



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:08 am BST

PDB ID : 1O9J
Title : The X-ray crystal structure of eta-crystallin
Authors : Purkiss, A.G.; Van Montfort, R.; Wistow, G.; Slingsby, C.
Deposited on : 2002-12-15
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

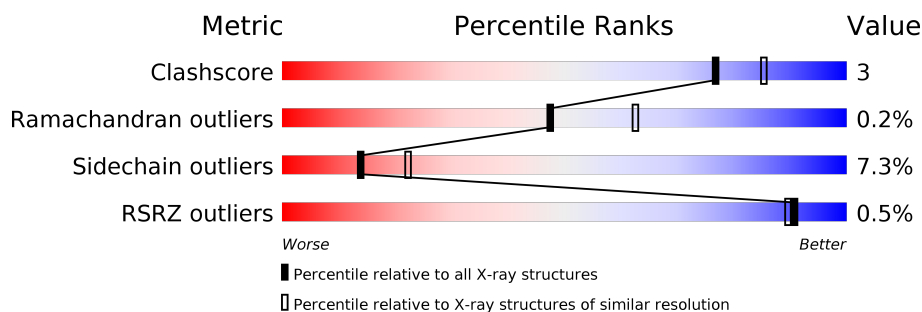
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 respectively. 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	501	 86% 12% ..
1	B	501	 86% 11% ..
1	C	501	 84% 14% .
1	D	501	 84% 14% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

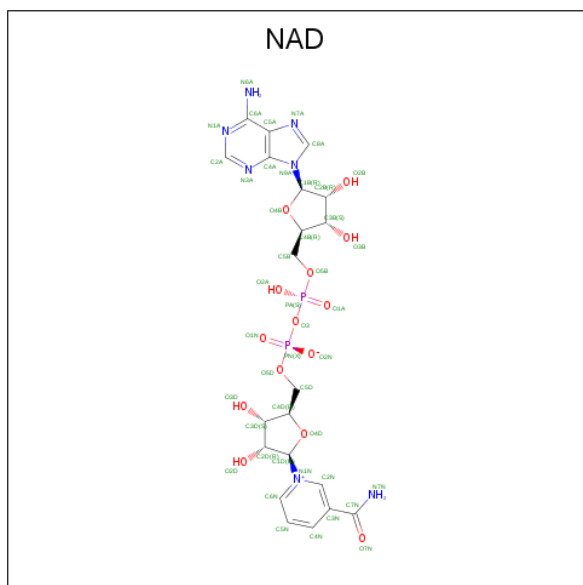
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DTU	D	901	X	-	-	-

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 ALDEHYDE DEHYDROGENASE, CYTOSOLIC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total 3784	C 2409	N 638	O 714	S 23	0	0	0
1	B	494	Total 3785	C 2409	N 638	O 715	S 23	0	0	0
1	C	494	Total 3785	C 2409	N 638	O 715	S 23	0	0	0
1	D	494	Total 3785	C 2409	N 638	O 715	S 23	0	0	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



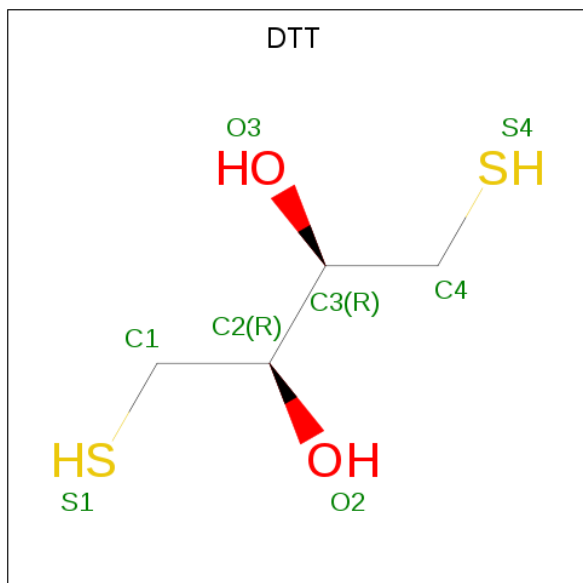
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

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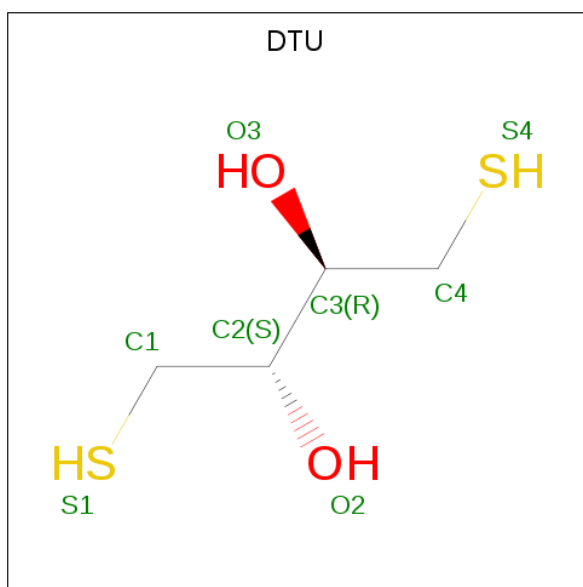
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 4 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTU) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	O	S	0	0
			8	4	2	2		

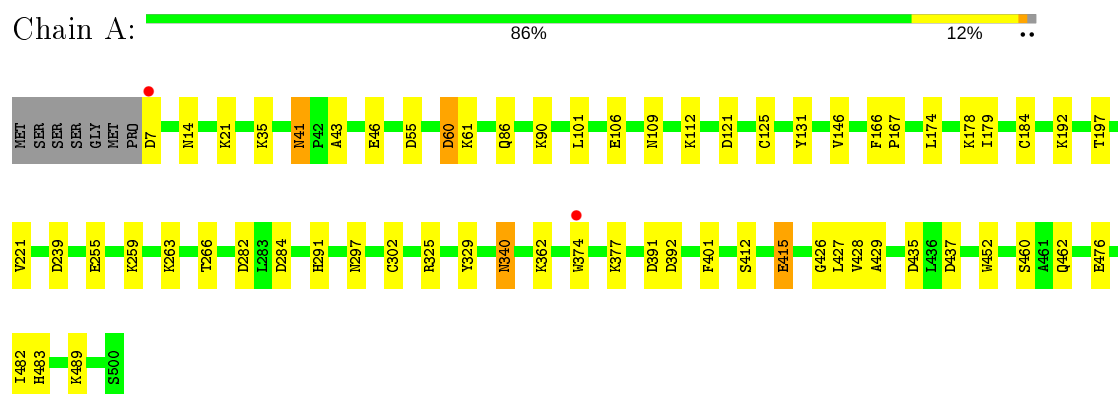
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	95	Total	O	0	0
			95	95		
5	B	145	Total	O	0	0
			145	145		
5	C	84	Total	O	0	0
			84	84		
5	D	130	Total	O	0	0
			130	130		

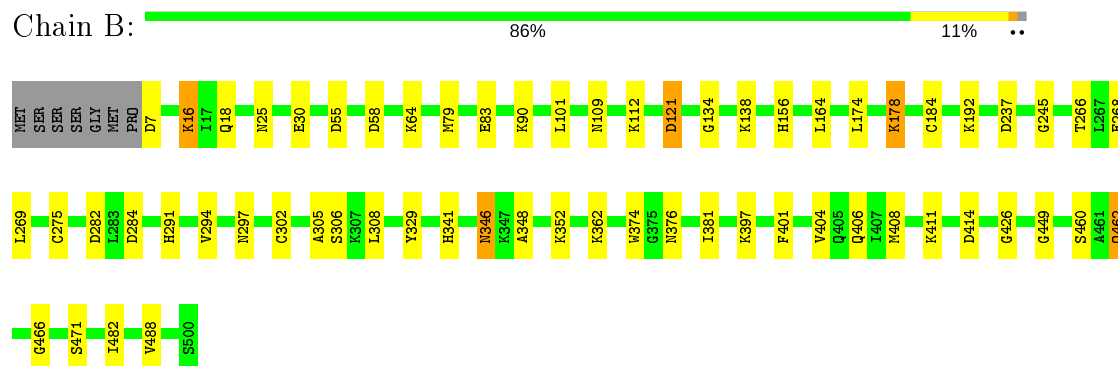
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

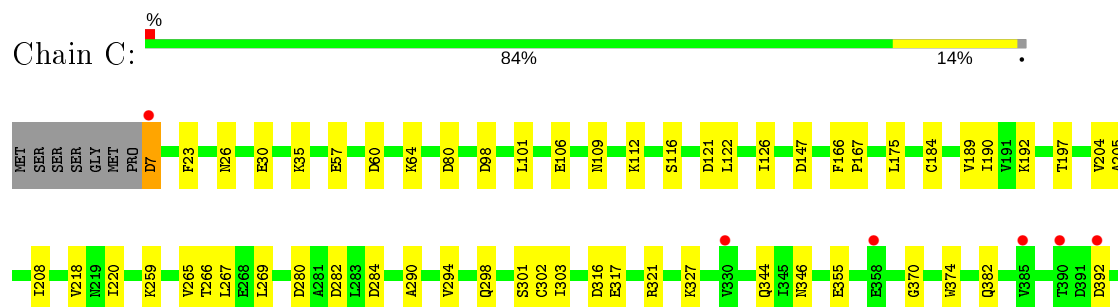
• Molecule 1: ALDEHYDE DEHYDROGENASE, CYTOSOLIC 1

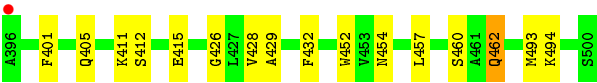


• Molecule 1: ALDEHYDE DEHYDROGENASE, CYTOSOLIC 1

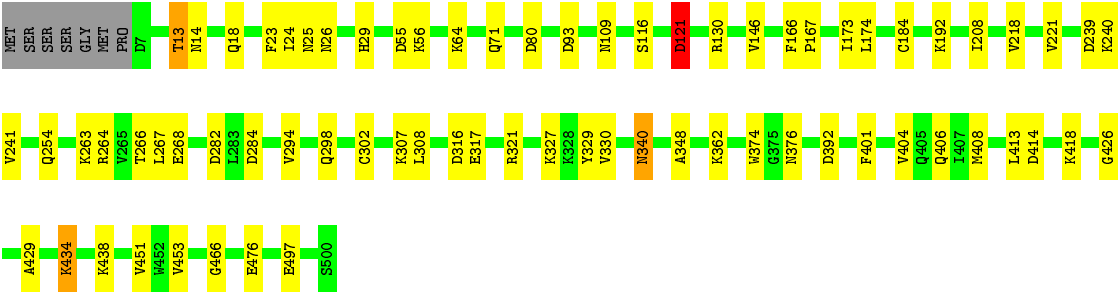
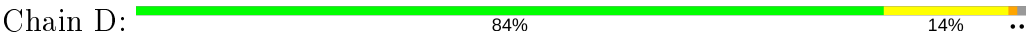


• Molecule 1: ALDEHYDE DEHYDROGENASE, CYTOSOLIC 1





● Molecule 1: ALDEHYDE DEHYDROGENASE, CYTOSOLIC 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.87Å 136.41Å 84.99Å 90.00° 102.62° 90.00°	Depositor
Resolution (Å)	41.52 – 2.40 41.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.2 (41.52-2.40) 96.2 (41.47-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.22 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.180 , 0.254 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15785	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, DTU, DTT

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	0.52	0/3865	0.73	10/5233 (0.2%)
1	B	0.57	0/3866	0.74	7/5233 (0.1%)
1	C	0.50	0/3866	0.71	10/5233 (0.2%)
1	D	0.55	0/3866	0.74	10/5233 (0.2%)
All	All	0.54	0/15463	0.73	37/20932 (0.2%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	ASP	CB-CG-OD2	7.32	124.89	118.30
1	C	316	ASP	CB-CG-OD2	7.27	124.84	118.30
1	B	121	ASP	CB-CG-OD2	7.07	124.66	118.30
1	D	414	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	282	ASP	CB-CG-OD2	6.94	124.54	118.30
1	A	392	ASP	CB-CG-OD2	6.93	124.54	118.30
1	C	282	ASP	CB-CG-OD2	6.77	124.39	118.30
1	C	60	ASP	CB-CG-OD2	6.57	124.22	118.30
1	D	316	ASP	CB-CG-OD2	6.50	124.15	118.30
1	C	147	ASP	CB-CG-OD2	6.38	124.04	118.30
1	D	93	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	282	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	55	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	55	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	7	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	437	ASP	CB-CG-OD2	5.84	123.56	118.30
1	C	280	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	391	ASP	CB-CG-OD2	5.69	123.42	118.30
1	D	121	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	58	ASP	CB-CG-OD2	5.59	123.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	121	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	60	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	392	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	7	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	7	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	80	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	98	ASP	CB-CG-OD2	5.27	123.04	118.30
1	D	239	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	239	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	392	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	284	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	237	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	130	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	D	55	ASP	CB-CG-OD2	5.15	122.93	118.30
1	C	121	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	80	ASP	CB-CG-OD2	5.03	122.82	118.30

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	3784	0	3773	24	0
1	B	3785	0	3773	22	0
1	C	3785	0	3773	25	0
1	D	3785	0	3773	25	0
2	A	44	0	26	1	0
2	B	44	0	26	2	0
2	C	44	0	26	2	0
2	D	44	0	26	3	0
3	B	8	0	10	1	0
4	D	8	0	10	2	0
5	A	95	0	0	0	0
5	B	145	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	84	0	0	0	0
5	D	130	0	0	0	0
All	All	15785	0	15216	91	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 3.

All (91) 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:B:302:CYS:SG	2:B:1501:NAD:C4N	2.52	0.97
1:D:302:CYS:SG	2:D:1501:NAD:C4N	2.61	0.88
1:C:302:CYS:SG	2:C:1501:NAD:C4N	2.61	0.88
1:A:302:CYS:SG	2:A:1501:NAD:C4N	2.71	0.79
1:A:41:ASN:C	1:A:41:ASN:HD22	1.92	0.73
1:C:302:CYS:SG	2:C:1501:NAD:C3N	2.77	0.72
1:B:348:ALA:HB2	4:D:901:DTU:H4C1	1.70	0.71
1:B:302:CYS:SG	2:B:1501:NAD:C3N	2.77	0.71
1:A:178:LYS:NZ	1:A:476:GLU:OE1	2.27	0.68
1:A:428:VAL:HG11	1:A:452:TRP:CZ3	2.29	0.68
1:B:348:ALA:HB2	4:D:901:DTU:C4	2.25	0.67
1:D:330:VAL:H	1:D:340:ASN:HD21	1.44	0.66
1:C:428:VAL:HG11	1:C:452:TRP:CZ3	2.35	0.61
1:B:156:HIS:CD2	1:B:488:VAL:HG22	2.37	0.60
1:A:427:LEU:HG	1:A:428:VAL:HG23	1.84	0.59
1:A:221:VAL:HG23	1:A:221:VAL:O	2.03	0.59
1:B:16:LYS:HD2	1:B:18:GLN:HE21	1.70	0.57
1:A:166:PHE:HB2	1:A:167:PRO:HD2	1.88	0.56
1:B:294:VAL:HG22	1:B:305:ALA:O	2.05	0.55
1:C:462:GLN:HG2	1:D:146:VAL:HG12	1.89	0.54
1:A:166:PHE:HB2	1:A:167:PRO:CD	2.37	0.54
1:A:109:ASN:HD21	1:A:197:THR:HA	1.71	0.54
1:D:330:VAL:H	1:D:340:ASN:ND2	2.04	0.54
1:C:370:GLY:HA2	1:C:382:GLN:HE21	1.73	0.54
1:A:41:ASN:ND2	1:A:43:ALA:H	2.06	0.54
1:C:294:VAL:HG21	1:C:405:GLN:HG3	1.90	0.53
1:D:404:VAL:HG12	1:D:406:GLN:OE1	2.08	0.53
1:D:208:ILE:HD13	1:D:218:VAL:HG11	1.90	0.53
1:C:166:PHE:HB2	1:C:167:PRO:CD	2.40	0.52
1:B:346:ASN:HD22	1:B:346:ASN:C	2.14	0.51
1:B:291:HIS:HE1	1:B:329:TYR:OH	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASN:ND2	1:A:41:ASN:C	2.63	0.51
1:C:101:LEU:HD23	1:C:101:LEU:C	2.32	0.50
1:D:268:GLU:HG3	1:D:476:GLU:OE1	2.11	0.50
1:A:291:HIS:CD2	1:A:325:ARG:HG3	2.47	0.50
1:A:412:SER:OG	1:A:415:GLU:HB3	2.12	0.49
1:C:175:LEU:HD21	1:C:204:VAL:HG11	1.95	0.49
1:D:166:PHE:HB2	1:D:167:PRO:CD	2.42	0.49
1:C:265:VAL:HG12	1:C:267:LEU:HD13	1.94	0.49
1:A:109:ASN:ND2	1:A:197:THR:HA	2.28	0.49
3:B:900:DTT:H2	1:D:348:ALA:HB2	1.95	0.48
1:B:16:LYS:CD	1:B:18:GLN:HE21	2.25	0.48
1:C:290:ALA:O	1:C:294:VAL:HG23	2.14	0.48
1:D:302:CYS:SG	2:D:1501:NAD:C3N	3.02	0.48
1:A:146:VAL:HA	1:B:462:GLN:CG	2.44	0.48
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.49	0.47
1:B:341:HIS:HE1	1:B:381:ILE:O	1.98	0.47
1:D:254:GLN:HG2	1:D:267:LEU:HD11	1.97	0.47
1:C:267:LEU:HG	1:C:269:LEU:HD21	1.98	0.46
1:C:298:GLN:HB3	1:C:344:GLN:HE22	1.79	0.46
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.51	0.46
1:A:131:TYR:CE1	1:A:462:GLN:HG3	2.51	0.46
1:B:291:HIS:HD2	5:B:2104:HOH:O	1.98	0.46
1:B:134:GLY:O	1:B:138:LYS:HD2	2.15	0.46
1:C:432:PHE:CD1	1:C:454:ASN:HA	2.51	0.45
1:D:434:LYS:HB3	1:D:434:LYS:NZ	2.31	0.45
1:A:101:LEU:HD23	1:A:101:LEU:C	2.36	0.45
1:C:208:ILE:HD13	1:C:218:VAL:HG11	1.97	0.45
1:C:462:GLN:CG	1:D:146:VAL:HA	2.47	0.45
1:B:101:LEU:HD23	1:B:101:LEU:C	2.37	0.45
1:B:79:MET:HG2	1:B:83:GLU:HB2	1.97	0.45
1:C:109:ASN:ND2	1:C:197:THR:HA	2.32	0.45
1:A:41:ASN:HD22	1:A:43:ALA:H	1.64	0.44
1:D:13:THR:HG23	1:D:14:ASN:HD22	1.82	0.44
1:D:302:CYS:SG	2:D:1501:NAD:H4N	2.54	0.44
1:B:404:VAL:HG12	1:B:406:GLN:OE1	2.18	0.44
1:A:291:HIS:CD2	1:A:325:ARG:CG	3.01	0.43
1:C:493:MET:HG2	1:D:453:VAL:HB	2.00	0.43
1:C:303:ILE:HD12	1:C:457:LEU:HD23	2.00	0.43
1:A:340:ASN:C	1:A:340:ASN:HD22	2.22	0.43
1:A:255:GLU:OE2	1:A:259:LYS:NZ	2.47	0.43
1:B:245:GLY:O	1:B:269:LEU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:TYR:HA	1:D:340:ASN:HD21	1.84	0.42
1:C:189:VAL:C	1:C:190:ILE:HD13	2.40	0.42
1:D:24:ILE:HB	1:D:29:HIS:CD2	2.54	0.41
1:D:241:VAL:HG12	1:D:263:LYS:HD3	2.02	0.41
1:A:428:VAL:HG12	1:A:429:ALA:N	2.36	0.41
1:D:284:ASP:OD1	1:D:321:ARG:NH1	2.53	0.41
1:D:268:GLU:OE1	1:D:466:GLY:HA2	2.21	0.41
1:A:291:HIS:HE1	1:A:329:TYR:OH	2.03	0.41
1:C:428:VAL:HG12	1:C:429:ALA:N	2.36	0.41
1:D:121:ASP:HA	1:D:173:ILE:HD11	2.01	0.41
1:C:122:LEU:O	1:C:126:ILE:HD12	2.21	0.41
1:C:205:ALA:HB2	1:C:220:ILE:HD12	2.03	0.41
1:D:240:LYS:HG3	1:D:264:ARG:HB2	2.03	0.41
1:D:429:ALA:O	1:D:451:VAL:HA	2.20	0.41
1:B:112:LYS:HG2	1:B:297:ASN:ND2	2.35	0.41
1:B:164:LEU:HD13	1:B:178:LYS:HB3	2.03	0.40
1:A:146:VAL:HA	1:B:462:GLN:HG2	2.03	0.40
1:C:428:VAL:CG1	1:C:429:ALA:N	2.85	0.40
1:B:449:GLY:HA3	1:B:466:GLY:O	2.22	0.40

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	492/501 (98%)	474 (96%)	17 (4%)	1 (0%)	47 62
1	B	492/501 (98%)	474 (96%)	17 (4%)	1 (0%)	47 62
1	C	492/501 (98%)	472 (96%)	19 (4%)	1 (0%)	47 62
1	D	492/501 (98%)	476 (97%)	15 (3%)	1 (0%)	47 62
All	All	1968/2004 (98%)	1896 (96%)	68 (4%)	4 (0%)	47 62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	426	GLY
1	A	426	GLY
1	D	426	GLY
1	B	426	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	402/408 (98%)	372 (92%)	30 (8%)	13	21
1	B	402/408 (98%)	372 (92%)	30 (8%)	13	21
1	C	402/408 (98%)	375 (93%)	27 (7%)	16	26
1	D	402/408 (98%)	371 (92%)	31 (8%)	13	20
All	All	1608/1632 (98%)	1490 (93%)	118 (7%)	14	22

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	21	LYS
1	A	35	LYS
1	A	41	ASN
1	A	46	GLU
1	A	60	ASP
1	A	61	LYS
1	A	86	GLN
1	A	90	LYS
1	A	106	GLU
1	A	112	LYS
1	A	125	CYS
1	A	174	LEU
1	A	179	ILE
1	A	184	CYS
1	A	192	LYS

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Mol	Chain	Res	Type
1	A	263	LYS
1	A	266	THR
1	A	284	ASP
1	A	297	ASN
1	A	340	ASN
1	A	362	LYS
1	A	374	TRP
1	A	377	LYS
1	A	401	PHE
1	A	415	GLU
1	A	460	SER
1	A	482	ILE
1	A	483	HIS
1	A	489	LYS
1	B	16	LYS
1	B	25	ASN
1	B	30	GLU
1	B	64	LYS
1	B	90	LYS
1	B	109	ASN
1	B	121	ASP
1	B	174	LEU
1	B	178	LYS
1	B	184	CYS
1	B	192	LYS
1	B	266	THR
1	B	268	GLU
1	B	275	CYS
1	B	306	SER
1	B	308	LEU
1	B	346	ASN
1	B	352	LYS
1	B	362	LYS
1	B	374	TRP
1	B	376	ASN
1	B	397	LYS
1	B	401	PHE
1	B	408	MET
1	B	411	LYS
1	B	414	ASP
1	B	460	SER
1	B	462	GLN

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Mol	Chain	Res	Type
1	B	471	SER
1	B	482	ILE
1	C	7	ASP
1	C	30	GLU
1	C	35	LYS
1	C	57	GLU
1	C	64	LYS
1	C	106	GLU
1	C	112	LYS
1	C	116	SER
1	C	184	CYS
1	C	192	LYS
1	C	259	LYS
1	C	266	THR
1	C	284	ASP
1	C	301	SER
1	C	317	GLU
1	C	321	ARG
1	C	327	LYS
1	C	346	ASN
1	C	355	GLU
1	C	374	TRP
1	C	401	PHE
1	C	411	LYS
1	C	412	SER
1	C	415	GLU
1	C	460	SER
1	C	462	GLN
1	C	494	LYS
1	D	13	THR
1	D	18	GLN
1	D	25	ASN
1	D	56	LYS
1	D	64	LYS
1	D	71	GLN
1	D	109	ASN
1	D	116	SER
1	D	121	ASP
1	D	174	LEU
1	D	184	CYS
1	D	192	LYS
1	D	221	VAL

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Mol	Chain	Res	Type
1	D	266	THR
1	D	294	VAL
1	D	298	GLN
1	D	307	LYS
1	D	308	LEU
1	D	317	GLU
1	D	327	LYS
1	D	340	ASN
1	D	362	LYS
1	D	374	TRP
1	D	376	ASN
1	D	401	PHE
1	D	408	MET
1	D	413	LEU
1	D	418	LYS
1	D	434	LYS
1	D	438	LYS
1	D	497	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	41	ASN
1	A	109	ASN
1	A	291	HIS
1	A	300	GLN
1	A	340	ASN
1	A	405	GLN
1	B	18	GLN
1	B	25	ASN
1	B	156	HIS
1	B	291	HIS
1	B	297	ASN
1	B	341	HIS
1	B	346	ASN
1	B	376	ASN
1	C	109	ASN
1	C	344	GLN
1	C	346	ASN
1	C	351	ASN
1	C	382	GLN

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Mol	Chain	Res	Type
1	C	388	ASN
1	D	14	ASN
1	D	25	ASN
1	D	29	HIS
1	D	340	ASN
1	D	405	GLN
1	D	473	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	$\# Z > 2$
4	DTU	D	901	-	7,7,7	0.71	0	4,8,8	1.50	0
2	NAD	A	1501	-	42,48,48	1.67	2 (4%)	50,73,73	1.42	4 (8%)
2	NAD	C	1501	-	42,48,48	1.70	4 (9%)	50,73,73	1.25	4 (8%)
2	NAD	B	1501	-	42,48,48	1.70	3 (7%)	50,73,73	1.30	4 (8%)
2	NAD	D	1501	-	42,48,48	1.73	5 (11%)	50,73,73	1.35	5 (10%)
3	DTT	B	900	-	7,7,7	0.85	0	4,8,8	1.07	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
4	DTU	D	901	-	2/2/2/2	6/8/8/8	-
2	NAD	A	1501	-	-	4/26/62/62	0/5/5/5
2	NAD	C	1501	-	-	4/26/62/62	0/5/5/5
2	NAD	B	1501	-	-	2/26/62/62	0/5/5/5
2	NAD	D	1501	-	-	5/26/62/62	0/5/5/5
3	DTT	B	900	-	-	2/8/8/8	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1501	NAD	O7N-C7N	8.48	1.40	1.24
2	C	1501	NAD	O7N-C7N	8.35	1.40	1.24
2	A	1501	NAD	O7N-C7N	8.20	1.39	1.24
2	B	1501	NAD	O7N-C7N	7.86	1.39	1.24
2	B	1501	NAD	C2A-N3A	4.66	1.39	1.32
2	A	1501	NAD	C2A-N3A	4.29	1.39	1.32
2	D	1501	NAD	C2A-N3A	4.26	1.39	1.32
2	C	1501	NAD	C2A-N3A	4.03	1.38	1.32
2	B	1501	NAD	C2A-N1A	2.87	1.39	1.33
2	C	1501	NAD	C2A-N1A	2.87	1.39	1.33
2	D	1501	NAD	C2N-N1N	2.25	1.37	1.35
2	D	1501	NAD	C2A-N1A	2.22	1.38	1.33
2	D	1501	NAD	C2B-C1B	-2.06	1.50	1.53
2	C	1501	NAD	C2B-C1B	-2.01	1.50	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	NAD	N3A-C2A-N1A	-5.63	119.88	128.68
2	D	1501	NAD	N3A-C2A-N1A	-5.04	120.81	128.68
2	B	1501	NAD	N3A-C2A-N1A	-4.97	120.91	128.68
2	B	1501	NAD	C3N-C7N-N7N	4.70	123.39	117.75
2	C	1501	NAD	N3A-C2A-N1A	-4.63	121.44	128.68
2	A	1501	NAD	C3N-C7N-N7N	4.61	123.28	117.75
2	C	1501	NAD	C3N-C7N-N7N	4.12	122.69	117.75
2	D	1501	NAD	C3N-C7N-N7N	3.78	122.29	117.75
2	A	1501	NAD	PN-O3-PA	-3.58	120.53	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1501	NAD	O7N-C7N-N7N	-3.26	117.95	122.58
2	D	1501	NAD	PN-O3-PA	-3.16	121.97	132.83
2	B	1501	NAD	O7N-C7N-N7N	-3.06	118.22	122.58
2	C	1501	NAD	PN-O3-PA	-2.65	123.75	132.83
2	A	1501	NAD	O7N-C7N-N7N	-2.48	119.05	122.58
2	D	1501	NAD	C1B-N9A-C4A	-2.26	122.67	126.64
2	C	1501	NAD	O7N-C7N-N7N	-2.05	119.66	122.58
2	B	1501	NAD	C1B-N9A-C4A	-2.05	123.04	126.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	901	DTU	C2
4	D	901	DTU	C3

All (23) torsion outliers are listed below:

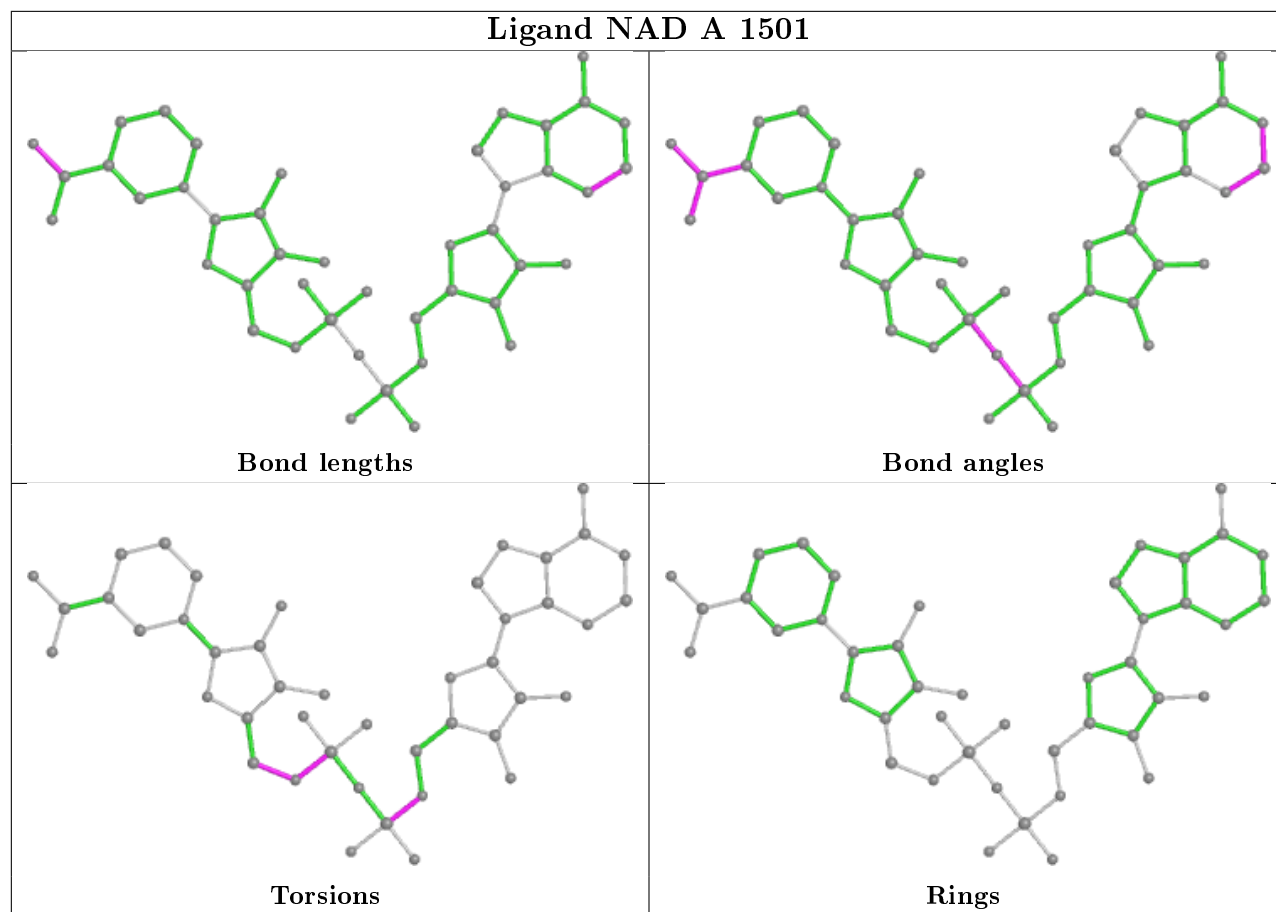
Mol	Chain	Res	Type	Atoms
4	D	901	DTU	S1-C1-C2-O2
4	D	901	DTU	S1-C1-C2-C3
4	D	901	DTU	C2-C3-C4-S4
4	D	901	DTU	O3-C3-C4-S4
2	A	1501	NAD	C5D-O5D-PN-O1N
2	C	1501	NAD	C5B-O5B-PA-O3
2	B	1501	NAD	C5D-O5D-PN-O1N
2	D	1501	NAD	C5B-O5B-PA-O1A
2	D	1501	NAD	C5B-O5B-PA-O3
3	B	900	DTT	C2-C3-C4-S4
3	B	900	DTT	O3-C3-C4-S4
4	D	901	DTU	O2-C2-C3-C4
2	A	1501	NAD	C4D-C5D-O5D-PN
2	B	1501	NAD	C5D-O5D-PN-O3
2	D	1501	NAD	C5D-O5D-PN-O3
2	D	1501	NAD	C4D-C5D-O5D-PN
4	D	901	DTU	C1-C2-C3-C4
2	C	1501	NAD	C5B-O5B-PA-O1A
2	C	1501	NAD	C5B-O5B-PA-O2A
2	D	1501	NAD	C5D-O5D-PN-O1N
2	C	1501	NAD	C4D-C5D-O5D-PN
2	A	1501	NAD	C5D-O5D-PN-O3
2	A	1501	NAD	C5B-O5B-PA-O1A

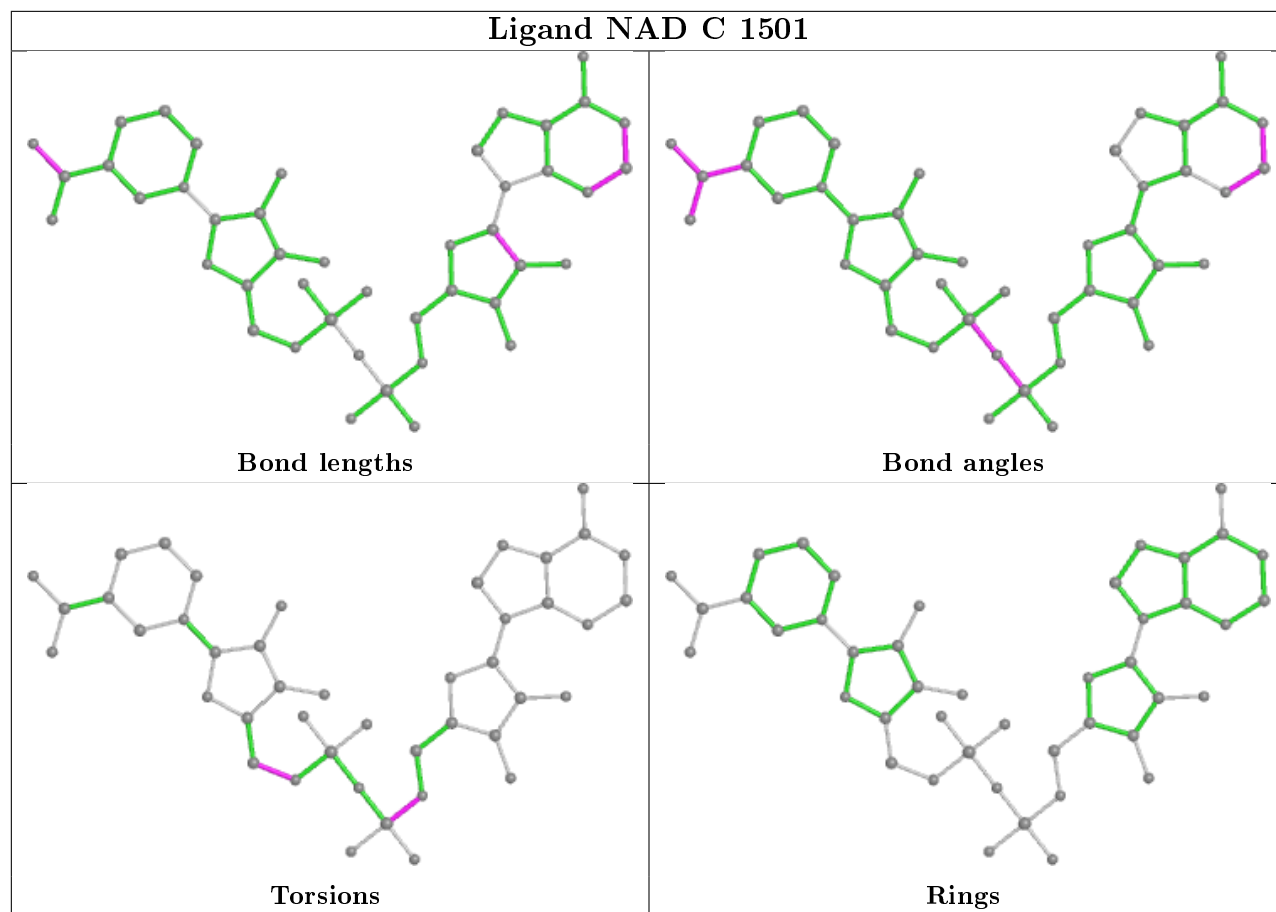
There are no ring outliers.

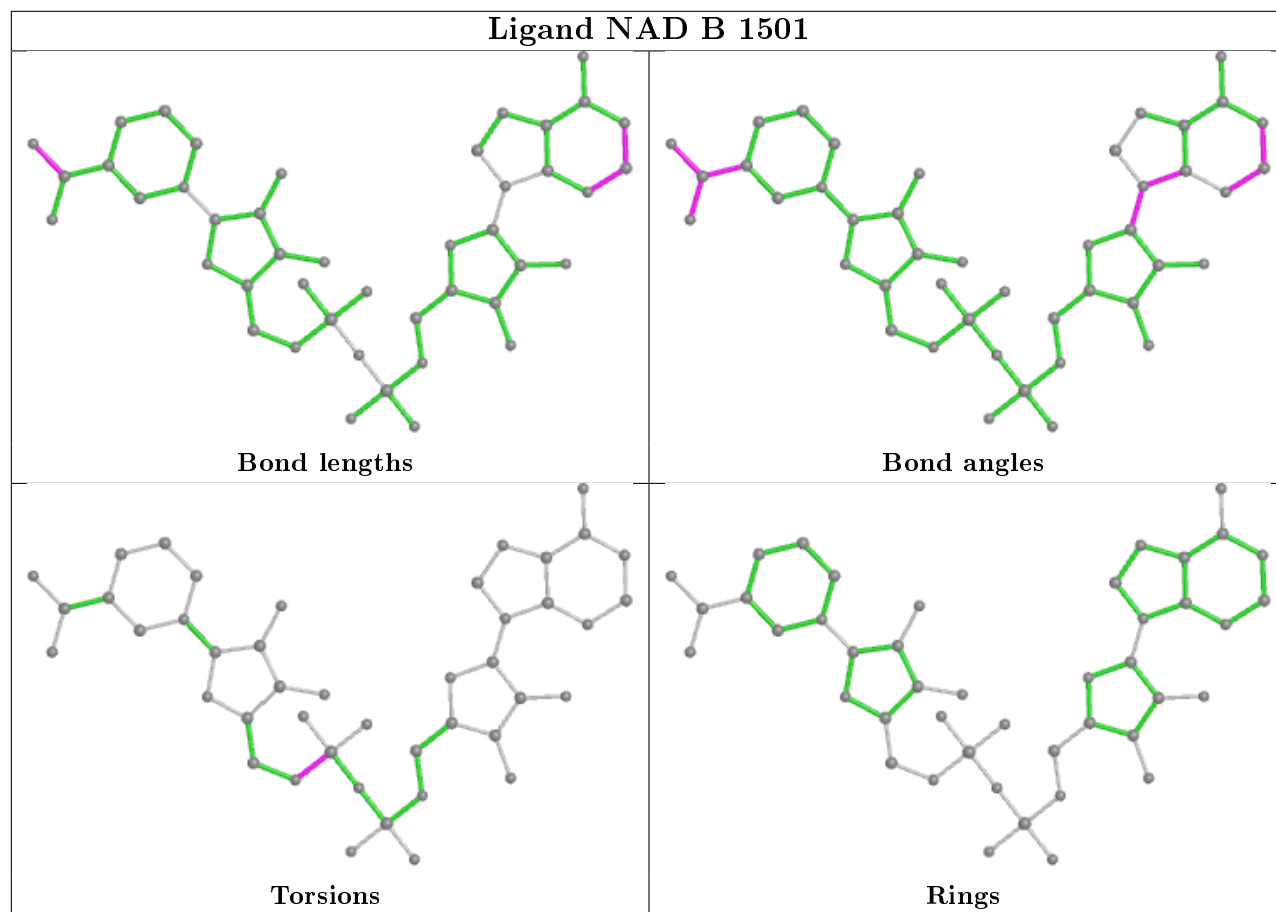
6 monomers are involved in 11 short contacts:

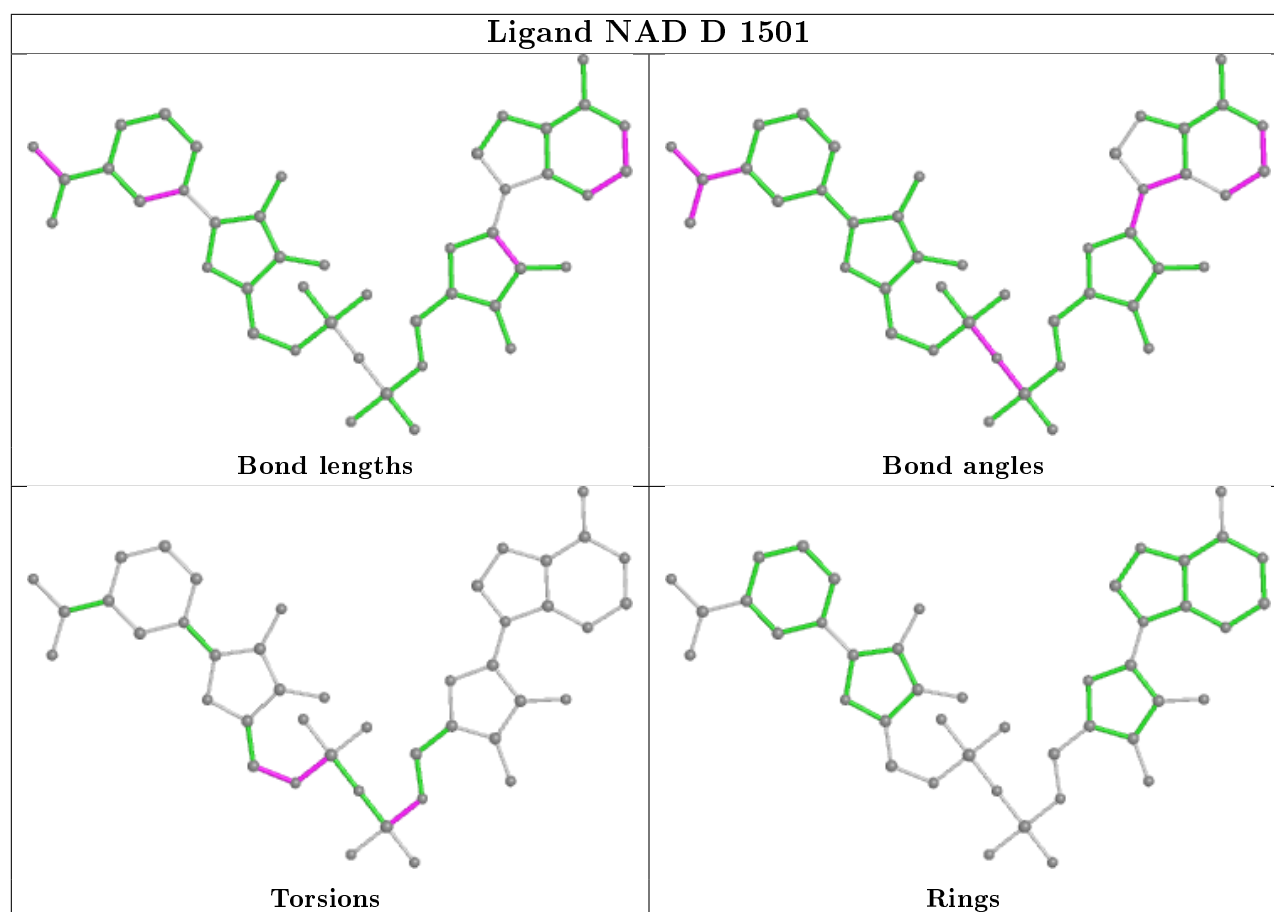
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	901	DTU	2	0
2	A	1501	NAD	1	0
2	C	1501	NAD	2	0
2	B	1501	NAD	2	0
2	D	1501	NAD	3	0
3	B	900	DTT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	494/501 (98%)	-0.26	2 (0%) 92 91	15, 26, 41, 51	0
1	B	494/501 (98%)	-0.37	0 100 100	13, 21, 32, 41	0
1	C	494/501 (98%)	-0.14	7 (1%) 75 73	13, 27, 44, 53	0
1	D	494/501 (98%)	-0.46	0 100 100	11, 20, 29, 44	0
All	All	1976/2004 (98%)	-0.31	9 (0%) 91 89	11, 23, 40, 53	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	ASP	3.3
1	C	7	ASP	2.7
1	C	330	VAL	2.6
1	C	385	VAL	2.5
1	C	390	THR	2.3
1	C	396	ALA	2.3
1	C	392	ASP	2.2
1	A	374	TRP	2.0
1	C	358	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

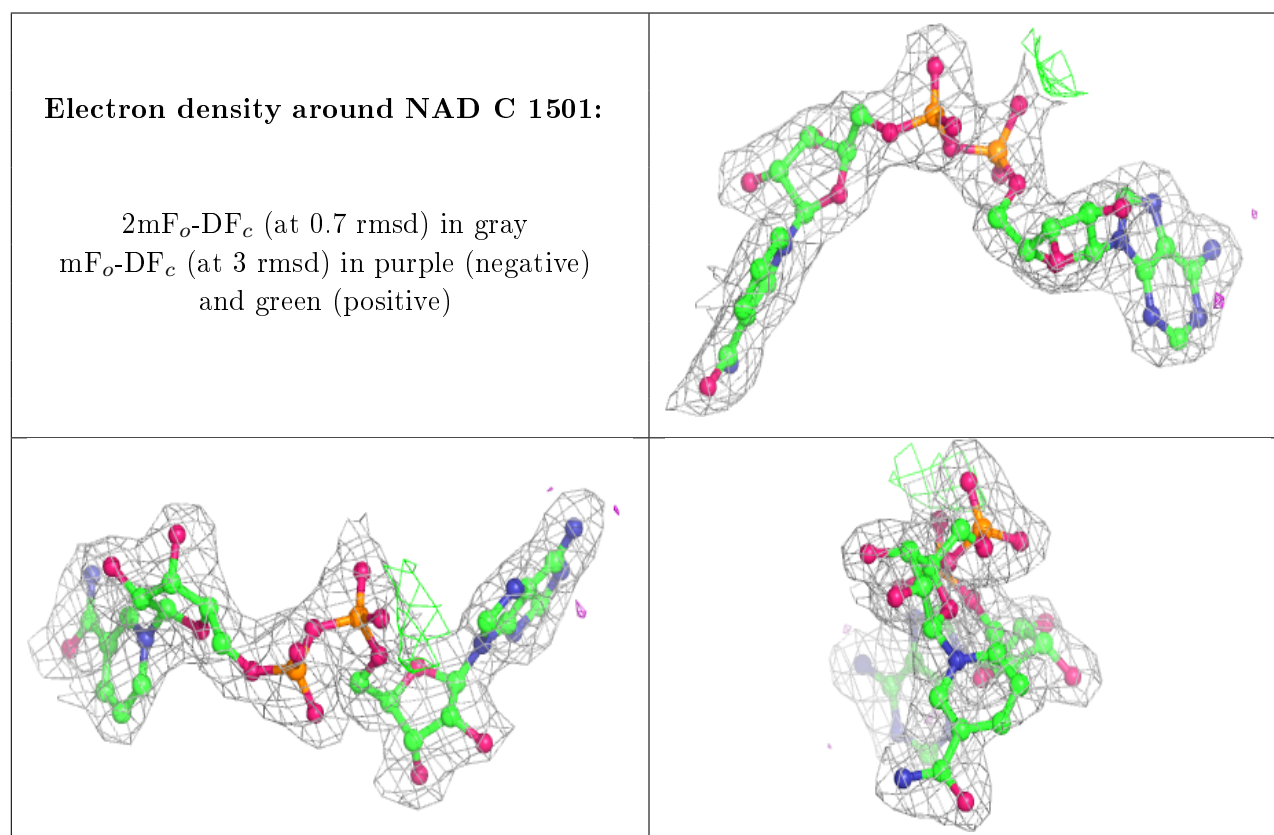
There are no carbohydrates in this entry.

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. 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.

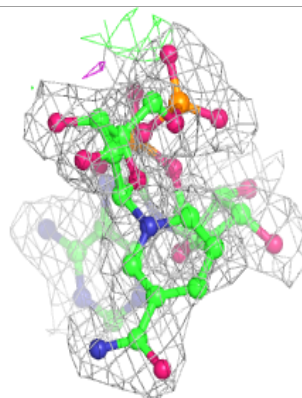
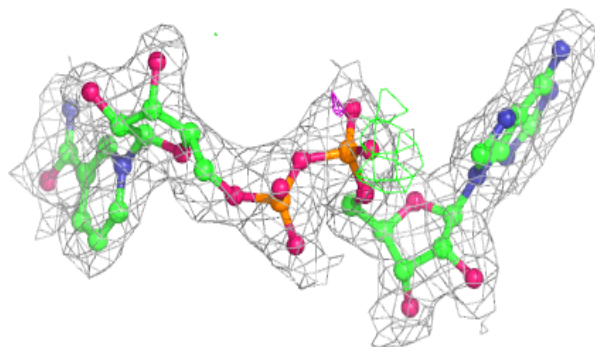
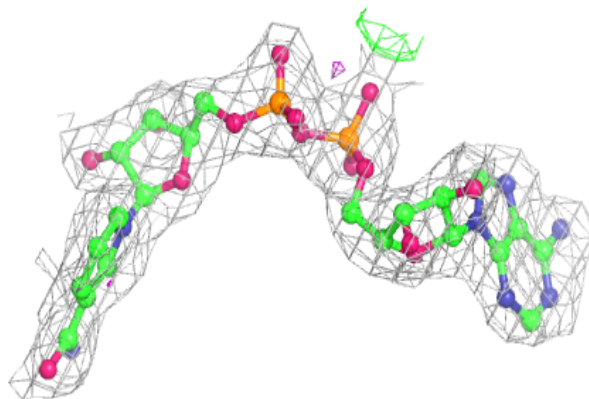
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DTU	D	901	8/8	0.80	0.31	32,39,44,45	0
3	DTT	B	900	8/8	0.85	0.30	26,36,41,44	0
2	NAD	C	1501	44/44	0.95	0.13	20,25,29,30	0
2	NAD	B	1501	44/44	0.96	0.13	14,22,25,26	0
2	NAD	D	1501	44/44	0.96	0.12	16,20,23,24	0
2	NAD	A	1501	44/44	0.96	0.12	18,25,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

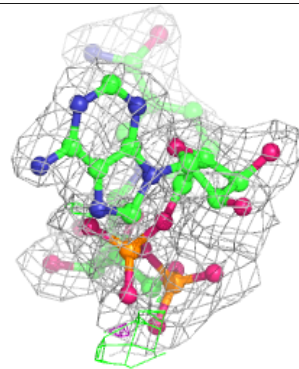
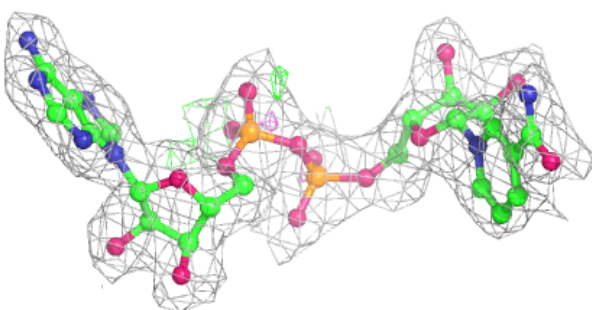
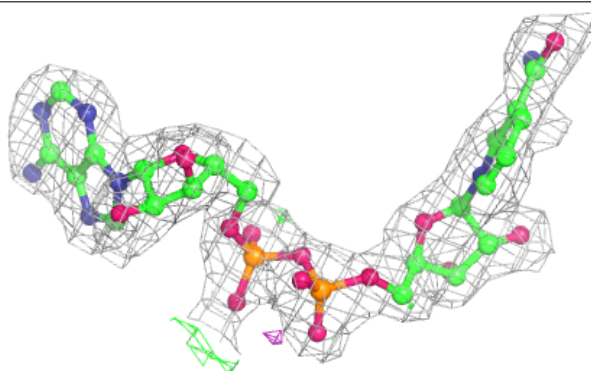


Electron density around NAD B 1501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

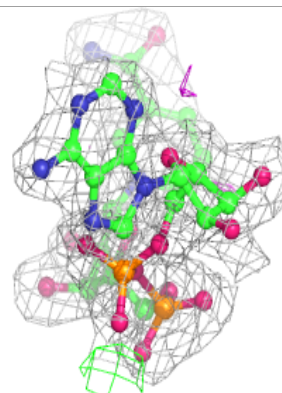
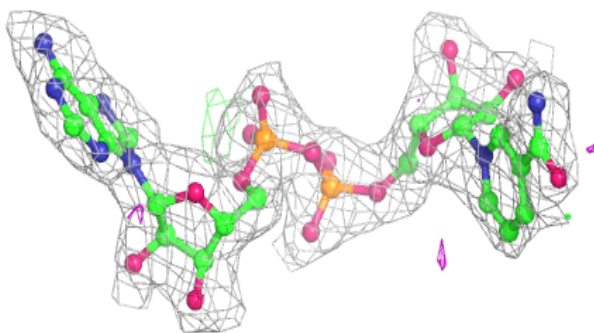
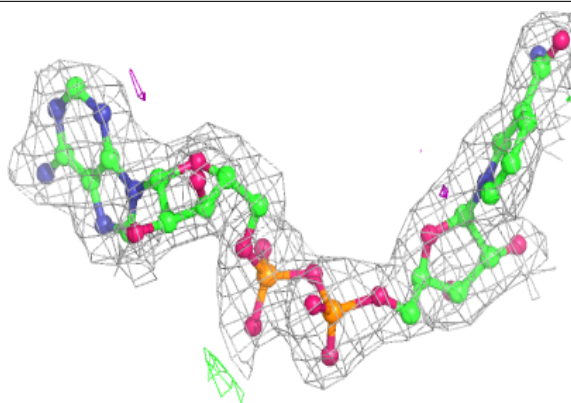
**Electron density around NAD D 1501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAD A 1501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.