



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:47 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 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>

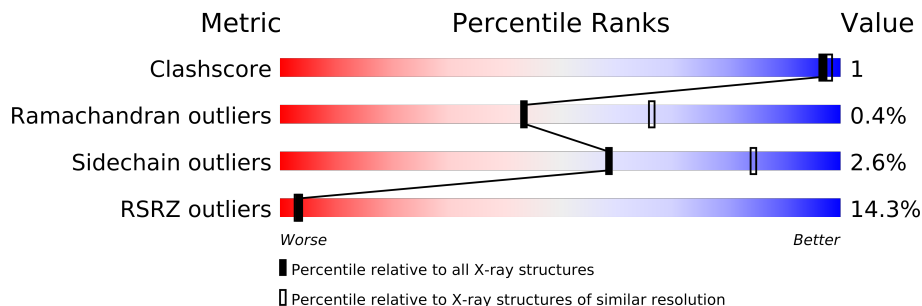
The following versions of software and data (see [references](#)) were used in the production of this report:

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 24719 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
			6415	4082	1095	1208	30			

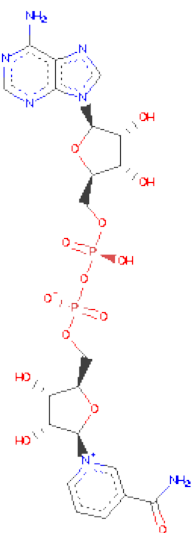
- Molecule 2 is a protein called Exotoxin A.

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.

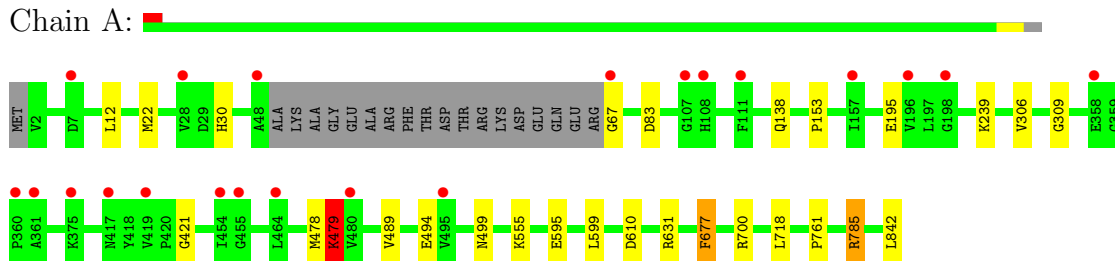
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	116	Total	O	0	0
			116	116		
4	C	77	Total	O	0	0
			77	77		
4	D	142	Total	O	0	0
			142	142		
4	E	60	Total	O	0	0
			60	60		
4	F	88	Total	O	0	0
			88	88		

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.

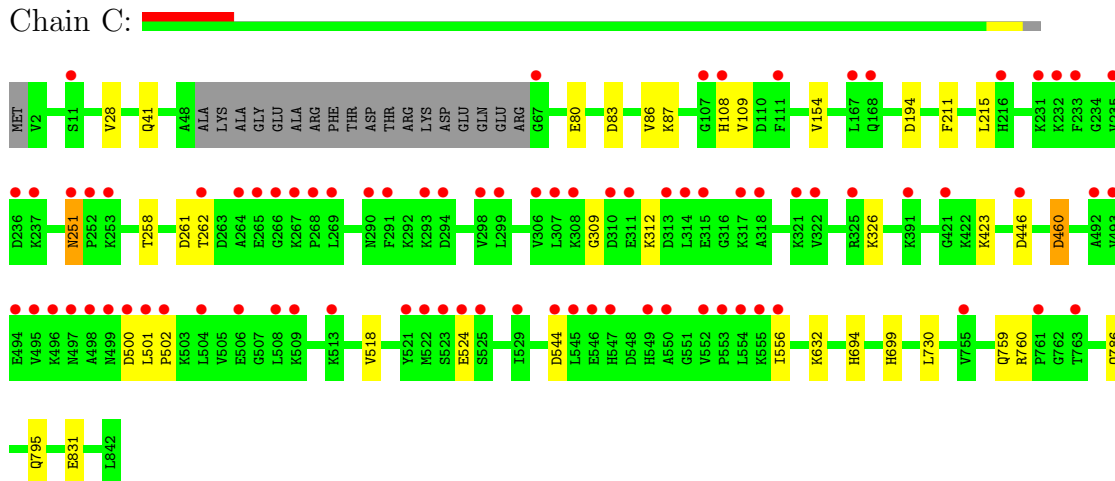
• Molecule 1: Elongation factor 2

Chain A:



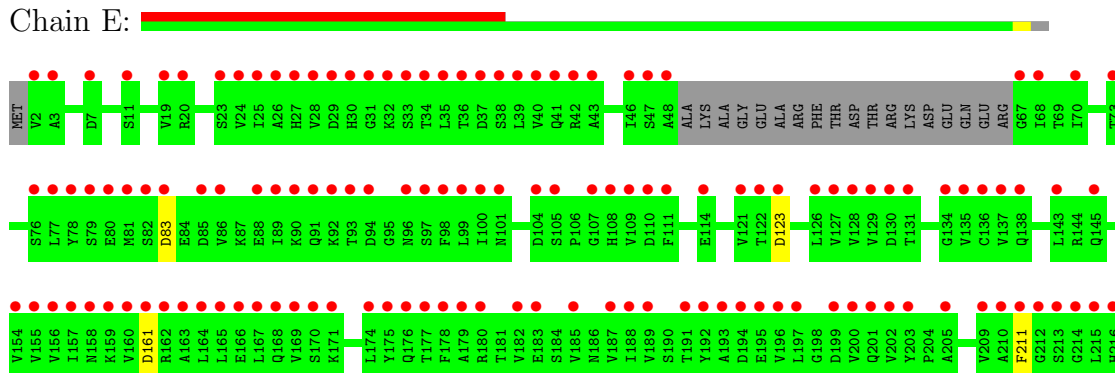
• Molecule 1: Elongation factor 2

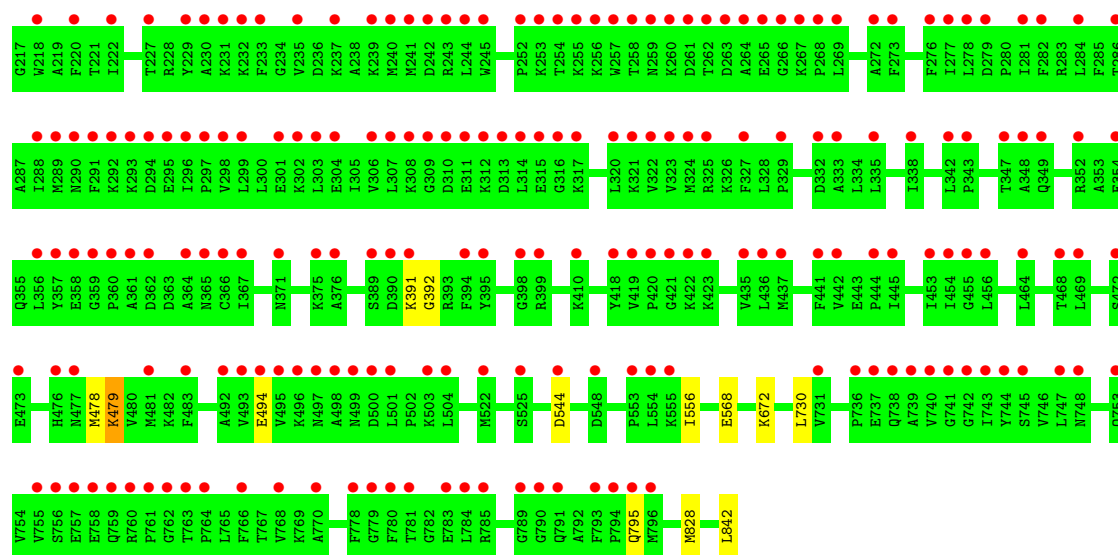
Chain C:



• Molecule 1: Elongation factor 2

Chain E:





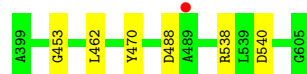
- Molecule 2: Exotoxin A

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	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 0.215 , (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)	0.33 , 38.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	3 of 162490 reflections (0.002%)	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.*

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	0.40	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 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	4	0
1	C	6415	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	6415	0	0	3	0
2	B	1592	0	0	2	0
2	D	1584	0	0	1	0
2	F	1584	0	0	5	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	0	0
4	B	116	0	0	0	0
4	C	77	0	0	0	0
4	D	142	0	0	0	0
4	E	60	0	0	0	0
4	F	88	0	0	0	0
All	All	24719	0	78	24	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 1.

All (24) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:785:ARG:NH1	1:A:785:ARG:CG	2.66	0.57
2:B:470:TYR:CD2	3:B:700:NAD:H2D	2.44	0.52
1:E:478:MET:O	1:E:479:LYS:C	2.48	0.52
2:F:488:ASP:N	2:F:492:ARG:O	2.43	0.51
1:E:123:ASP:N	1:E:123:ASP:OD1	2.44	0.49
2:D:470:TYR:CD2	3:D:701:NAD:H2D	2.47	0.49
1:A:478:MET:O	1:A:479:LYS:C	2.52	0.47
2:F:508:LEU:N	2:F:509:PRO:CD	2.77	0.47
1:C:108:HIS:ND1	1:C:109:VAL:N	2.64	0.46
1:A:677:PHE:N	1:A:677:PHE:CD2	2.83	0.46
1:C:699:DDE:CAC	1:C:699:DDE:NAD	2.76	0.44
1:C:460:ASP:OD1	1:C:460:ASP:N	2.51	0.44
2:F:470:TYR:CD2	3:F:702:NAD:H2D	2.53	0.44
1:C:694:HIS:CE1	1:C:699:DDE:CD2	3.01	0.44
1:C:831:GLU:OE1	1:C:831:GLU:N	2.51	0.44
1:C:759:GLN:CG	1:C:760:ARG:N	2.81	0.43
2:B:508:LEU:N	2:B:509:PRO:CD	2.81	0.43
1:C:251:ASN:ND2	1:C:251:ASN:C	2.73	0.42
1:E:391:LYS:CG	1:E:392:GLY:N	2.83	0.41
2:F:488:ASP:OD1	2:F:489:ALA:N	2.53	0.41
1:A:494:GLU:O	1:A:555:LYS:N	2.54	0.41
1:C:261:ASP:N	1:C:261:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:501:LEU:N	1:C:502:PRO:CD	2.84	0.40
2:F:553:GLU:OE1	3:F:702:NAD:H6N	2.21	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%)	780 (95%)	34 (4%)	4 (0%)	38	60
1	C	818/842 (97%)	776 (95%)	39 (5%)	3 (0%)	43	66
1	E	818/842 (97%)	750 (92%)	65 (8%)	3 (0%)	43	66
2	B	206/207 (100%)	200 (97%)	6 (3%)	0	100	100
2	D	205/207 (99%)	199 (97%)	5 (2%)	1 (0%)	38	60
2	F	205/207 (99%)	201 (98%)	3 (2%)	1 (0%)	38	60
All	All	3070/3147 (98%)	2906 (95%)	152 (5%)	12 (0%)	43	66

All (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
2	D	453	GLY
1	E	795	GLN
2	F	453	GLY
1	C	446	ASP
1	C	795	GLN
1	E	556	ILE
1	A	421	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%)	678 (97%)	21 (3%)	53	80
1	C	699/714 (98%)	674 (96%)	25 (4%)	47	73
1	E	699/714 (98%)	689 (99%)	10 (1%)	78	94
2	B	161/160 (101%)	158 (98%)	3 (2%)	69	90
2	D	160/160 (100%)	156 (98%)	4 (2%)	60	85
2	F	160/160 (100%)	155 (97%)	5 (3%)	52	79
All	All	2578/2622 (98%)	2510 (97%)	68 (3%)	59	84

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	22	MET
1	A	30	HIS
1	A	83	ASP
1	A	138	GLN
1	A	153	PRO
1	A	195	GLU
1	A	239	LYS
1	A	306	VAL
1	A	479	LYS
1	A	489	VAL
1	A	499	ASN
1	A	595	GLU
1	A	599	LEU
1	A	610	ASP
1	A	631	ARG
1	A	677	PHE
1	A	700	ARG
1	A	718	LEU
1	A	785	ARG
1	A	842	LEU
2	B	462	LEU
2	B	513	ARG

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Mol	Chain	Res	Type
2	B	540	ASP
1	C	28	VAL
1	C	41	GLN
1	C	80	GLU
1	C	83	ASP
1	C	86	VAL
1	C	87	LYS
1	C	154	VAL
1	C	194	ASP
1	C	211	PHE
1	C	215	LEU
1	C	251	ASN
1	C	258	THR
1	C	262	THR
1	C	312	LYS
1	C	326	LYS
1	C	423	LYS
1	C	460	ASP
1	C	500	ASP
1	C	518	VAL
1	C	524	GLU
1	C	544	ASP
1	C	556	ILE
1	C	632	LYS
1	C	730	LEU
1	C	786	GLN
2	D	462	LEU
2	D	488	ASP
2	D	538	ARG
2	D	540	ASP
1	E	83	ASP
1	E	161	ASP
1	E	211	PHE
1	E	494	GLU
1	E	544	ASP
1	E	568	GLU
1	E	672	LYS
1	E	730	LEU
1	E	828	MET
1	E	842	LEU
2	F	462	LEU
2	F	494	ARG

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Mol	Chain	Res	Type
2	F	540	ASP
2	F	547	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	6.31	2 (25%)	7,12,30	0.47	0
1	DDE	C	699	1	20,20,21	4.19	5 (25%)	26,28,30	1.61	6 (23%)
1	DDE	E	699	1	20,20,21	4.30	5 (25%)	26,28,30	1.38	5 (19%)

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	-	1/19/21/23	0/1/1/1
1	DDE	E	699	1	-	0/19/21/23	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	699	DDE	O-C	18.15	1.23	1.11
1	A	699	DDE	O-C	17.62	1.23	1.11
1	C	699	DDE	O-C	17.60	1.23	1.11
1	C	699	DDE	CD2-CG	-3.56	1.33	1.36
1	E	699	DDE	CD2-CG	-3.10	1.33	1.36
1	E	699	DDE	CA-C	3.02	1.54	1.48
1	C	699	DDE	CA-C	2.93	1.53	1.48
1	A	699	DDE	CA-C	2.67	1.53	1.48
1	C	699	DDE	CD2-NE2	-2.62	1.33	1.36
1	E	699	DDE	CD2-NE2	-2.55	1.33	1.36
1	E	699	DDE	CBW-NCB	-2.39	1.48	1.54
1	C	699	DDE	CBW-NCB	-2.24	1.49	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	699	DDE	CB-CG-CD2	-3.92	124.85	131.13
1	C	699	DDE	CB-CG-CD2	-3.75	125.12	131.13
1	C	699	DDE	C-CA-N	-3.64	110.19	113.83
1	C	699	DDE	CAU-CBW-NCB	-3.59	109.24	112.64
1	E	699	DDE	C-CA-N	-3.14	110.69	113.83
1	C	699	DDE	CG-CB-CA	-2.51	110.41	113.85
1	E	699	DDE	NE2-CE1-ND1	-2.29	107.63	111.41
1	C	699	DDE	CAT-CE1-ND1	2.22	127.25	123.63
1	C	699	DDE	NE2-CE1-ND1	-2.18	107.81	111.41
1	E	699	DDE	CG-CB-CA	-2.11	110.96	113.85
1	E	699	DDE	CAT-CE1-ND1	2.11	127.08	123.63

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	699	DDE	CAU-CAT-CE1-NE2

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	0.74	1 (2%)	73,73,73	1.90	9 (12%)
3	NAD	D	701	-	48,48,48	0.74	1 (2%)	73,73,73	1.84	10 (13%)
3	NAD	F	702	-	48,48,48	0.77	1 (2%)	73,73,73	2.04	9 (12%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	NAD	C4A-N9A	-2.71	1.33	1.37
3	F	702	NAD	C4A-N9A	-2.71	1.33	1.37
3	D	701	NAD	C4A-N9A	-2.67	1.33	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	702	NAD	O4B-C1B-N9A	9.41	117.19	108.44
3	B	700	NAD	N3A-C2A-N1A	-8.91	121.26	128.71
3	F	702	NAD	N3A-C2A-N1A	-8.78	121.36	128.71
3	D	701	NAD	N3A-C2A-N1A	-8.68	121.46	128.71
3	B	700	NAD	O4B-C1B-N9A	8.07	115.95	108.44
3	D	701	NAD	O4B-C1B-N9A	7.29	115.22	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	702	NAD	C4B-O4B-C1B	-6.14	103.08	109.75
3	B	700	NAD	C4B-O4B-C1B	-5.34	103.95	109.75
3	D	701	NAD	C4B-O4B-C1B	-4.83	104.50	109.75
3	F	702	NAD	N3A-C4A-N9A	4.47	133.50	125.43
3	B	700	NAD	N3A-C4A-N9A	4.00	132.65	125.43
3	D	701	NAD	N3A-C4A-N9A	3.97	132.61	125.43
3	D	701	NAD	C3D-C2D-C1D	3.62	106.58	100.91
3	B	700	NAD	C3D-C2D-C1D	3.58	106.50	100.91
3	F	702	NAD	C3D-C2D-C1D	3.50	106.38	100.91
3	F	702	NAD	C5A-C4A-N3A	-2.99	119.19	125.70
3	D	701	NAD	C5A-C4A-N3A	-2.72	119.77	125.70
3	B	700	NAD	C5A-C4A-N3A	-2.65	119.92	125.70
3	F	702	NAD	PN-O3-PA	-2.54	122.05	132.95
3	D	701	NAD	PN-O3-PA	-2.33	122.95	132.95
3	B	700	NAD	PN-O3-PA	-2.31	123.04	132.95
3	F	702	NAD	C2A-N3A-C4A	2.19	120.23	114.01
3	D	701	NAD	C4A-C5A-N7A	-2.16	107.67	109.52
3	B	700	NAD	C2A-N3A-C4A	2.11	120.01	114.01
3	D	701	NAD	C2A-N3A-C4A	2.10	119.98	114.01
3	B	700	NAD	C4A-C5A-N7A	-2.08	107.74	109.52
3	F	702	NAD	C4A-C5A-N7A	-2.05	107.76	109.52
3	D	701	NAD	C2D-C1D-N1N	-2.05	110.38	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%)	0.03	21 (2%) 53 55	12, 51, 91, 113	0
1	C	823/842 (97%)	0.43	82 (9%) 8 7	13, 60, 136, 178	0
1	E	823/842 (97%)	1.94	334 (40%) 1 0	10, 124, 182, 229	0
2	B	207/207 (100%)	-0.30	2 (0%) 79 81	10, 22, 54, 89	0
2	D	207/207 (100%)	-0.32	1 (0%) 88 90	9, 21, 52, 95	0
2	F	207/207 (100%)	-0.29	2 (0%) 79 81	12, 27, 62, 91	0
All	All	3090/3147 (98%)	0.58	442 (14%) 3 3	9, 53, 159, 229	0

All (442) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	67	GLY	12.9
1	E	314	LEU	12.2
1	E	163	ALA	10.9
1	E	311	GLU	10.4
1	E	108	HIS	10.1
1	E	761	PRO	9.7
1	E	166	GLU	9.7
1	E	167	LEU	8.5
1	E	245	TRP	8.3
1	E	200	VAL	8.1
1	E	310	ASP	7.9
1	E	307	LEU	7.7
1	E	193	ALA	7.7
1	E	68	ILE	7.6
1	E	789	GLY	7.5
1	E	258	THR	7.5
1	E	367	ILE	7.5
1	E	169	VAL	7.5
1	E	790	GLY	7.4

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Mol	Chain	Res	Type	RSRZ
1	C	495	VAL	7.4
1	E	298	VAL	7.4
1	E	239	LYS	7.4
1	E	187	VAL	7.3
1	E	740	VAL	7.3
1	E	157	ILE	7.2
1	E	107	GLY	7.1
1	E	196	VAL	7.0
1	E	86	VAL	7.0
1	E	795	GLN	6.9
1	E	744	TYR	6.9
1	E	175	TYR	6.8
1	E	88	GLU	6.8
1	E	315	GLU	6.7
1	E	231	LYS	6.7
1	E	308	LYS	6.6
1	E	36	THR	6.6
1	E	195	GLU	6.5
1	E	26	ALA	6.4
1	E	290	ASN	6.4
1	E	420	PRO	6.3
1	E	361	ALA	6.2
1	E	76	SER	6.2
1	C	494	GLU	6.2
1	E	197	LEU	6.2
1	E	110	ASP	6.1
1	E	28	VAL	6.1
1	E	299	LEU	6.1
1	C	499	ASN	6.1
1	E	233	PHE	5.9
1	E	260	LYS	5.9
1	E	321	LYS	5.8
1	E	766	PHE	5.8
1	E	553	PRO	5.8
1	E	111	PHE	5.7
1	E	160	VAL	5.7
1	E	218	TRP	5.7
1	E	419	VAL	5.7
1	E	192	TYR	5.6
1	E	264	ALA	5.5
1	E	137	VAL	5.5
1	E	32	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	216	HIS	5.5
1	E	759	GLN	5.5
1	E	760	ARG	5.5
1	E	317	LYS	5.5
1	E	212	GLY	5.5
1	E	211	PHE	5.4
1	E	194	ASP	5.4
1	E	281	ILE	5.4
1	E	745	SER	5.3
1	E	770	ALA	5.3
1	C	306	VAL	5.3
1	C	498	ALA	5.3
1	E	257	TRP	5.2
2	D	489	ALA	5.2
1	C	550	ALA	5.2
1	C	522	MET	5.2
1	E	335	LEU	5.2
1	E	81	MET	5.2
1	E	203	TYR	5.1
1	E	129	VAL	5.1
1	E	179	ALA	5.1
1	C	549	HIS	5.0
1	E	269	LEU	5.0
1	E	737	GLU	5.0
1	C	523	SER	5.0
1	E	78	TYR	5.0
1	E	376	ALA	5.0
1	E	358	GLU	5.0
1	E	131	THR	5.0
1	E	89	ILE	5.0
1	E	312	LYS	4.9
1	E	763	THR	4.9
1	E	421	GLY	4.8
1	E	91	GLN	4.8
1	E	356	LEU	4.8
1	E	309	GLY	4.8
1	E	360	PRO	4.8
1	E	342	LEU	4.8
1	E	755	VAL	4.8
1	C	493	VAL	4.7
1	E	268	PRO	4.7
1	E	343	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	237	LYS	4.7
1	E	254	THR	4.7
1	E	282	PHE	4.7
1	E	47	SER	4.7
1	E	739	ALA	4.7
1	E	499	ASN	4.7
1	E	294	ASP	4.6
1	E	178	PHE	4.6
1	E	34	THR	4.6
1	E	262	THR	4.6
1	C	504	LEU	4.5
1	E	27	HIS	4.5
1	E	747	LEU	4.5
1	E	48	ALA	4.5
1	E	359	GLY	4.5
1	E	215	LEU	4.5
1	E	156	VAL	4.4
1	E	256	LYS	4.4
1	E	289	MET	4.4
1	E	267	LYS	4.4
1	C	496	LYS	4.4
1	E	497	ASN	4.4
1	E	261	ASP	4.4
1	E	277	ILE	4.4
1	E	781	THR	4.3
1	E	98	PHE	4.3
1	E	293	LYS	4.3
1	E	96	ASN	4.3
1	E	762	GLY	4.3
1	E	266	GLY	4.3
1	C	252	PRO	4.3
1	E	83	ASP	4.3
1	E	255	LYS	4.3
1	E	180	ARG	4.2
1	E	296	ILE	4.2
1	E	158	ASN	4.2
1	E	232	LYS	4.2
1	C	298	VAL	4.2
1	E	259	ASN	4.2
1	E	168	GLN	4.2
1	E	741	GLY	4.2
1	C	513	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	317	LYS	4.1
1	E	164	LEU	4.1
1	E	554	LEU	4.1
1	E	128	VAL	4.1
1	E	768	VAL	4.1
1	E	227	THR	4.1
1	C	502	PRO	4.1
1	E	441	PHE	4.1
1	E	278	LEU	4.0
1	E	422	LYS	4.0
1	C	310	ASP	4.0
1	E	366	CYS	4.0
1	E	375	LYS	4.0
1	E	46	ILE	4.0
2	B	489	ALA	4.0
1	C	556	ILE	4.0
1	E	37	ASP	4.0
1	E	240	MET	3.9
1	C	509	LYS	3.9
1	C	167	LEU	3.9
1	E	155	VAL	3.9
1	E	348	ALA	3.9
1	E	210	ALA	3.9
1	E	503	LYS	3.9
1	E	80	GLU	3.9
1	E	494	GLU	3.9
1	E	362	ASP	3.9
1	E	265	GLU	3.8
1	E	201	GLN	3.8
1	A	107	GLY	3.8
1	E	332	ASP	3.8
1	E	253	LYS	3.8
1	E	306	VAL	3.8
1	E	320	LEU	3.8
1	E	476	HIS	3.8
1	C	235	VAL	3.8
1	E	162	ARG	3.8
1	E	276	PHE	3.7
1	E	79	SER	3.7
1	A	67	GLY	3.7
1	C	299	LEU	3.7
1	E	743	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	143	LEU	3.6
1	C	231	LYS	3.6
1	C	269	LEU	3.6
1	C	311	GLU	3.6
1	E	135	VAL	3.6
1	C	108	HIS	3.6
1	E	291	PHE	3.6
1	A	361	ALA	3.6
1	E	498	ALA	3.6
1	E	445	ILE	3.6
1	E	85	ASP	3.6
1	E	500	ASP	3.6
1	E	93	THR	3.6
1	E	338	ILE	3.6
1	C	251	ASN	3.6
1	E	90	LYS	3.6
1	E	436	LEU	3.5
1	E	273	PHE	3.5
1	E	29	ASP	3.5
1	E	20	ARG	3.5
1	E	263	ASP	3.5
1	A	198	GLY	3.5
1	E	302	LYS	3.5
1	E	189	VAL	3.5
1	C	500	ASP	3.5
1	E	77	LEU	3.5
1	E	391	LYS	3.5
1	E	235	VAL	3.5
1	E	297	PRO	3.4
1	C	501	LEU	3.4
1	E	213	SER	3.4
1	E	41	GLN	3.4
1	E	748	ASN	3.4
1	C	67	GLY	3.4
1	E	316	GLY	3.4
1	E	284	LEU	3.4
1	E	242	ASP	3.4
1	E	444	PRO	3.4
1	C	216	HIS	3.4
1	C	265	GLU	3.4
1	E	453	ILE	3.4
1	E	454	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	170	SER	3.4
1	C	546	GLU	3.4
1	E	165	LEU	3.4
1	E	325	ARG	3.4
1	E	30	HIS	3.4
1	E	390	ASP	3.3
1	E	109	VAL	3.3
1	E	329	PRO	3.3
1	E	199	ASP	3.3
1	A	375	LYS	3.3
1	C	291	PHE	3.3
1	E	288	ILE	3.3
1	E	301	GLU	3.3
1	C	294	ASP	3.3
1	E	104	ASP	3.3
1	C	267	LYS	3.3
1	E	758	GLU	3.2
1	C	264	ALA	3.2
1	E	40	VAL	3.2
1	E	205	ALA	3.2
1	E	188	ILE	3.2
1	E	127	VAL	3.2
1	E	496	LYS	3.2
1	E	324	MET	3.2
1	E	92	LYS	3.2
1	E	794	PRO	3.2
1	C	293	LYS	3.2
1	E	185	VAL	3.2
1	E	229	TYR	3.2
1	E	442	VAL	3.1
1	C	232	LYS	3.1
1	E	423	LYS	3.1
1	C	553	PRO	3.1
1	E	136	CYS	3.1
1	E	286	THR	3.1
1	C	268	PRO	3.1
1	E	354	GLU	3.1
1	E	555	LYS	3.1
1	C	544	ASP	3.1
1	E	177	THR	3.1
1	E	222	ILE	3.0
1	E	202	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	323	VAL	3.0
1	C	262	THR	3.0
1	C	314	LEU	3.0
1	C	761	PRO	3.0
1	E	464	LEU	3.0
1	E	736	PRO	3.0
1	E	757	GLU	3.0
1	E	230	ALA	3.0
1	C	308	LYS	3.0
1	C	168	GLN	3.0
1	E	764	PRO	3.0
1	E	94	ASP	3.0
1	E	796	MET	3.0
1	A	111	PHE	3.0
1	E	394	PHE	3.0
1	E	97	SER	3.0
1	E	304	GLU	3.0
1	E	130	ASP	3.0
1	C	497	ASN	3.0
1	E	220	PHE	3.0
1	E	389	SER	3.0
1	E	134	GLY	2.9
1	E	313	ASP	2.9
1	E	477	ASN	2.9
1	E	548	ASP	2.9
1	C	321	LYS	2.9
1	E	455	GLY	2.9
1	E	322	VAL	2.9
1	C	253	LYS	2.9
1	A	417	ASN	2.9
1	E	70	ILE	2.9
1	E	779	GLY	2.9
1	C	315	GLU	2.9
1	E	472	SER	2.9
1	E	209	VAL	2.9
1	E	23	SER	2.8
1	E	25	ILE	2.8
1	E	395	TYR	2.8
1	E	43	ALA	2.8
1	E	272	ALA	2.8
1	E	42	ARG	2.8
1	E	780	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	473	GLU	2.8
2	F	461	ASP	2.8
1	E	292	LYS	2.8
1	E	738	GLN	2.8
1	E	161	ASP	2.8
1	E	522	MET	2.8
1	E	742	GLY	2.8
1	E	3	ALA	2.7
1	E	24	VAL	2.7
1	A	196	VAL	2.7
1	E	145	GLN	2.7
1	E	100	ILE	2.7
1	E	756	SER	2.7
1	E	176	GLN	2.7
1	E	295	GLU	2.7
1	A	360	PRO	2.7
1	E	99	LEU	2.7
1	E	214	GLY	2.7
1	E	793	PHE	2.7
2	B	461	ASP	2.7
1	E	483	PHE	2.7
1	E	159	LYS	2.7
1	E	171	LYS	2.7
1	C	111	PHE	2.6
1	E	784	LEU	2.6
1	C	313	ASP	2.6
1	E	243	ARG	2.6
1	C	266	GLY	2.6
1	E	252	PRO	2.6
1	E	303	LEU	2.6
1	E	525	SER	2.6
1	C	233	PHE	2.6
1	E	347	THR	2.6
1	C	107	GLY	2.6
1	E	241	MET	2.6
1	E	279	ASP	2.6
1	C	492	ALA	2.5
1	C	529	ILE	2.5
1	C	290	ASN	2.5
1	C	552	VAL	2.5
1	E	333	ALA	2.5
1	E	469	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	555	LYS	2.5
1	E	123	ASP	2.5
1	E	31	GLY	2.5
1	E	38	SER	2.5
1	A	419	VAL	2.5
1	E	183	GLU	2.5
1	E	365	ASN	2.5
1	C	521	TYR	2.4
1	E	2	VAL	2.4
1	E	437	MET	2.4
1	E	456	LEU	2.4
1	C	446	ASP	2.4
1	E	182	VAL	2.4
1	E	418	TYR	2.4
1	E	154	VAL	2.4
1	C	236	ASP	2.4
1	C	525	SER	2.4
1	E	33	SER	2.4
1	E	82	SER	2.4
1	A	157	ILE	2.4
1	C	421	GLY	2.3
1	E	191	THR	2.3
1	E	138	GLN	2.3
1	E	501	LEU	2.3
1	E	371	ASN	2.3
1	A	108	HIS	2.3
1	E	398	GLY	2.3
1	E	785	ARG	2.3
1	C	11	SER	2.3
1	A	48	ALA	2.3
1	C	307	LEU	2.3
1	E	35	LEU	2.3
1	C	506	GLU	2.3
1	C	318	ALA	2.3
1	E	731	VAL	2.3
1	E	504	LEU	2.3
1	E	492	ALA	2.3
1	A	28	VAL	2.3
1	C	763	THR	2.3
1	E	410	LYS	2.2
1	A	454	ILE	2.2
1	C	391	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	399	ARG	2.2
1	E	778	PHE	2.2
1	A	358	GLU	2.2
1	E	544	ASP	2.2
1	E	364	ALA	2.2
1	E	495	VAL	2.2
1	E	349	GLN	2.2
1	C	322	VAL	2.2
1	E	783	GLU	2.2
1	C	545	LEU	2.2
1	E	753	GLN	2.2
1	C	524	GLU	2.2
1	C	755	VAL	2.2
1	E	7	ASP	2.2
1	E	174	LEU	2.2
1	E	121	VAL	2.2
1	E	327	PHE	2.2
1	E	791	GLN	2.2
1	E	11	SER	2.1
1	E	73	THR	2.1
1	E	122	THR	2.1
1	E	493	VAL	2.1
1	E	126	LEU	2.1
2	F	489	ALA	2.1
1	E	101	ASN	2.1
1	E	105	SER	2.1
1	E	352	ARG	2.1
1	A	480	VAL	2.1
1	E	244	LEU	2.1
1	E	357	TYR	2.1
1	E	468	THR	2.1
1	A	455	GLY	2.1
1	C	554	LEU	2.1
1	A	495	VAL	2.0
1	E	19	VAL	2.0
1	E	481	MET	2.0
1	E	39	LEU	2.0
1	E	435	VAL	2.0
1	A	7	ASP	2.0
1	C	325	ARG	2.0
1	E	114	GLU	2.0
1	C	237	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	464	LEU	2.0
1	C	508	LEU	2.0
1	C	547	HIS	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	E	699	20/21	0.23	1.04	30,62,75,79	0
1	DDE	A	699	10/21	0.17	0.87	40,49,57,57	0
1	DDE	C	699	20/21	0.18	0.55	14,61,107,114	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	B	700	44/44	0.14	-0.34	4,20,39,42	0
3	NAD	F	702	44/44	0.14	-0.44	11,24,38,48	0
3	NAD	D	701	44/44	0.13	-0.47	7,22,38,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.