312	LYS	4.7
1	E	128	VAL	4.7
1	E	77	LEU	4.7
1	E	474	THR	4.7
1	E	164	LEU	4.7
1	E	180	ARG	4.6
1	E	551	GLY	4.6
1	C	501	LEU	4.6
1	C	496	LYS	4.6
1	E	759	GLN	4.6
1	C	505	VAL	4.6
1	E	67	GLY	4.6
1	E	288	ILE	4.6
1	E	493	VAL	4.5
1	E	760	ARG	4.5
1	E	80	GLU	4.5
1	E	501	LEU	4.5
1	E	360	PRO	4.5
1	E	242	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	777	SER	4.5
1	E	282	PHE	4.5
1	E	227	THR	4.4
1	E	126	LEU	4.4
1	E	362	ASP	4.4
1	E	232	LYS	4.4
1	E	222	ILE	4.4
1	E	76	SER	4.3
1	E	154	VAL	4.3
1	E	298	VAL	4.3
1	E	19	VAL	4.3
1	E	365	ASN	4.3
1	E	500	ASP	4.3
1	E	48	ALA	4.3
1	E	187	VAL	4.3
1	A	475	ALA	4.2
1	C	524	GLU	4.2
1	C	509	LYS	4.2
1	E	418	TYR	4.2
1	E	83	ASP	4.2
1	E	226	ALA	4.2
1	E	322	VAL	4.2
1	E	762	GLY	4.2
1	E	176	GLN	4.2
1	E	421	GLY	4.2
1	E	169	VAL	4.2
1	E	79	SER	4.2
1	E	258	THR	4.2
1	C	528	HIS	4.2
1	C	513	LYS	4.1
1	E	739	ALA	4.1
1	E	45	ILE	4.1
1	E	143	LEU	4.1
1	E	506	GLU	4.1
1	E	317	LYS	4.1
1	E	166	GLU	4.1
1	E	182	VAL	4.1
1	E	203	TYR	4.0
1	E	343	PRO	4.0
1	C	311	GLU	4.0
1	E	131	THR	4.0
1	E	309	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	552	VAL	4.0
1	E	229	TYR	4.0
1	C	546	GLU	4.0
1	E	740	VAL	4.0
1	E	361	ALA	4.0
1	E	319	LEU	3.9
1	E	496	LYS	3.9
1	C	500	ASP	3.9
1	E	46	ILE	3.9
1	E	735	CYS	3.9
1	E	422	LYS	3.9
1	C	291	PHE	3.9
1	E	441	PHE	3.9
1	C	2	VAL	3.9
1	E	475	ALA	3.9
1	E	105	SER	3.9
1	E	25	ILE	3.9
1	E	24	VAL	3.8
1	E	794	PRO	3.8
1	E	737	GLU	3.8
1	C	498	ALA	3.8
1	E	550	ALA	3.8
1	E	96	ASN	3.8
1	E	329	PRO	3.7
1	E	358	GLU	3.7
1	E	260	LYS	3.7
1	E	747	LEU	3.7
1	E	306	VAL	3.7
1	E	284	LEU	3.7
1	E	205	ALA	3.6
2	F	489	ALA	3.6
1	C	553	PRO	3.6
1	E	511	LEU	3.6
1	C	504	LEU	3.6
1	E	497	ASN	3.6
1	E	185	VAL	3.6
1	E	296	ILE	3.6
1	E	410	LYS	3.6
1	E	472	SER	3.6
1	E	268	PRO	3.6
1	E	790	GLY	3.5
1	E	218	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	495	VAL	3.5
1	E	106	PRO	3.5
1	E	155	VAL	3.5
1	E	736	PRO	3.5
1	C	313	ASP	3.5
1	E	257	TRP	3.5
1	E	165	LEU	3.4
1	E	508	LEU	3.4
1	E	730	LEU	3.4
1	E	795	GLN	3.4
1	E	241	MET	3.4
1	E	216	HIS	3.4
1	E	149	GLU	3.4
1	E	340	LEU	3.4
1	C	314	LEU	3.4
1	E	188	ILE	3.4
1	C	4	PHE	3.4
1	E	301	GLU	3.4
1	E	744	TYR	3.3
1	E	223	ARG	3.3
1	E	294	ASP	3.3
1	E	552	VAL	3.3
1	C	545	LEU	3.3
1	E	781	THR	3.3
1	E	47	SER	3.3
1	C	167	LEU	3.3
1	E	522	MET	3.3
1	C	497	ASN	3.3
1	E	293	LYS	3.3
1	E	197	LEU	3.2
1	E	423	LYS	3.2
1	E	780	PHE	3.2
1	C	511	LEU	3.2
1	E	556	ILE	3.2
1	E	499	ASN	3.2
1	E	503	LYS	3.2
1	E	111	PHE	3.2
1	E	123	ASP	3.2
1	E	36	THR	3.2
1	E	32	LYS	3.1
1	E	295	GLU	3.1
1	E	256	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	741	GLY	3.1
1	C	300	LEU	3.1
1	A	420	PRO	3.1
1	E	510	ARG	3.1
1	E	369	ILE	3.1
1	E	547	HIS	3.1
1	E	230	ALA	3.1
1	C	112	SER	3.1
2	F	490	ARG	3.0
1	C	555	LYS	3.0
1	E	144	ARG	3.0
1	E	70	ILE	3.0
1	E	127	VAL	3.0
1	E	137	VAL	3.0
1	E	342	LEU	3.0
1	E	541	CYS	3.0
1	E	200	VAL	3.0
1	E	42	ARG	3.0
1	E	431	ILE	3.0
1	E	357	TYR	3.0
1	E	548	ASP	3.0
1	A	361	ALA	2.9
1	E	145	GLN	2.9
1	C	740	VAL	2.9
1	E	38	SER	2.9
1	E	4	PHE	2.9
1	E	31	GLY	2.9
1	E	94	ASP	2.9
1	E	424	ASP	2.9
1	E	754	VAL	2.9
1	E	254	THR	2.9
1	E	324	MET	2.9
1	E	290	ASN	2.9
1	E	757	GLU	2.9
1	E	297	PRO	2.8
1	E	445	ILE	2.8
1	E	505	VAL	2.8
1	E	91	GLN	2.8
1	E	477	ASN	2.8
1	E	326	LYS	2.8
1	E	292	LYS	2.8
1	E	9	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	796	MET	2.8
1	C	554	LEU	2.8
1	E	75	ILE	2.8
1	E	134	GLY	2.8
1	C	503	LYS	2.8
1	E	125	ALA	2.8
1	E	755	VAL	2.8
1	E	546	GLU	2.8
1	E	135	VAL	2.8
1	E	305	ILE	2.8
1	C	3	ALA	2.7
1	E	161	ASP	2.7
2	D	489	ALA	2.7
1	C	285	PHE	2.7
1	E	304	GLU	2.7
1	E	325	ARG	2.7
1	E	255	LYS	2.7
1	C	307	LEU	2.7
1	E	302	LYS	2.7
1	E	148	GLY	2.7
1	E	395	TYR	2.7
1	C	310	ASP	2.7
1	A	365	ASN	2.7
1	E	93	THR	2.7
1	E	784	LEU	2.7
1	E	68	ILE	2.7
1	E	243	ARG	2.6
1	E	41	GLN	2.6
1	E	130	ASP	2.6
1	E	171	LYS	2.6
1	E	768	VAL	2.6
1	C	309	GLY	2.6
1	E	437	MET	2.6
1	E	151	ILE	2.6
1	E	156	VAL	2.6
1	E	104	ASP	2.6
1	E	199	ASP	2.6
1	E	147	LEU	2.6
1	E	494	GLU	2.6
1	C	492	ALA	2.5
1	E	390	ASP	2.5
1	E	523	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	244	LEU	2.5
1	E	162	ARG	2.5
1	E	207	GLY	2.5
1	A	46	ILE	2.5
1	E	85	ASP	2.5
1	E	542	LEU	2.4
1	E	265	GLU	2.4
1	C	154	VAL	2.4
1	C	306	VAL	2.4
1	E	471	THR	2.4
1	E	103	ILE	2.4
1	E	287	ALA	2.4
1	E	376	ALA	2.4
1	C	252	PRO	2.4
1	E	401	PHE	2.4
1	C	510	ARG	2.4
1	E	412	ARG	2.4
1	E	763	THR	2.4
1	E	90	LYS	2.4
1	E	119	LEU	2.4
1	E	337	MET	2.3
1	E	113	SER	2.3
1	E	356	LEU	2.3
1	E	377	ASP	2.3
1	E	388	THR	2.3
1	E	526	GLY	2.3
1	E	772	LEU	2.3
1	E	354	GLU	2.3
1	E	375	LYS	2.3
1	E	158	ASN	2.3
1	E	502	PRO	2.3
1	E	211	PHE	2.3
1	C	323	VAL	2.3
1	E	209	VAL	2.3
1	E	549	HIS	2.3
1	E	208	THR	2.3
1	E	347	THR	2.3
1	C	251	ASN	2.3
1	E	115	VAL	2.3
1	C	299	LEU	2.2
1	E	473	GLU	2.2
1	E	120	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	235	VAL	2.2
1	E	73	THR	2.2
1	E	261	ASP	2.2
1	E	545	LEU	2.2
1	E	267	LYS	2.2
1	C	162	ARG	2.2
1	C	547	HIS	2.2
1	C	556	ILE	2.2
1	E	286	THR	2.2
1	E	328	LEU	2.2
1	E	82	SER	2.2
1	E	756	SER	2.2
1	C	109	VAL	2.2
1	E	177	THR	2.2
1	C	445	ILE	2.2
1	C	265	GLU	2.2
1	C	232	LYS	2.2
1	C	507	GLY	2.2
1	E	2	VAL	2.2
1	A	84	GLU	2.2
1	E	349	GLN	2.2
1	C	521	TYR	2.2
1	E	274	ASN	2.1
1	E	443	GLU	2.1
1	E	34	THR	2.1
1	E	121	VAL	2.1
1	E	3	ALA	2.1
1	E	27	HIS	2.1
1	A	553	PRO	2.1
1	A	496	LYS	2.1
1	E	189	VAL	2.1
1	E	394	PHE	2.1
1	E	425	ASP	2.1
1	C	526	GLY	2.1
1	E	20	ARG	2.1
1	E	782	GLY	2.1
1	C	46	ILE	2.1
1	E	300	LEU	2.1
1	E	153	PRO	2.1
1	A	423	LYS	2.1
1	C	269	LEU	2.1
1	E	201	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	758	GLU	2.0
1	C	163	ALA	2.0
1	E	101	ASN	2.0
1	A	360	PRO	2.0
1	E	481	MET	2.0
1	A	310	ASP	2.0
1	E	10	ARG	2.0
1	C	320	LEU	2.0
1	E	264	ALA	2.0
1	C	421	GLY	2.0
1	E	122	THR	2.0

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	DDE	C	699	20/21	0.22	1.43	22,85,126,129	0
1	DDE	A	699	10/21	0.13	-0.33	43,61,74,78	0
1	DDE	E	699	10/21	0.12	-1.22	38,49,69,70	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAD	F	702	44/44	0.15	-0.15	7,34,59,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAD	D	701	44/44	0.16	-0.18	12,29,51,56	0
3	NAD	B	700	44/44	0.15	-0.22	17,33,54,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.