



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:59 PM UTC

PDB ID : 1EBF / pdb\_00001ebf  
Title : HOMOSERINE DEHYDROGENASE FROM S. CEREVISIAE COMPLEX WITH NAD+  
Authors : DeLaBarre, B.; Thompson, P.R.; Wright, G.D.; Berghuis, A.M.  
Deposited on : 2000-01-24  
Resolution : 2.30 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

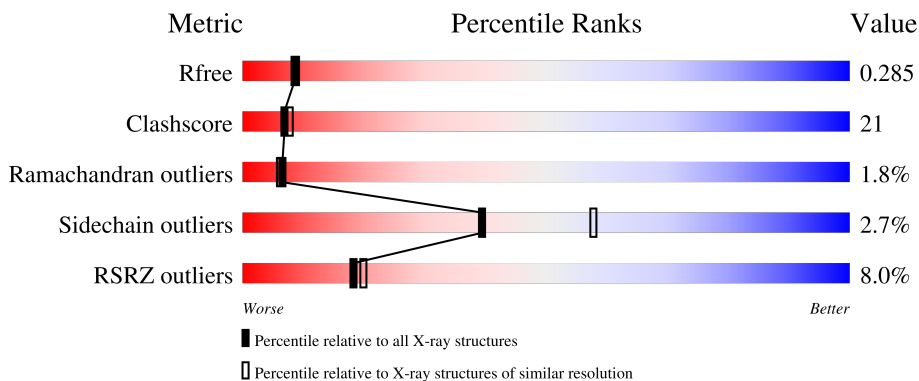
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	358	
1	B	358	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5719 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

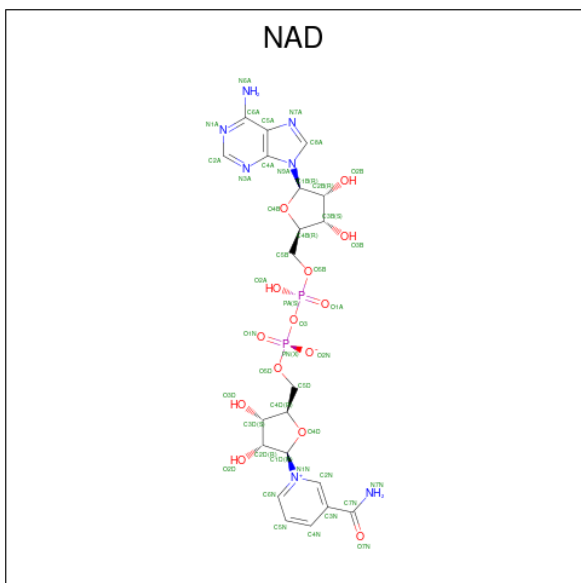
- Molecule 1 is a protein called HOMOSERINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	Total 2710	C 1737	N 443	O 529	S 1	0	0	0
1	B	358	Total 2710	C 1737	N 443	O 529	S 1	0	0	0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	Total 1	Na 1	0	0
2	B	1	Total 1	Na 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

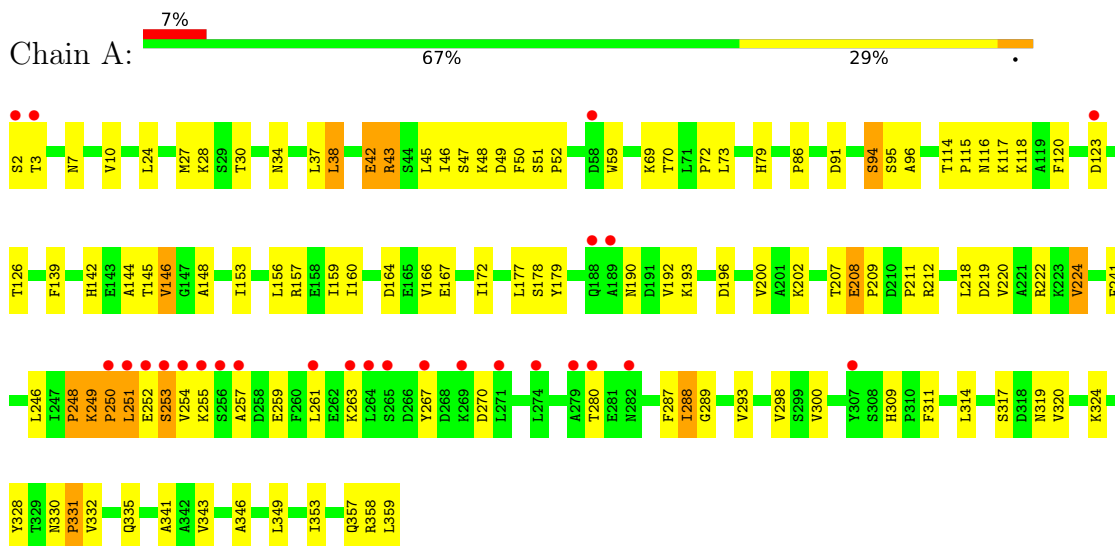
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total 122	O 122	0	0
4	B	131	Total 131	O 131	0	0

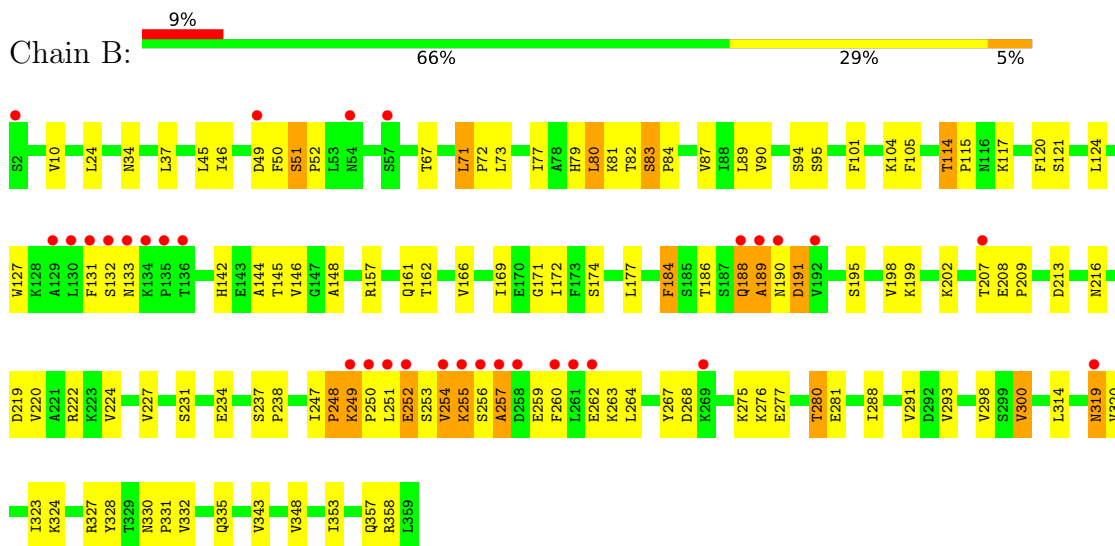
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: HOMOSERINE DEHYDROGENASE



- Molecule 1: HOMOSERINE DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.40Å 80.40Å 250.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.96 – 2.30 35.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	85.7 (35.96-2.30) 95.2 (35.96-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.20Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.269 0.234 , 0.285	Depositor DCC
$R_{free}$ test set	2870 reflections (7.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtrriage
Anisotropy	0.118	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.45	0/2757	1.02	18/3741 (0.5%)
1	B	0.44	0/2757	1.01	16/3741 (0.4%)
All	All	0.44	0/5514	1.02	34/7482 (0.5%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	THR	N-CA-C	10.37	117.47	108.13
1	A	114	THR	N-CA-C	10.31	117.41	108.13
1	A	330	ASN	N-CA-C	-8.54	99.30	110.07
1	A	251	LEU	N-CA-C	-8.02	104.46	112.97
1	B	332	VAL	N-CA-C	-7.94	96.80	108.87
1	B	288	ILE	N-CA-C	7.09	119.15	108.80
1	A	288	ILE	N-CA-C	7.03	118.94	108.96
1	B	51	SER	N-CA-C	-7.00	100.98	110.36
1	A	332	VAL	N-CA-C	-6.95	97.60	108.23
1	A	95	SER	N-CA-C	6.53	119.18	109.59
1	B	330	ASN	N-CA-C	-6.43	100.29	109.62
1	A	319	ASN	N-CA-C	-6.29	100.90	110.14
1	B	323	ILE	N-CA-C	6.09	116.38	107.37
1	B	83	SER	CA-C-N	6.05	126.17	119.87
1	B	83	SER	C-N-CA	6.05	126.17	119.87
1	B	72	PRO	N-CA-C	-5.84	102.29	111.34
1	A	51	SER	N-CA-C	-5.76	102.34	110.29
1	A	73	LEU	N-CA-C	5.75	118.29	111.33
1	A	10	VAL	N-CA-C	5.70	116.79	108.58
1	A	208	GLU	N-CA-C	-5.69	102.23	110.08
1	A	30	THR	N-CA-C	-5.60	105.94	112.89
1	A	72	PRO	N-CA-C	-5.56	102.46	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	SER	N-CA-C	5.50	117.67	109.25
1	B	94	SER	N-CA-C	-5.45	104.03	111.56
1	B	45	LEU	N-CA-C	-5.41	99.69	108.52
1	A	341	ALA	N-CA-C	5.41	117.62	111.02
1	A	96	ALA	N-CA-C	-5.40	105.47	111.36
1	A	289	GLY	N-CA-C	-5.37	101.53	111.04
1	A	94	SER	N-CA-C	-5.26	104.45	111.87
1	B	184	PHE	N-CA-C	5.16	116.59	110.97
1	B	71	LEU	N-CA-C	5.14	116.36	109.83
1	A	331	PRO	N-CA-C	5.13	119.15	111.14
1	B	293	VAL	N-CA-C	5.11	115.88	110.72
1	B	188	GLN	N-CA-C	5.07	117.46	109.39

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2710	0	2782	118	0
1	B	2710	0	2782	123	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	44	0	26	0	0
4	A	122	0	0	1	0
4	B	131	0	0	0	0
All	All	5719	0	5590	234	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 21.

All (234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LYS:HB3	1:A:250:PRO:HD2	1.17	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ILE:O	1:B:319:ASN:HB2	1.53	1.05
1:B:291:VAL:HG22	1:B:298:VAL:HG22	1.42	1.01
1:A:249:LYS:HB3	1:A:250:PRO:CD	2.00	0.91
1:B:251:LEU:HD22	1:B:267:TYR:OH	1.72	0.89
1:A:314:LEU:HD21	1:A:320:VAL:HG21	1.53	0.88
1:B:142:HIS:HD2	1:B:145:THR:HG21	1.39	0.87
1:B:320:VAL:HG12	1:B:335:GLN:CB	2.03	0.87
1:A:142:HIS:HE1	1:A:157:ARG:HH21	1.22	0.86
1:B:255:LYS:HD3	1:B:259:GLU:HG3	1.56	0.86
1:A:255:LYS:HD2	1:A:259:GLU:HG3	1.59	0.82
1:B:145:THR:HG23	1:B:146:VAL:HG23	1.59	0.82
1:A:146:VAL:HG13	1:A:153:ILE:HD11	1.61	0.82
1:B:320:VAL:HG12	1:B:335:GLN:HB2	1.63	0.81
1:A:207:THR:HG21	1:A:211:PRO:HG3	1.63	0.80
1:B:220:VAL:O	1:B:224:VAL:HG23	1.82	0.79
1:A:212:ARG:NH2	1:A:257:ALA:H	1.81	0.78
1:A:249:LYS:CB	1:A:250:PRO:HD2	2.09	0.78
1:B:10:VAL:HG22	1:B:90:VAL:CG2	2.14	0.78
1:A:255:LYS:HD2	1:A:259:GLU:CG	2.14	0.77
1:B:255:LYS:HD3	1:B:259:GLU:CG	2.14	0.77
1:B:249:LYS:HB3	1:B:250:PRO:CD	2.13	0.77
1:A:220:VAL:O	1:A:224:VAL:HG12	1.85	0.76
1:B:117:LYS:HG2	1:B:145:THR:OG1	1.84	0.76
1:B:324:LYS:HG2	1:B:331:PRO:HG3	1.68	0.76
1:B:157:ARG:O	1:B:161:GLN:HG3	1.87	0.75
1:A:346:ALA:HB1	1:B:162:THR:HG21	1.69	0.75
1:A:346:ALA:CB	1:B:162:THR:HG21	2.16	0.74
1:A:27:MET:CE	1:A:353:ILE:HD11	2.18	0.74
1:B:249:LYS:H	1:B:249:LYS:HD2	1.53	0.73
1:B:10:VAL:HG22	1:B:90:VAL:HG21	1.68	0.72
1:A:27:MET:HE3	1:A:349:LEU:HD21	1.73	0.71
1:A:190:ASN:HD22	1:A:192:VAL:HG23	1.54	0.71
1:A:320:VAL:HG22	1:A:335:GLN:HG2	1.72	0.71
1:A:27:MET:HE1	1:A:353:ILE:HD11	1.72	0.71
1:A:142:HIS:CE1	1:A:157:ARG:HH21	2.08	0.71
1:A:218:LEU:O	1:A:222:ARG:HG3	1.90	0.70
1:A:42:GLU:CD	1:A:42:GLU:H	2.00	0.70
1:B:249:LYS:HD2	1:B:249:LYS:N	2.09	0.68
1:B:142:HIS:O	1:B:145:THR:HG22	1.94	0.68
1:B:202:LYS:HA	1:B:207:THR:HG22	1.76	0.67
1:B:248:PRO:O	1:B:249:LYS:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:HD12	1:A:46:ILE:HG22	1.76	0.66
1:A:353:ILE:O	1:A:357:GLN:HG3	1.96	0.65
1:A:207:THR:HG22	1:A:208:GLU:O	1.98	0.64
1:B:314:LEU:HD21	1:B:320:VAL:HG11	1.79	0.64
1:B:320:VAL:HG12	1:B:335:GLN:HB3	1.78	0.63
1:A:202:LYS:HD2	1:A:261:LEU:HD11	1.81	0.63
1:A:190:ASN:ND2	1:A:192:VAL:HG23	2.14	0.62
1:A:159:ILE:CG2	1:A:164:ASP:HB3	2.29	0.62
1:A:252:GLU:HG3	1:A:253:SER:H	1.64	0.62
1:A:34:ASN:OD1	1:A:52:PRO:HG3	2.00	0.62
1:A:49:ASP:O	1:A:50:PHE:HB2	1.99	0.62
1:B:222:ARG:HG3	1:B:222:ARG:HH11	1.65	0.62
1:A:314:LEU:CD2	1:A:320:VAL:HG21	2.29	0.62
1:B:319:ASN:C	1:B:319:ASN:HD22	2.08	0.62
1:A:357:GLN:HB3	1:B:358:ARG:HG3	1.82	0.61
1:B:115:PRO:HG3	1:B:348:VAL:HG21	1.83	0.61
1:B:34:ASN:OD1	1:B:52:PRO:HG3	2.01	0.60
1:B:190:ASN:HD22	1:B:275:LYS:NZ	1.99	0.60
1:B:121:SER:OG	1:B:222:ARG:HD2	2.02	0.60
1:B:142:HIS:CD2	1:B:145:THR:HG21	2.28	0.60
1:B:247:ILE:HG23	1:B:260:PHE:CE1	2.36	0.60
1:A:190:ASN:HD22	1:A:192:VAL:H	1.49	0.60
1:A:250:PRO:C	1:A:252:GLU:H	2.10	0.60
1:B:90:VAL:HG23	1:B:90:VAL:O	2.02	0.60
1:A:156:LEU:O	1:A:160:ILE:HG12	2.02	0.59
1:A:255:LYS:HE3	1:A:263:LYS:HG2	1.83	0.59
1:A:328:TYR:OH	1:B:343:VAL:HG13	2.01	0.59
1:B:314:LEU:HD21	1:B:320:VAL:CG1	2.32	0.59
1:A:160:ILE:HD11	1:A:166:VAL:HG23	1.82	0.59
1:A:167:GLU:HA	1:A:293:VAL:HG22	1.83	0.59
1:A:69:LYS:HD2	1:A:70:THR:N	2.18	0.58
1:B:249:LYS:HB2	1:B:251:LEU:CD1	2.33	0.58
1:A:166:VAL:O	1:A:293:VAL:HG21	2.04	0.58
1:B:256:SER:O	1:B:257:ALA:HB3	2.02	0.58
1:A:193:LYS:HB2	1:A:196:ASP:OD2	2.04	0.57
1:B:247:ILE:HG21	1:B:252:GLU:HB2	1.85	0.57
1:A:248:PRO:O	1:A:249:LYS:O	2.23	0.56
1:A:159:ILE:HG23	1:A:164:ASP:HB3	1.87	0.56
1:A:207:THR:CG2	1:A:211:PRO:HA	2.35	0.56
1:A:69:LYS:HE3	1:A:70:THR:O	2.06	0.56
1:A:251:LEU:HD22	1:A:267:TYR:OH	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:CD1	1:A:46:ILE:HG22	2.36	0.56
1:A:172:ILE:HD12	1:A:314:LEU:HD11	1.87	0.56
1:B:190:ASN:O	1:B:191:ASP:HB2	2.04	0.56
1:B:280:THR:HG22	1:B:281:GLU:HG3	1.87	0.55
1:A:252:GLU:O	1:A:254:VAL:N	2.31	0.55
1:A:123:ASP:HB2	1:A:126:THR:OG1	2.06	0.55
1:A:167:GLU:HA	1:A:293:VAL:CG2	2.37	0.55
1:B:79:HIS:O	1:B:82:THR:HB	2.05	0.55
1:A:324:LYS:CE	1:A:331:PRO:HG3	2.36	0.55
1:A:212:ARG:HH22	1:A:257:ALA:H	1.56	0.54
1:A:86:PRO:CB	1:A:359:LEU:HD13	2.38	0.54
1:A:343:VAL:HG13	1:B:328:TYR:OH	2.06	0.54
1:A:42:GLU:CD	1:A:42:GLU:N	2.64	0.54
1:A:86:PRO:HB3	1:A:359:LEU:HD13	1.90	0.53
1:A:34:ASN:CG	1:A:52:PRO:HG3	2.33	0.53
1:B:73:LEU:HD12	1:B:101:PHE:CD1	2.43	0.53
1:A:179:TYR:HB2	1:A:317:SER:HB3	1.91	0.53
1:A:69:LYS:HD2	1:A:70:THR:H	1.74	0.52
1:A:255:LYS:HD2	1:A:259:GLU:HG2	1.92	0.52
1:B:314:LEU:HD11	1:B:320:VAL:HG13	1.90	0.52
1:B:115:PRO:HG3	1:B:348:VAL:CG2	2.39	0.52
1:A:116:ASN:OD1	1:A:118:LYS:HG2	2.09	0.52
1:B:219:ASP:O	1:B:222:ARG:HB2	2.08	0.52
1:A:207:THR:HG21	1:A:211:PRO:CG	2.37	0.52
1:A:349:LEU:HD23	1:B:162:THR:HG23	1.91	0.52
1:A:224:VAL:CG2	1:A:298:VAL:HG13	2.40	0.51
1:B:254:VAL:HB	1:B:255:LYS:HE3	1.91	0.51
1:B:89:LEU:HD22	1:B:105:PHE:CE2	2.45	0.51
1:B:171:GLY:HA3	1:B:320:VAL:O	2.09	0.51
1:B:174:SER:HB3	1:B:177:LEU:HB2	1.92	0.51
1:B:131:PHE:O	1:B:133:ASN:N	2.41	0.51
1:B:256:SER:O	1:B:257:ALA:CB	2.59	0.51
1:A:252:GLU:C	1:A:254:VAL:H	2.15	0.51
1:A:196:ASP:O	1:A:200:VAL:HG23	2.11	0.50
1:B:188:GLN:O	1:B:188:GLN:HG2	2.12	0.50
1:B:249:LYS:HB3	1:B:250:PRO:HD3	1.92	0.50
1:B:37:LEU:HD23	1:B:37:LEU:C	2.37	0.50
1:B:324:LYS:HE3	1:B:331:PRO:HG3	1.94	0.50
1:B:222:ARG:HG3	1:B:222:ARG:NH1	2.25	0.50
1:A:328:TYR:CZ	1:B:343:VAL:HG13	2.46	0.49
1:A:159:ILE:HG23	1:A:164:ASP:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:GLN:O	1:B:189:ALA:C	2.54	0.49
1:B:198:VAL:HG21	1:B:264:LEU:HD23	1.95	0.49
1:B:186:THR:HB	1:B:188:GLN:NE2	2.28	0.49
1:A:324:LYS:HE3	1:A:331:PRO:HG3	1.94	0.49
1:B:162:THR:CG2	1:B:327:ARG:HH12	2.26	0.49
1:B:249:LYS:HB3	1:B:250:PRO:HD2	1.93	0.49
1:A:27:MET:HE2	1:A:353:ILE:HD11	1.93	0.48
1:B:198:VAL:HG23	1:B:199:LYS:N	2.29	0.48
1:A:207:THR:HG22	1:A:208:GLU:N	2.28	0.48
1:B:77:ILE:O	1:B:81:LYS:HG3	2.13	0.48
1:B:247:ILE:HG21	1:B:252:GLU:CB	2.43	0.48
1:B:46:ILE:HD11	1:B:71:LEU:HD13	1.96	0.48
1:B:249:LYS:C	1:B:251:LEU:HD12	2.39	0.48
1:A:177:LEU:HD13	1:A:287:PHE:CD2	2.49	0.47
1:A:159:ILE:HG22	1:A:164:ASP:HB3	1.96	0.47
1:B:207:THR:HG23	1:B:208:GLU:O	2.15	0.47
1:B:213:ASP:HA	1:B:216:ASN:ND2	2.29	0.47
1:B:252:GLU:HG2	1:B:253:SER:N	2.29	0.47
1:B:162:THR:HG22	1:B:327:ARG:HH12	1.78	0.47
1:A:288:ILE:HD12	1:A:288:ILE:C	2.41	0.46
1:B:10:VAL:HA	1:B:90:VAL:HG22	1.98	0.46
1:B:50:PHE:CE2	1:B:83:SER:HB2	2.50	0.46
1:B:166:VAL:HG11	1:B:231:SER:CB	2.45	0.46
1:B:169:ILE:HG21	1:B:227:VAL:HG11	1.97	0.46
1:B:195:SER:O	1:B:198:VAL:HG22	2.15	0.46
1:A:120:PHE:CZ	1:A:142:HIS:HB3	2.51	0.46
1:B:120:PHE:CZ	1:B:142:HIS:HB3	2.50	0.46
1:A:202:LYS:CD	1:A:261:LEU:HD11	2.45	0.46
1:A:241:PHE:HE1	1:A:300:VAL:HG23	1.80	0.46
1:A:27:MET:HE1	1:A:349:LEU:HG	1.97	0.46
1:B:49:ASP:OD1	1:B:51:SER:HB3	2.15	0.46
1:A:48:LYS:HD2	1:A:79:HIS:CE1	2.50	0.46
1:A:142:HIS:HB2	1:A:145:THR:CG2	2.46	0.46
1:B:255:LYS:N	1:B:255:LYS:HE2	2.30	0.46
1:A:94:SER:O	1:A:118:LYS:HE3	2.16	0.45
1:B:67:THR:HG22	1:B:67:THR:O	2.17	0.45
1:A:38:LEU:HB3	1:A:45:LEU:HB2	1.97	0.45
1:A:224:VAL:HG21	1:A:298:VAL:HG13	1.98	0.45
1:A:251:LEU:HD21	1:A:263:LYS:CE	2.46	0.45
1:B:195:SER:HB2	1:B:268:ASP:OD2	2.17	0.45
1:B:144:ALA:HA	1:B:148:ALA:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:MET:HE3	1:A:349:LEU:CD2	2.45	0.45
1:A:252:GLU:C	1:A:254:VAL:N	2.75	0.45
1:B:255:LYS:HE2	1:B:255:LYS:CA	2.47	0.45
1:B:277:GLU:HG2	1:B:281:GLU:OE2	2.16	0.45
1:A:91:ASP:O	1:A:115:PRO:HD2	2.17	0.45
1:B:263:LYS:O	1:B:263:LYS:HD3	2.17	0.45
1:A:117:LYS:HE3	1:A:219:ASP:OD2	2.16	0.44
1:A:208:GLU:O	1:A:209:PRO:C	2.59	0.44
1:A:190:ASN:ND2	1:A:192:VAL:CG2	2.80	0.44
1:B:237:SER:HB2	1:B:238:PRO:HD2	1.99	0.44
1:A:159:ILE:HD12	4:A:2113:HOH:O	2.15	0.44
1:A:251:LEU:HD21	1:A:263:LYS:CG	2.48	0.44
1:B:255:LYS:HE2	1:B:255:LYS:HA	1.99	0.44
1:A:314:LEU:CD2	1:A:335:GLN:HE21	2.31	0.43
1:B:83:SER:HA	1:B:84:PRO:HD3	1.76	0.43
1:B:124:LEU:HD21	1:B:234:GLU:HB3	2.01	0.43
1:B:80:LEU:HG	1:B:87:VAL:HG11	2.00	0.43
1:B:353:ILE:O	1:B:357:GLN:HG3	2.18	0.43
1:B:257:ALA:C	1:B:259:GLU:N	2.76	0.43
1:A:146:VAL:O	1:A:146:VAL:HG22	2.18	0.43
1:A:172:ILE:CG2	1:A:178:SER:HB2	2.49	0.43
1:A:139:PHE:CE1	1:A:358:ARG:HG2	2.54	0.43
1:A:249:LYS:CB	1:A:250:PRO:CD	2.80	0.43
1:B:49:ASP:O	1:B:50:PHE:HB2	2.19	0.43
1:B:251:LEU:HD22	1:B:267:TYR:CZ	2.54	0.43
1:B:184:PHE:CE1	1:B:275:LYS:HD2	2.54	0.43
1:A:47:SER:OG	1:A:50:PHE:N	2.48	0.42
1:A:48:LYS:HD2	1:A:48:LYS:HA	1.85	0.42
1:A:250:PRO:HA	1:A:252:GLU:HG2	2.00	0.42
1:B:77:ILE:HD13	1:B:104:LYS:HB3	2.00	0.42
1:B:202:LYS:HA	1:B:207:THR:CG2	2.47	0.42
1:B:247:ILE:CG2	1:B:252:GLU:HB3	2.50	0.42
1:B:249:LYS:HB2	1:B:251:LEU:HD11	2.01	0.42
1:B:255:LYS:HD3	1:B:259:GLU:HG2	1.98	0.42
1:A:142:HIS:HB2	1:A:145:THR:HG23	2.01	0.42
1:A:251:LEU:O	1:A:251:LEU:HG	2.20	0.42
1:B:324:LYS:CG	1:B:331:PRO:HG3	2.42	0.42
1:A:42:GLU:HG3	1:A:43:ARG:CZ	2.50	0.42
1:B:190:ASN:CG	1:B:191:ASP:H	2.28	0.42
1:A:42:GLU:HG2	1:A:43:ARG:H	1.83	0.42
1:B:10:VAL:HG22	1:B:90:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASP:HA	1:B:216:ASN:HD21	1.84	0.41
1:B:208:GLU:O	1:B:209:PRO:C	2.63	0.41
1:A:252:GLU:H	1:A:252:GLU:HG2	1.71	0.41
1:B:73:LEU:HD12	1:B:101:PHE:CE1	2.55	0.41
1:B:191:ASP:CG	1:B:191:ASP:O	2.63	0.41
1:B:276:LYS:HE3	1:B:276:LYS:HB2	1.90	0.41
1:A:172:ILE:HG21	1:A:178:SER:HB2	2.03	0.41
1:A:324:LYS:HE2	1:A:331:PRO:HG3	2.02	0.41
1:B:262:GLU:OE1	1:B:262:GLU:HA	2.20	0.41
1:B:10:VAL:HG13	1:B:90:VAL:HG23	2.03	0.41
1:B:120:PHE:HB3	1:B:127:TRP:HZ3	1.85	0.41
1:B:114:THR:HA	1:B:115:PRO:HD3	1.83	0.41
1:A:146:VAL:CG1	1:A:153:ILE:HD11	2.42	0.41
1:B:220:VAL:CG2	1:B:300:VAL:HG21	2.51	0.41
1:A:241:PHE:CD1	1:A:298:VAL:HG12	2.56	0.41
1:A:249:LYS:O	1:A:251:LEU:N	2.54	0.41
1:A:309:HIS:HD2	1:A:311:PHE:HB2	1.86	0.41
1:B:267:TYR:CD1	1:B:267:TYR:N	2.89	0.40
1:A:2:SER:HB3	1:A:359:LEU:OXT	2.21	0.40
1:A:59:TRP:CD1	1:A:59:TRP:H	2.38	0.40
1:A:212:ARG:NH2	1:A:257:ALA:N	2.61	0.40
1:B:133:ASN:O	1:B:133:ASN:ND2	2.55	0.40
1:B:224:VAL:CG1	1:B:298:VAL:HG13	2.51	0.40
1:B:314:LEU:N	1:B:314:LEU:HD23	2.35	0.40
1:A:7:ASN:HD22	1:A:34:ASN:HB2	1.86	0.40
1:A:144:ALA:HA	1:A:148:ALA:O	2.21	0.40
1:B:73:LEU:HA	1:B:73:LEU:HD23	1.89	0.40
1:B:248:PRO:O	1:B:249:LYS:C	2.64	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	356/358 (99%)	325 (91%)	26 (7%)	5 (1%)	9	9
1	B	356/358 (99%)	330 (93%)	18 (5%)	8 (2%)	5	4
All	All	712/716 (99%)	655 (92%)	44 (6%)	13 (2%)	6	6

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	LYS
1	B	191	ASP
1	B	249	LYS
1	B	257	ALA
1	A	3	THR
1	A	253	SER
1	B	132	SER
1	B	189	ALA
1	B	254	VAL
1	B	255	LYS
1	A	250	PRO
1	B	248	PRO
1	A	248	PRO

### 5.3.2 Protein sidechains [i](#)

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	300/300 (100%)	290 (97%)	10 (3%)	33	50
1	B	300/300 (100%)	294 (98%)	6 (2%)	48	67
All	All	600/600 (100%)	584 (97%)	16 (3%)	39	58

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	28	LYS
1	A	38	LEU

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Mol	Chain	Res	Type
1	A	42	GLU
1	A	43	ARG
1	A	146	VAL
1	A	224	VAL
1	A	246	LEU
1	A	270	ASP
1	A	280	THR
1	B	24	LEU
1	B	80	LEU
1	B	252	GLU
1	B	280	THR
1	B	300	VAL
1	B	319	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	79	HIS
1	A	108	ASN
1	A	133	ASN
1	A	137	ASN
1	A	142	HIS
1	A	190	ASN
1	A	273	GLN
1	A	309	HIS
1	A	330	ASN
1	A	335	GLN
1	B	7	ASN
1	B	133	ASN
1	B	142	HIS
1	B	188	GLN
1	B	190	ASN
1	B	319	ASN
1	B	330	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	A	2109	-	46,48,48	2.60	10 (21%)	64,73,73	1.54	6 (9%)

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	A	2109	-	-	8/30/62/62	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2109	NAD	C4N-C3N	9.36	1.53	1.39
3	A	2109	NAD	C2N-C3N	7.10	1.50	1.39
3	A	2109	NAD	C5N-C4N	6.58	1.50	1.38
3	A	2109	NAD	PN-O3	6.57	1.66	1.59
3	A	2109	NAD	C2N-N1N	4.19	1.39	1.35
3	A	2109	NAD	C6N-N1N	3.76	1.43	1.35
3	A	2109	NAD	C7N-N7N	3.09	1.38	1.33
3	A	2109	NAD	PA-O3	-2.74	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2109	NAD	O7N-C7N	2.54	1.28	1.24
3	A	2109	NAD	C2A-N1A	2.17	1.37	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2109	NAD	C5N-C4N-C3N	-8.02	112.48	120.36
3	A	2109	NAD	C6N-N1N-C2N	-3.75	118.69	121.88
3	A	2109	NAD	C3N-C7N-N7N	3.62	122.20	117.74
3	A	2109	NAD	C6N-C5N-C4N	3.59	124.62	119.45
3	A	2109	NAD	O2N-PN-O5D	2.44	118.64	107.57
3	A	2109	NAD	C5N-C6N-N1N	2.10	123.25	120.38

There are no chirality outliers.

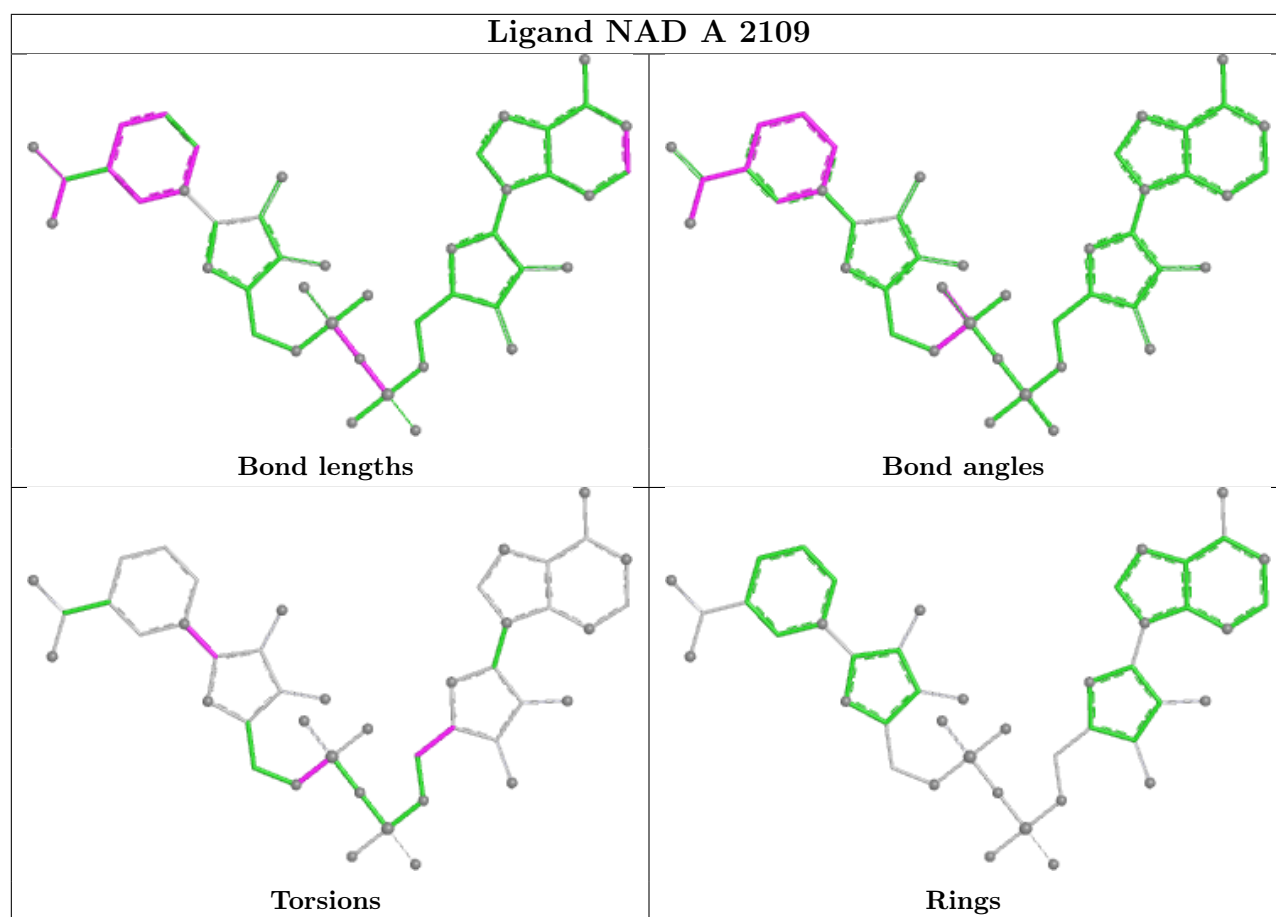
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2109	NAD	C5D-O5D-PN-O3
3	A	2109	NAD	C5D-O5D-PN-O2N
3	A	2109	NAD	O4D-C1D-N1N-C2N
3	A	2109	NAD	O4D-C1D-N1N-C6N
3	A	2109	NAD	C2D-C1D-N1N-C6N
3	A	2109	NAD	C5D-O5D-PN-O1N
3	A	2109	NAD	C2D-C1D-N1N-C2N
3	A	2109	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

No monomer is involved in short contacts.

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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	358/358 (100%)	0.24	26 (7%) 21 23	10, 22, 59, 80	0
1	B	358/358 (100%)	0.33	31 (8%) 16 17	11, 24, 57, 72	0
All	All	716/716 (100%)	0.28	57 (7%) 18 20	10, 23, 59, 80	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	LEU	7.2
1	B	130	LEU	6.2
1	A	3	THR	5.5
1	A	254	VAL	5.4
1	B	131	PHE	5.1
1	B	133	ASN	5.1
1	A	250	PRO	5.0
1	B	261	LEU	4.3
1	B	250	PRO	4.2
1	B	134	LYS	3.8
1	B	254	VAL	3.8
1	A	255	LYS	3.8
1	B	136	THR	3.7
1	B	135	PRO	3.7
1	A	257	ALA	3.6
1	B	129	ALA	3.4
1	A	253	SER	3.4
1	B	251	LEU	3.1
1	B	257	ALA	3.0
1	B	256	SER	3.0
1	B	132	SER	2.9
1	B	252	GLU	2.9
1	A	280	THR	2.7
1	A	58	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	258	ASP	2.7
1	B	262	GLU	2.7
1	A	123	ASP	2.7
1	B	260	PHE	2.6
1	A	269	LYS	2.6
1	B	54	ASN	2.5
1	B	319	ASN	2.5
1	A	265	SER	2.5
1	B	49	ASP	2.5
1	B	192	VAL	2.4
1	A	261	LEU	2.4
1	B	255	LYS	2.4
1	A	256	SER	2.4
1	A	274	LEU	2.4
1	A	282	ASN	2.3
1	A	279	ALA	2.3
1	B	190	ASN	2.3
1	A	267	TYR	2.3
1	B	2	SER	2.3
1	A	252	GLU	2.3
1	A	264	LEU	2.2
1	A	271	LEU	2.2
1	A	2	SER	2.2
1	A	263	LYS	2.2
1	A	189	ALA	2.2
1	B	189	ALA	2.2
1	A	307	TYR	2.1
1	B	57	SER	2.1
1	B	269	LYS	2.1
1	B	249	LYS	2.1
1	B	188	GLN	2.0
1	B	207	THR	2.0
1	A	188	GLN	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](#)

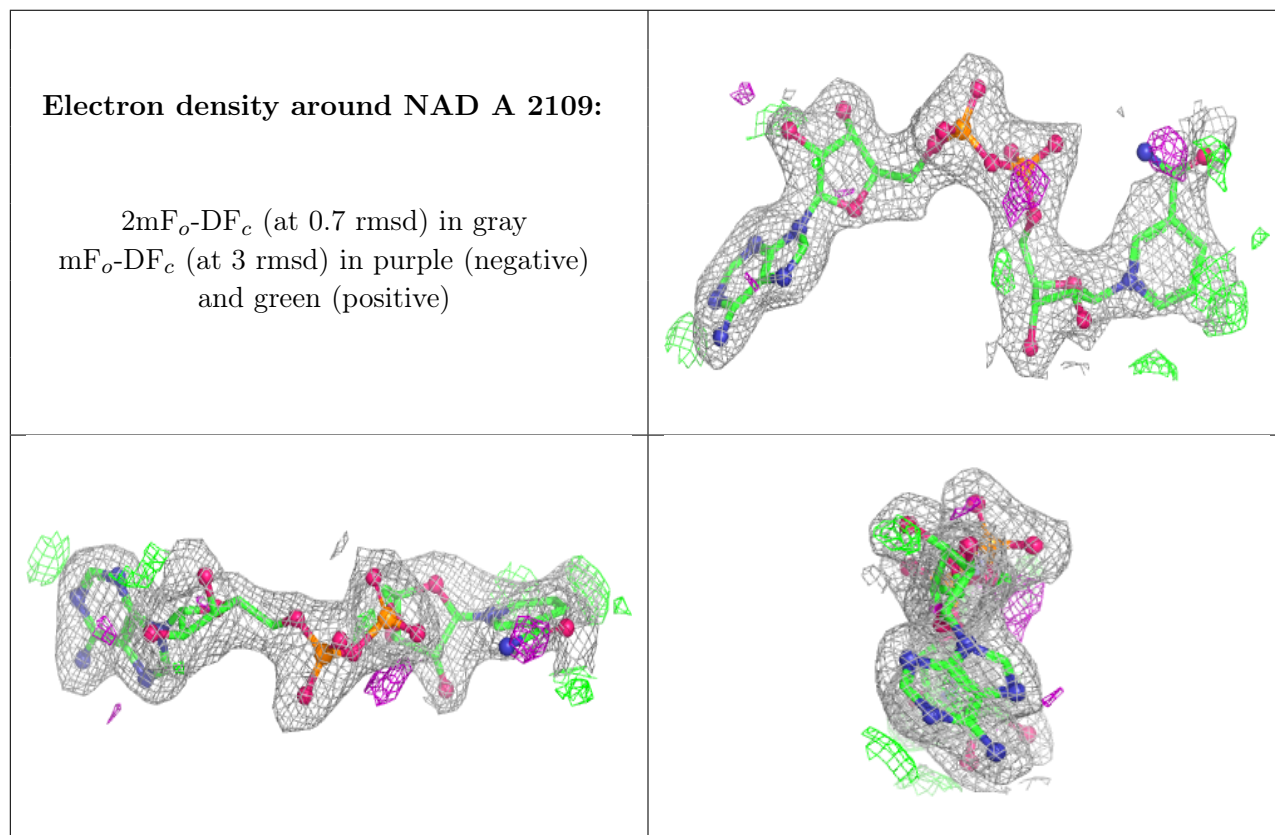
There are no oligosaccharides in this entry.

## 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	NAD	A	2109	44/44	0.91	0.11	18,28,42,47	0
2	NA	B	2114	1/1	0.93	0.08	35,35,35,35	0
2	NA	A	2104	1/1	0.96	0.12	29,29,29,29	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.