



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:28 PM EDT

PDB ID : 1BXS / pdb_00001bxs
Title : SHEEP LIVER CLASS 1 ALDEHYDE DEHYDROGENASE WITH NAD BOUND
Authors : Moore, S.A.; Baker, H.M.; Blythe, T.J.; Kitson, K.E.; Kitson, T.M.; Baker, E.N.
Deposited on : 1998-10-08
Resolution : 2.35 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 types of validation reports are described at

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

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

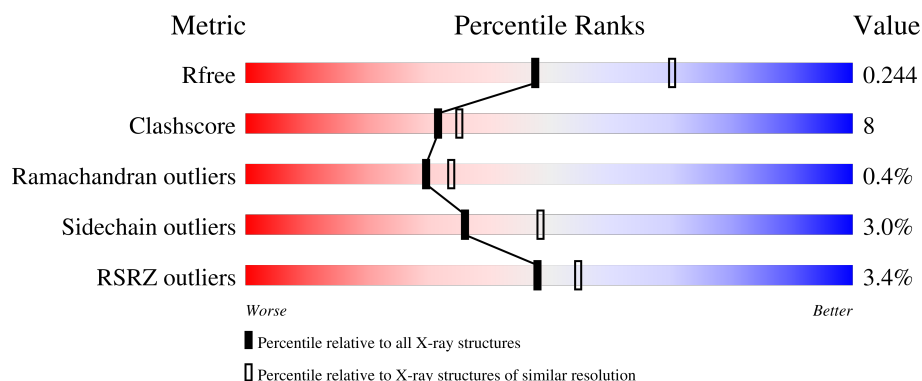
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 ≥ 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	2% 77% 20% ..
1	B	501	4% 78% 19% ..
1	C	501	4% 79% 17% ..
1	D	501	4% 79% 18% ..

2 Entry composition [i](#)

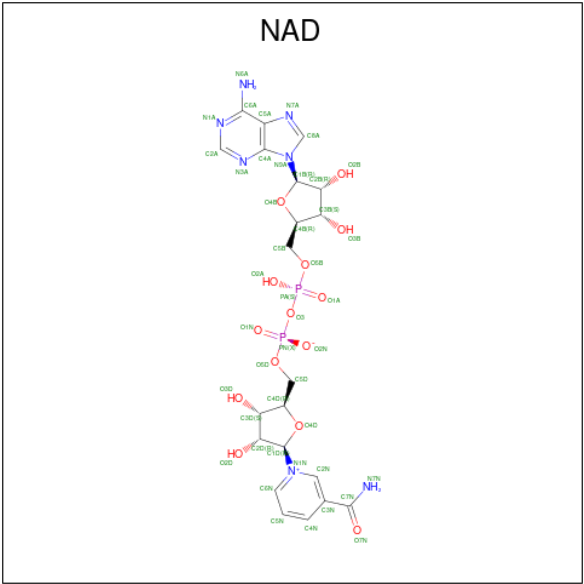
There are 3 unique types of molecules in this entry. The entry contains 15444 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3785	2411	634	718	22			
1	B	494	Total	C	N	O	S	0	0	0
			3785	2411	634	718	22			
1	C	494	Total	C	N	O	S	0	0	0
			3785	2411	634	718	22			
1	D	494	Total	C	N	O	S	0	0	0
			3785	2411	634	718	22			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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		

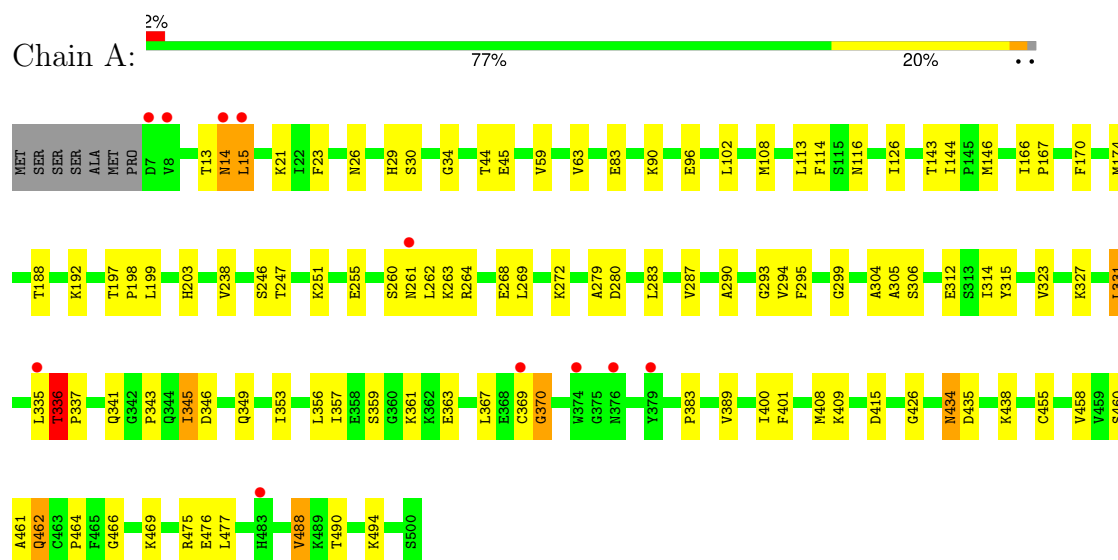
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	32	Total	O	0	0
			32	32		
3	C	32	Total	O	0	0
			32	32		
3	D	32	Total	O	0	0
			32	32		

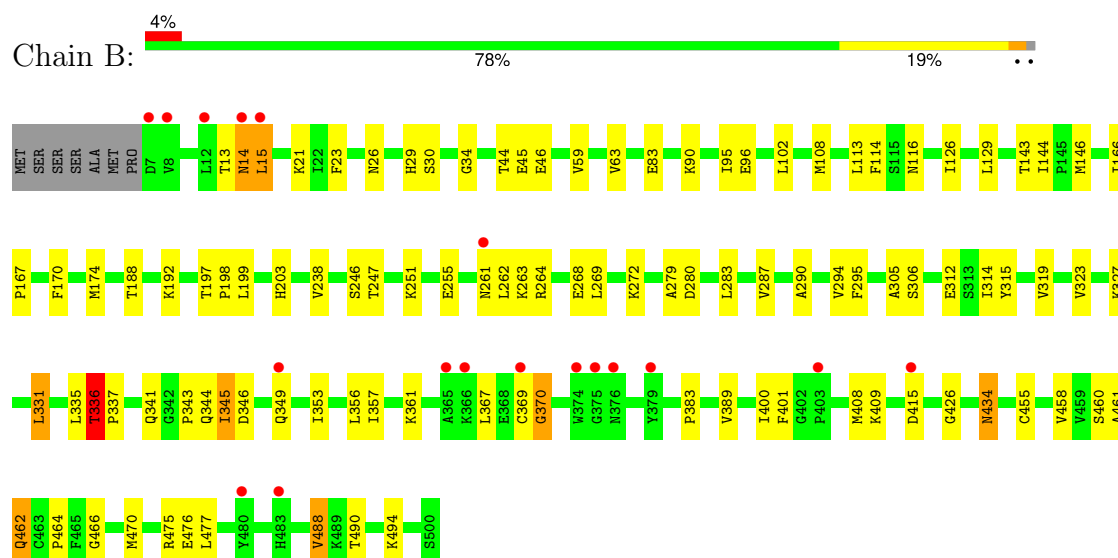
3 Residue-property plots

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.

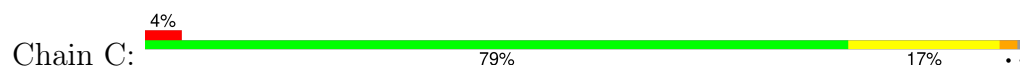
• Molecule 1: ALDEHYDE DEHYDROGENASE

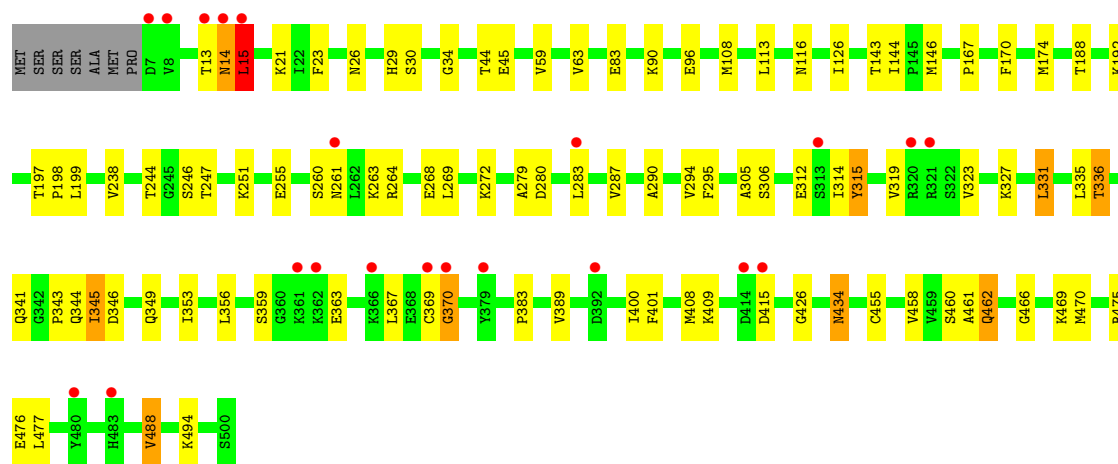


• Molecule 1: ALDEHYDE DEHYDROGENASE

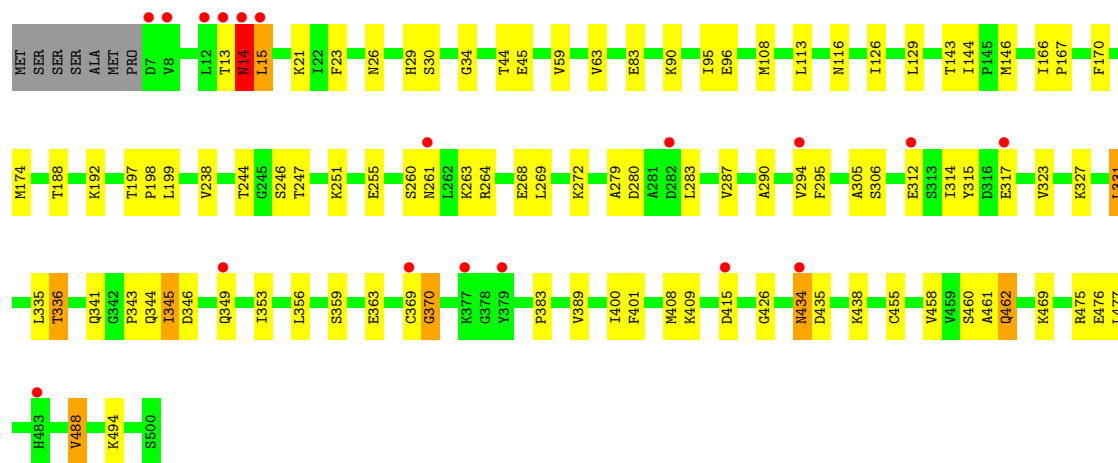
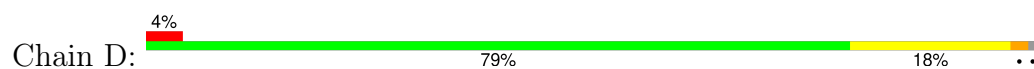


• Molecule 1: ALDEHYDE DEHYDROGENASE





● Molecule 1: ALDEHYDE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.69Å 87.62Å 90.84Å 110.47° 105.63° 103.56°	Depositor
Resolution (Å)	100.00 – 2.35 78.51 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.5 (100.00-2.35) 95.5 (78.51-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.34Å)	Xtriage
Refinement program	CNS 0.3C	Depositor
R, R_{free}	0.235 , 0.259 0.224 , 0.244	Depositor DCC
R_{free} test set	8274 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15444	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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

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	0/3868	1.04	18/5234 (0.3%)
1	B	0.52	0/3868	1.03	17/5234 (0.3%)
1	C	0.53	0/3868	1.03	18/5234 (0.3%)
1	D	0.52	0/3868	1.04	20/5234 (0.4%)
All	All	0.52	0/15472	1.03	73/20936 (0.3%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	ILE	N-CA-C	8.27	117.01	107.84
1	A	166	ILE	N-CA-C	8.21	116.95	107.84
1	D	166	ILE	N-CA-C	8.12	116.86	107.84
1	A	336	THR	CA-C-N	7.46	127.92	119.93
1	A	336	THR	C-N-CA	7.46	127.92	119.93
1	C	336	THR	CA-C-N	7.45	127.90	119.93
1	C	336	THR	C-N-CA	7.45	127.90	119.93
1	A	260	SER	N-CA-C	7.43	120.75	108.48
1	B	199	LEU	N-CA-C	7.38	120.02	111.02
1	C	199	LEU	N-CA-C	7.27	119.89	111.02
1	D	199	LEU	N-CA-C	7.26	119.88	111.02
1	A	199	LEU	N-CA-C	7.25	119.86	111.02
1	C	260	SER	N-CA-C	7.12	120.23	108.48
1	B	144	ILE	N-CA-C	7.03	115.64	107.77
1	A	144	ILE	N-CA-C	6.87	115.47	107.77
1	B	336	THR	CA-C-N	6.86	126.90	119.90
1	B	336	THR	C-N-CA	6.86	126.90	119.90
1	C	144	ILE	N-CA-C	6.82	115.41	107.77
1	D	144	ILE	N-CA-C	6.81	115.40	107.77
1	B	143	THR	N-CA-C	-6.73	97.44	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	THR	N-CA-C	-6.65	97.57	108.41
1	C	143	THR	N-CA-C	-6.64	97.58	108.41
1	D	143	THR	N-CA-C	-6.58	97.69	108.41
1	C	345	ILE	N-CA-C	6.47	116.64	110.42
1	D	345	ILE	N-CA-C	6.44	116.61	110.42
1	A	13	THR	N-CA-C	6.41	121.62	113.55
1	C	13	THR	N-CA-C	6.36	121.56	113.55
1	D	13	THR	N-CA-C	6.22	120.89	113.12
1	A	345	ILE	N-CA-C	6.19	116.36	110.42
1	D	260	SER	N-CA-C	6.09	118.53	108.48
1	A	197	THR	N-CA-C	6.07	118.34	109.30
1	C	197	THR	N-CA-C	6.06	118.33	109.30
1	C	344	GLN	N-CA-C	-6.04	102.73	110.53
1	C	315	TYR	N-CA-C	6.00	117.52	110.97
1	B	13	THR	N-CA-C	6.00	120.91	112.93
1	D	197	THR	N-CA-C	5.98	118.20	109.30
1	B	197	THR	N-CA-C	5.93	118.13	109.30
1	B	295	PHE	N-CA-C	5.86	120.27	113.18
1	A	295	PHE	N-CA-C	5.79	120.18	113.18
1	C	295	PHE	N-CA-C	5.72	120.10	113.18
1	A	469	LYS	N-CA-C	5.69	116.96	108.31
1	D	295	PHE	N-CA-C	5.69	120.06	113.18
1	B	34	GLY	N-CA-C	-5.68	107.93	114.69
1	D	344	GLN	N-CA-C	-5.65	103.24	110.53
1	B	114	PHE	N-CA-C	5.65	117.11	111.07
1	C	469	LYS	N-CA-C	5.60	116.82	108.31
1	D	469	LYS	N-CA-C	5.60	116.82	108.31
1	D	14	ASN	CA-C-N	-5.57	113.08	121.05
1	D	14	ASN	C-N-CA	-5.57	113.08	121.05
1	A	315	TYR	N-CA-C	5.52	116.99	110.97
1	D	315	TYR	N-CA-C	5.48	116.94	110.97
1	D	336	THR	CA-C-N	5.46	125.78	119.93
1	D	336	THR	C-N-CA	5.46	125.78	119.93
1	D	30	SER	N-CA-C	-5.42	102.50	110.52
1	A	30	SER	N-CA-C	-5.39	102.54	110.52
1	B	30	SER	N-CA-C	-5.37	102.57	110.52
1	B	315	TYR	N-CA-C	5.33	116.78	110.97
1	C	34	GLY	N-CA-C	-5.32	108.36	114.69
1	B	344	GLN	N-CA-C	-5.32	103.67	110.53
1	C	30	SER	N-CA-C	-5.28	102.70	110.52
1	A	188	THR	N-CA-C	-5.28	100.80	109.40
1	D	34	GLY	N-CA-C	-5.26	108.43	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	488	VAL	N-CA-C	5.25	115.81	108.89
1	B	188	THR	N-CA-C	-5.23	100.87	109.40
1	D	188	THR	N-CA-C	-5.23	100.88	109.40
1	B	345	ILE	N-CA-C	5.21	115.42	110.42
1	B	488	VAL	N-CA-C	5.20	115.75	108.89
1	D	488	VAL	N-CA-C	5.19	115.74	108.89
1	C	188	THR	N-CA-C	-5.17	100.96	109.40
1	A	488	VAL	N-CA-C	5.15	115.69	108.89
1	A	34	GLY	N-CA-C	-5.15	108.56	114.69
1	A	114	PHE	N-CA-C	5.13	116.56	111.07
1	C	15	LEU	N-CA-C	5.08	117.53	109.96

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	3785	0	3733	72	0
1	B	3785	0	3733	73	0
1	C	3785	0	3733	63	1
1	D	3785	0	3733	61	1
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	32	0	0	0	0
3	B	32	0	0	0	0
3	C	32	0	0	0	0
3	D	32	0	0	0	0
All	All	15444	0	15036	246	1

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 8.

All (246) 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:261:ASN:HD21	1:A:263:LYS:HE3	1.27	0.96
1:A:268:GLU:HG3	1:A:476:GLU:OE2	1.72	0.90
1:C:268:GLU:HG3	1:C:476:GLU:OE2	1.73	0.88
1:C:261:ASN:HD21	1:C:263:LYS:HE3	1.37	0.88
1:D:268:GLU:HG3	1:D:476:GLU:OE2	1.73	0.88
1:B:268:GLU:HG3	1:B:476:GLU:OE2	1.74	0.87
1:B:108:MET:HG2	1:B:335:LEU:HD11	1.57	0.86
1:D:108:MET:HG2	1:D:335:LEU:HD11	1.57	0.86
1:B:261:ASN:HD21	1:B:263:LYS:HE3	1.42	0.85
1:C:108:MET:HG2	1:C:335:LEU:HD11	1.56	0.84
1:A:108:MET:HG2	1:A:335:LEU:HD11	1.58	0.83
1:D:261:ASN:HD21	1:D:263:LYS:HE3	1.51	0.76
1:A:146:MET:HE3	1:B:460:SER:HB2	1.71	0.71
1:A:460:SER:HB2	1:B:146:MET:HE3	1.74	0.69
1:C:460:SER:HB2	1:D:146:MET:HE3	1.74	0.69
1:D:247:THR:HA	1:D:269:LEU:HD13	1.78	0.65
1:B:247:THR:HA	1:B:269:LEU:HD13	1.79	0.65
1:B:323:VAL:HG13	1:B:369:CYS:SG	2.37	0.64
1:C:247:THR:HA	1:C:269:LEU:HD13	1.79	0.64
1:D:323:VAL:HG13	1:D:369:CYS:SG	2.39	0.62
1:A:247:THR:HA	1:A:269:LEU:HD13	1.81	0.62
1:C:389:VAL:O	1:C:408:MET:HG3	2.00	0.62
1:D:192:LYS:HD3	1:D:192:LYS:C	2.25	0.62
1:D:44:THR:O	1:D:45:GLU:HB2	2.00	0.61
1:B:192:LYS:HD3	1:B:192:LYS:C	2.25	0.61
1:C:146:MET:HE3	1:D:460:SER:HB2	1.81	0.61
1:A:192:LYS:HD3	1:A:192:LYS:C	2.25	0.61
1:B:312:GLU:HG2	1:B:409:LYS:HG2	1.82	0.61
1:A:261:ASN:ND2	1:A:263:LYS:HE3	2.09	0.61
1:A:312:GLU:HG2	1:A:409:LYS:HG2	1.83	0.61
1:B:44:THR:O	1:B:45:GLU:HB2	2.01	0.61
1:C:192:LYS:HD3	1:C:192:LYS:C	2.26	0.61
1:A:323:VAL:HG13	1:A:369:CYS:SG	2.41	0.61
1:C:312:GLU:HG2	1:C:409:LYS:HG2	1.83	0.60
1:B:323:VAL:O	1:B:327:LYS:HG3	2.02	0.60
1:B:246:SER:HB3	2:B:550:NAD:O4D	2.03	0.59
1:C:44:THR:O	1:C:45:GLU:HB2	2.00	0.59
1:D:312:GLU:HG2	1:D:409:LYS:HG2	1.85	0.59
1:B:238:VAL:O	1:B:261:ASN:ND2	2.36	0.59
1:A:251:LYS:O	1:A:255:GLU:HG3	2.03	0.58
1:A:44:THR:O	1:A:45:GLU:HB2	2.01	0.58
1:D:251:LYS:O	1:D:255:GLU:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:VAL:O	1:D:408:MET:HG3	2.04	0.58
1:B:251:LYS:O	1:B:255:GLU:HG3	2.04	0.57
1:C:323:VAL:O	1:C:327:LYS:HG3	2.05	0.57
1:A:246:SER:HB3	2:A:550:NAD:O4D	2.04	0.57
1:C:251:LYS:O	1:C:255:GLU:HG3	2.04	0.57
1:A:389:VAL:O	1:A:408:MET:HG3	2.04	0.57
1:D:108:MET:CG	1:D:335:LEU:HD11	2.32	0.57
1:C:238:VAL:O	1:C:261:ASN:ND2	2.38	0.57
1:A:323:VAL:O	1:A:327:LYS:HG3	2.05	0.56
1:C:170:PHE:O	1:C:174:MET:HG2	2.05	0.56
1:A:170:PHE:O	1:A:174:MET:HG2	2.05	0.56
1:C:246:SER:HB3	2:C:550:NAD:O4D	2.05	0.56
1:A:96:GLU:HG3	1:A:126:ILE:HD13	1.88	0.56
1:B:170:PHE:O	1:B:174:MET:HG2	2.05	0.56
1:B:389:VAL:O	1:B:408:MET:HG3	2.06	0.55
1:D:238:VAL:O	1:D:261:ASN:ND2	2.40	0.55
1:D:246:SER:HB3	2:D:550:NAD:O4D	2.07	0.55
1:D:170:PHE:O	1:D:174:MET:HG2	2.05	0.55
1:D:323:VAL:O	1:D:327:LYS:HG3	2.07	0.55
1:B:261:ASN:ND2	1:B:263:LYS:HB3	2.22	0.54
1:D:264:ARG:N	1:D:264:ARG:HD2	2.22	0.54
1:A:261:ASN:HD21	1:A:263:LYS:CE	2.11	0.54
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.42	0.54
1:C:323:VAL:HG13	1:C:369:CYS:SG	2.48	0.54
1:C:341:GLN:OE1	1:C:383:PRO:HG3	2.08	0.54
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.42	0.54
1:A:434:ASN:HD22	1:A:434:ASN:H	1.56	0.54
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.42	0.53
1:B:261:ASN:ND2	1:B:263:LYS:HE3	2.19	0.53
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.42	0.53
1:B:247:THR:HG22	1:B:269:LEU:HB3	1.91	0.53
1:C:434:ASN:HD22	1:C:434:ASN:H	1.57	0.53
1:D:434:ASN:HD22	1:D:434:ASN:H	1.57	0.53
1:B:434:ASN:H	1:B:434:ASN:HD22	1.57	0.53
1:A:341:GLN:OE1	1:A:383:PRO:HG3	2.09	0.53
1:C:261:ASN:ND2	1:C:263:LYS:HB3	2.24	0.53
1:D:247:THR:HG22	1:D:269:LEU:HB3	1.91	0.53
1:C:261:ASN:ND2	1:C:263:LYS:HE3	2.16	0.53
1:D:261:ASN:ND2	1:D:263:LYS:HB3	2.24	0.52
1:D:341:GLN:OE1	1:D:383:PRO:HG3	2.09	0.52
1:D:279:ALA:HA	1:D:314:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ARG:HD2	1:B:264:ARG:N	2.26	0.51
1:A:261:ASN:O	1:A:262:LEU:HB2	2.10	0.51
1:C:146:MET:HE1	1:D:458:VAL:HG12	1.93	0.51
1:A:356:LEU:HD13	1:A:400:ILE:HG12	1.93	0.50
1:B:113:LEU:HB2	1:B:116:ASN:HD22	1.75	0.50
1:B:264:ARG:HD2	1:B:264:ARG:H	1.76	0.50
1:B:369:CYS:O	1:B:370:GLY:C	2.54	0.50
1:A:247:THR:HG22	1:A:269:LEU:HB3	1.92	0.50
1:C:247:THR:HG22	1:C:269:LEU:HB3	1.93	0.50
1:A:261:ASN:ND2	1:A:263:LYS:HB3	2.27	0.50
1:A:238:VAL:O	1:A:261:ASN:ND2	2.44	0.50
1:D:113:LEU:HB2	1:D:116:ASN:HD22	1.75	0.50
1:A:494:LYS:HB2	1:B:455:CYS:HB3	1.93	0.50
1:C:264:ARG:HD2	1:C:264:ARG:N	2.27	0.50
1:A:113:LEU:HB2	1:A:116:ASN:HD22	1.77	0.49
1:A:455:CYS:HB3	1:B:494:LYS:HB2	1.95	0.49
1:B:96:GLU:HG3	1:B:126:ILE:HD13	1.94	0.49
1:B:261:ASN:HD21	1:B:263:LYS:HB3	1.77	0.49
1:C:356:LEU:HD13	1:C:400:ILE:HG12	1.94	0.49
1:A:280:ASP:HB2	1:A:434:ASN:HD21	1.78	0.49
1:B:319:VAL:O	1:B:323:VAL:HG23	2.13	0.49
1:B:356:LEU:HD13	1:B:400:ILE:HG12	1.94	0.49
1:B:341:GLN:OE1	1:B:383:PRO:HG3	2.12	0.49
1:C:113:LEU:HB2	1:C:116:ASN:HD22	1.78	0.49
1:A:264:ARG:HD2	1:A:264:ARG:N	2.28	0.48
1:A:458:VAL:HG12	1:B:146:MET:HE1	1.95	0.48
1:C:279:ALA:HA	1:C:314:ILE:HD13	1.93	0.48
1:B:279:ALA:HA	1:B:314:ILE:HD13	1.95	0.48
1:C:458:VAL:HG12	1:D:146:MET:HE1	1.95	0.48
1:D:264:ARG:HD2	1:D:264:ARG:H	1.77	0.48
1:A:279:ALA:HA	1:A:314:ILE:HD13	1.94	0.48
1:A:331:LEU:N	1:A:331:LEU:HD23	2.28	0.48
1:D:331:LEU:N	1:D:331:LEU:HD23	2.29	0.48
1:A:108:MET:CG	1:A:335:LEU:HD11	2.39	0.48
1:D:280:ASP:HB2	1:D:434:ASN:HD21	1.78	0.48
1:D:290:ALA:O	1:D:294:VAL:HG23	2.13	0.48
1:D:369:CYS:O	1:D:370:GLY:C	2.57	0.48
1:A:488:VAL:O	1:B:475:ARG:NH1	2.46	0.47
1:D:331:LEU:HD22	1:D:341:GLN:HB3	1.96	0.47
1:C:96:GLU:HG3	1:C:126:ILE:HD13	1.97	0.47
1:B:349:GLN:O	1:B:353:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LEU:HD22	1:A:341:GLN:HB3	1.95	0.47
1:D:349:GLN:O	1:D:353:ILE:HG13	2.15	0.47
1:D:356:LEU:HD13	1:D:400:ILE:HG12	1.96	0.47
1:A:261:ASN:O	1:B:470:MET:HG2	2.15	0.47
1:B:280:ASP:HB2	1:B:434:ASN:HD21	1.79	0.47
1:D:261:ASN:HD21	1:D:263:LYS:HB3	1.80	0.47
1:A:272:LYS:HD2	1:A:306:SER:OG	2.15	0.47
1:B:272:LYS:HD2	1:B:306:SER:OG	2.14	0.46
1:C:280:ASP:HB2	1:C:434:ASN:HD21	1.80	0.46
1:A:146:MET:HE3	1:B:460:SER:CB	2.41	0.46
1:C:460:SER:CB	1:D:146:MET:HE3	2.44	0.46
1:A:460:SER:CB	1:B:146:MET:HE3	2.44	0.46
1:D:96:GLU:HG3	1:D:126:ILE:HD13	1.98	0.46
1:A:14:ASN:O	1:A:15:LEU:C	2.58	0.46
1:D:14:ASN:O	1:D:15:LEU:C	2.56	0.46
1:A:247:THR:HG22	1:A:269:LEU:CB	2.46	0.46
1:B:331:LEU:N	1:B:331:LEU:HD23	2.31	0.46
1:C:272:LYS:HD2	1:C:306:SER:OG	2.16	0.46
1:C:455:CYS:HB3	1:D:494:LYS:HB2	1.98	0.46
1:B:90:LYS:HD2	1:B:90:LYS:HA	1.79	0.46
1:B:261:ASN:O	1:B:262:LEU:HB2	2.14	0.45
1:D:247:THR:HG22	1:D:269:LEU:CB	2.46	0.45
1:C:345:ILE:HG23	1:C:346:ASP:N	2.31	0.45
1:A:369:CYS:O	1:A:370:GLY:C	2.60	0.45
1:A:475:ARG:NH1	1:B:488:VAL:O	2.48	0.45
1:C:470:MET:HG2	1:D:261:ASN:O	2.16	0.45
1:A:490:THR:OG1	1:B:464:PRO:HG2	2.16	0.45
1:B:247:THR:HG22	1:B:269:LEU:CB	2.46	0.45
1:D:462:GLN:CD	1:D:462:GLN:H	2.25	0.45
1:A:264:ARG:HD2	1:A:264:ARG:H	1.82	0.45
1:C:331:LEU:HD23	1:C:331:LEU:N	2.32	0.45
1:C:294:VAL:HG22	1:C:305:ALA:O	2.17	0.45
1:C:261:ASN:HD21	1:C:263:LYS:HB3	1.81	0.44
1:A:290:ALA:O	1:A:294:VAL:HG23	2.17	0.44
1:A:434:ASN:HD22	1:A:434:ASN:N	2.12	0.44
1:C:434:ASN:HD22	1:C:434:ASN:N	2.13	0.44
1:B:353:ILE:O	1:B:357:ILE:HG13	2.17	0.44
1:B:462:GLN:CD	1:B:462:GLN:H	2.26	0.44
1:C:462:GLN:CD	1:C:462:GLN:H	2.25	0.44
1:B:312:GLU:HG2	1:B:409:LYS:CG	2.47	0.44
1:B:361:LYS:HD3	1:B:367:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:VAL:HG22	1:B:305:ALA:O	2.18	0.44
1:C:247:THR:HG22	1:C:269:LEU:CB	2.48	0.44
1:C:331:LEU:HD22	1:C:341:GLN:HB3	1.99	0.44
1:A:294:VAL:HG22	1:A:305:ALA:O	2.18	0.44
1:B:345:ILE:HG23	1:B:346:ASP:N	2.32	0.44
1:C:264:ARG:HD2	1:C:264:ARG:H	1.83	0.44
1:C:290:ALA:O	1:C:294:VAL:HG23	2.17	0.44
1:D:283:LEU:O	1:D:287:VAL:HG23	2.18	0.44
1:A:361:LYS:HD3	1:A:367:LEU:HD22	1.99	0.44
1:B:95:ILE:HD12	1:B:129:LEU:HD12	2.00	0.44
1:B:108:MET:CG	1:B:335:LEU:HD11	2.37	0.44
1:B:21:LYS:HB3	1:B:29:HIS:O	2.18	0.44
1:D:280:ASP:HB2	1:D:434:ASN:ND2	2.33	0.44
1:A:280:ASP:HB2	1:A:434:ASN:ND2	2.33	0.43
1:C:466:GLY:HA3	1:C:475:ARG:HE	1.83	0.43
1:B:290:ALA:O	1:B:294:VAL:HG23	2.18	0.43
1:B:461:ALA:HA	1:B:477:LEU:HD13	1.99	0.43
1:D:294:VAL:HG22	1:D:305:ALA:O	2.19	0.43
1:A:462:GLN:CD	1:A:462:GLN:H	2.26	0.43
1:B:261:ASN:HD21	1:B:263:LYS:CE	2.23	0.43
1:A:146:MET:HE1	1:B:458:VAL:HG12	1.99	0.43
1:A:283:LEU:O	1:A:287:VAL:HG23	2.18	0.43
1:A:349:GLN:O	1:A:353:ILE:HG13	2.19	0.43
1:A:461:ALA:HA	1:A:477:LEU:HD13	2.00	0.43
1:D:272:LYS:HD2	1:D:306:SER:OG	2.18	0.43
1:D:461:ALA:HA	1:D:477:LEU:HD13	1.99	0.43
1:A:312:GLU:HG2	1:A:409:LYS:CG	2.48	0.43
1:B:102:LEU:HD21	1:B:203:HIS:CD2	2.54	0.43
1:C:461:ALA:HA	1:C:477:LEU:HD13	1.99	0.43
1:C:494:LYS:HB2	1:D:455:CYS:HB3	2.01	0.43
1:D:90:LYS:HD2	1:D:90:LYS:HA	1.78	0.43
1:B:14:ASN:HD22	1:B:14:ASN:HA	1.55	0.42
1:D:272:LYS:HD2	1:D:272:LYS:HA	1.91	0.42
1:A:21:LYS:HB3	1:A:29:HIS:O	2.19	0.42
1:A:336:THR:HA	1:A:337:PRO:HD3	1.85	0.42
1:B:280:ASP:HB2	1:B:434:ASN:ND2	2.34	0.42
1:B:434:ASN:HD22	1:B:434:ASN:N	2.13	0.42
1:C:312:GLU:HG2	1:C:409:LYS:CG	2.48	0.42
1:A:464:PRO:HG2	1:B:490:THR:OG1	2.18	0.42
1:B:283:LEU:O	1:B:287:VAL:HG23	2.19	0.42
1:C:475:ARG:NH1	1:D:488:VAL:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:HD2	1:A:90:LYS:HA	1.77	0.42
1:A:359:SER:O	1:A:363:GLU:HG3	2.20	0.42
1:A:466:GLY:HA3	1:A:475:ARG:HE	1.85	0.42
1:D:21:LYS:HB3	1:D:29:HIS:O	2.20	0.42
1:B:14:ASN:O	1:B:15:LEU:C	2.59	0.42
1:C:90:LYS:HD2	1:C:90:LYS:HA	1.77	0.42
1:D:434:ASN:HD22	1:D:434:ASN:N	2.13	0.42
1:A:14:ASN:HD22	1:A:14:ASN:HA	1.54	0.42
1:C:108:MET:CG	1:C:335:LEU:HD11	2.39	0.42
1:B:336:THR:HA	1:B:337:PRO:HD3	1.90	0.42
1:D:345:ILE:HG23	1:D:346:ASP:N	2.34	0.42
1:C:14:ASN:O	1:C:15:LEU:C	2.62	0.42
1:C:21:LYS:HB3	1:C:29:HIS:O	2.20	0.42
1:A:345:ILE:HG23	1:A:346:ASP:N	2.35	0.41
1:C:14:ASN:HD22	1:C:14:ASN:HA	1.56	0.41
1:A:353:ILE:O	1:A:357:ILE:HG13	2.21	0.41
1:A:102:LEU:HD21	1:A:203:HIS:CD2	2.56	0.41
1:C:283:LEU:O	1:C:287:VAL:HG23	2.20	0.41
1:C:359:SER:O	1:C:363:GLU:HG3	2.21	0.41
1:C:280:ASP:HB2	1:C:434:ASN:ND2	2.35	0.41
1:C:349:GLN:O	1:C:353:ILE:HG13	2.20	0.41
1:D:174:MET:HE2	1:D:244:THR:HG21	2.02	0.41
1:D:435:ASP:OD2	1:D:438:LYS:HG3	2.21	0.41
1:B:331:LEU:HD22	1:B:341:GLN:HB3	2.03	0.41
1:B:466:GLY:HA3	1:B:475:ARG:HE	1.85	0.41
1:D:59:VAL:O	1:D:63:VAL:HG23	2.21	0.41
1:A:59:VAL:O	1:A:63:VAL:HG23	2.21	0.41
1:A:294:VAL:O	1:A:299:GLY:HA2	2.21	0.41
1:A:435:ASP:OD2	1:A:438:LYS:HG3	2.21	0.41
1:C:315:TYR:O	1:C:319:VAL:HG23	2.20	0.41
1:B:261:ASN:OD1	1:B:263:LYS:HG2	2.21	0.41
1:C:369:CYS:O	1:C:370:GLY:C	2.64	0.41
1:D:95:ILE:HD12	1:D:129:LEU:HD12	2.03	0.41
1:A:293:GLY:O	1:A:304:ALA:HA	2.21	0.40
1:B:44:THR:OG1	1:B:46:GLU:HG2	2.21	0.40
1:B:59:VAL:O	1:B:63:VAL:HG23	2.21	0.40
1:C:59:VAL:O	1:C:63:VAL:HG23	2.21	0.40
1:C:174:MET:HE2	1:C:244:THR:HG21	2.04	0.40
1:C:488:VAL:O	1:D:475:ARG:NH1	2.53	0.40
1:D:359:SER:O	1:D:363:GLU:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:LEU:O	1:D:317:GLU:OE2[1_556]	2.12	0.08

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%)	472 (96%)	18 (4%)	2 (0%)	30	34
1	B	492/501 (98%)	470 (96%)	20 (4%)	2 (0%)	30	34
1	C	492/501 (98%)	471 (96%)	19 (4%)	2 (0%)	30	34
1	D	492/501 (98%)	472 (96%)	18 (4%)	2 (0%)	30	34
All	All	1968/2004 (98%)	1885 (96%)	75 (4%)	8 (0%)	30	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	GLY
1	B	370	GLY
1	C	370	GLY
1	D	370	GLY
1	A	426	GLY
1	B	426	GLY
1	C	426	GLY
1	D	426	GLY

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	404/415 (97%)	392 (97%)	12 (3%)	36	48
1	B	404/415 (97%)	392 (97%)	12 (3%)	36	48
1	C	404/415 (97%)	392 (97%)	12 (3%)	36	48
1	D	404/415 (97%)	392 (97%)	12 (3%)	36	48
All	All	1616/1660 (97%)	1568 (97%)	48 (3%)	36	48

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	15	LEU
1	A	83	GLU
1	A	167	PRO
1	A	198	PRO
1	A	331	LEU
1	A	336	THR
1	A	343	PRO
1	A	401	PHE
1	A	415	ASP
1	A	434	ASN
1	A	462	GLN
1	B	14	ASN
1	B	15	LEU
1	B	83	GLU
1	B	167	PRO
1	B	198	PRO
1	B	331	LEU
1	B	336	THR
1	B	343	PRO
1	B	401	PHE
1	B	415	ASP
1	B	434	ASN
1	B	462	GLN
1	C	14	ASN
1	C	15	LEU
1	C	83	GLU
1	C	167	PRO
1	C	198	PRO
1	C	331	LEU
1	C	336	THR

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Mol	Chain	Res	Type
1	C	343	PRO
1	C	401	PHE
1	C	415	ASP
1	C	434	ASN
1	C	462	GLN
1	D	14	ASN
1	D	15	LEU
1	D	83	GLU
1	D	167	PRO
1	D	198	PRO
1	D	331	LEU
1	D	336	THR
1	D	343	PRO
1	D	401	PHE
1	D	415	ASP
1	D	434	ASN
1	D	462	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	116	ASN
1	A	140	GLN
1	A	164	GLN
1	A	292	GLN
1	A	405	GLN
1	A	434	ASN
1	A	497	GLN
1	B	14	ASN
1	B	116	ASN
1	B	140	GLN
1	B	164	GLN
1	B	292	GLN
1	B	405	GLN
1	B	434	ASN
1	B	497	GLN
1	C	14	ASN
1	C	109	ASN
1	C	116	ASN
1	C	140	GLN
1	C	164	GLN

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Mol	Chain	Res	Type
1	C	292	GLN
1	C	405	GLN
1	C	434	ASN
1	C	497	GLN
1	D	14	ASN
1	D	109	ASN
1	D	116	ASN
1	D	140	GLN
1	D	164	GLN
1	D	292	GLN
1	D	405	GLN
1	D	434	ASN
1	D	497	GLN

5.3.3 RNA [i](#)

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](#)

4 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	$\# Z > 2$
2	NAD	B	550	-	46,48,48	1.92	7 (15%)	64,73,73	2.33	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	A	550	-	46,48,48	1.83	5 (10%)	64,73,73	2.25	15 (23%)
2	NAD	D	550	-	46,48,48	1.90	6 (13%)	64,73,73	2.22	13 (20%)
2	NAD	C	550	-	46,48,48	1.79	6 (13%)	64,73,73	2.34	17 (26%)

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
2	NAD	B	550	-	-	9/30/62/62	0/5/5/5
2	NAD	A	550	-	-	11/30/62/62	0/5/5/5
2	NAD	D	550	-	-	11/30/62/62	0/5/5/5
2	NAD	C	550	-	-	11/30/62/62	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	550	NAD	C2N-N1N	8.15	1.43	1.35
2	B	550	NAD	C2N-N1N	7.96	1.43	1.35
2	C	550	NAD	C2N-N1N	7.69	1.43	1.35
2	A	550	NAD	C2N-N1N	7.51	1.43	1.35
2	D	550	NAD	C6N-N1N	5.07	1.46	1.35
2	C	550	NAD	C6N-N1N	5.04	1.46	1.35
2	A	550	NAD	C6N-N1N	4.96	1.46	1.35
2	B	550	NAD	C6N-N1N	4.90	1.46	1.35
2	D	550	NAD	O4D-C1D	4.59	1.46	1.40
2	A	550	NAD	O4D-C1D	4.53	1.46	1.40
2	B	550	NAD	O4D-C1D	4.36	1.46	1.40
2	C	550	NAD	O4D-C1D	3.96	1.46	1.40
2	A	550	NAD	C5A-N7A	-3.85	1.32	1.39
2	D	550	NAD	C5A-N7A	-3.76	1.32	1.39
2	B	550	NAD	C5A-N7A	-3.72	1.32	1.39
2	B	550	NAD	PN-O3	3.49	1.63	1.59
2	C	550	NAD	C5A-N7A	-3.29	1.33	1.39
2	D	550	NAD	C4N-C3N	2.34	1.43	1.39
2	D	550	NAD	C3N-C7N	2.28	1.54	1.50
2	B	550	NAD	C4N-C3N	2.27	1.42	1.39
2	B	550	NAD	C3N-C7N	2.21	1.53	1.50
2	C	550	NAD	C4N-C3N	2.08	1.42	1.39
2	A	550	NAD	C4N-C3N	2.06	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	550	NAD	C3N-C7N	2.01	1.53	1.50

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	550	NAD	C4D-O4D-C1D	7.09	116.42	109.92
2	D	550	NAD	C4D-O4D-C1D	6.94	116.28	109.92
2	B	550	NAD	C4D-O4D-C1D	6.90	116.24	109.92
2	A	550	NAD	N3A-C4A-N9A	6.53	138.26	127.17
2	C	550	NAD	N3A-C4A-N9A	6.53	138.26	127.17
2	C	550	NAD	N3A-C2A-N1A	-6.36	118.96	128.58
2	B	550	NAD	C5A-C4A-N3A	-6.35	117.97	126.72
2	B	550	NAD	N3A-C4A-N9A	6.29	137.87	127.17
2	D	550	NAD	C5A-C4A-N3A	-6.23	118.14	126.72
2	B	550	NAD	C5N-C4N-C3N	6.20	126.46	120.36
2	D	550	NAD	N3A-C4A-N9A	6.11	137.56	127.17
2	A	550	NAD	C4D-O4D-C1D	6.06	115.47	109.92
2	B	550	NAD	N3A-C2A-N1A	-5.95	119.57	128.58
2	C	550	NAD	C5A-C4A-N3A	-5.90	118.59	126.72
2	A	550	NAD	C5A-C4A-N3A	-5.82	118.71	126.72
2	A	550	NAD	N3A-C2A-N1A	-5.73	119.91	128.58
2	D	550	NAD	C5N-C4N-C3N	5.70	125.97	120.36
2	D	550	NAD	N3A-C2A-N1A	-5.68	119.99	128.58
2	A	550	NAD	C5N-C4N-C3N	5.06	125.34	120.36
2	C	550	NAD	C5N-C4N-C3N	5.06	125.34	120.36
2	B	550	NAD	C6N-C5N-C4N	-4.19	113.40	119.45
2	B	550	NAD	C2A-N3A-C4A	4.13	121.91	111.83
2	C	550	NAD	C2A-N3A-C4A	4.12	121.91	111.83
2	D	550	NAD	C2A-N3A-C4A	4.07	121.77	111.83
2	A	550	NAD	C2A-N3A-C4A	3.87	121.28	111.83
2	A	550	NAD	O4B-C1B-N9A	3.78	115.34	108.09
2	D	550	NAD	C6N-C5N-C4N	-3.72	114.08	119.45
2	C	550	NAD	C6N-C5N-C4N	-3.63	114.22	119.45
2	A	550	NAD	C6N-C5N-C4N	-3.55	114.34	119.45
2	C	550	NAD	O4B-C1B-N9A	3.43	114.69	108.09
2	A	550	NAD	C6A-C5A-N7A	-3.27	125.78	132.09
2	B	550	NAD	O2B-C2B-C3B	3.16	121.96	111.82
2	A	550	NAD	C4A-C5A-N7A	3.14	114.17	110.58
2	B	550	NAD	O3D-C3D-C2D	3.07	121.65	111.82
2	C	550	NAD	C6A-C5A-N7A	-2.95	126.39	132.09
2	C	550	NAD	C4A-C5A-N7A	2.89	113.88	110.58
2	C	550	NAD	C2A-N1A-C6A	2.83	123.37	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	550	NAD	C6A-C5A-N7A	-2.73	126.82	132.09
2	B	550	NAD	C6A-C5A-N7A	-2.73	126.83	132.09
2	A	550	NAD	O3D-C3D-C4D	2.73	118.91	111.08
2	D	550	NAD	O2B-C2B-C3B	2.72	120.53	111.82
2	B	550	NAD	C2A-N1A-C6A	2.71	123.17	118.73
2	A	550	NAD	O2B-C2B-C3B	2.69	120.45	111.82
2	C	550	NAD	O2N-PN-O3	-2.68	100.04	107.27
2	A	550	NAD	C5A-C4A-N9A	-2.65	102.92	105.81
2	D	550	NAD	C2A-N1A-C6A	2.65	123.08	118.73
2	B	550	NAD	O5D-C5D-C4D	2.54	117.63	108.99
2	C	550	NAD	C5A-C4A-N9A	-2.52	103.07	105.81
2	A	550	NAD	C2A-N1A-C6A	2.41	122.69	118.73
2	C	550	NAD	C4A-N9A-C8A	2.34	108.19	105.74
2	D	550	NAD	O5D-C5D-C4D	2.25	116.67	108.99
2	B	550	NAD	C4A-C5A-N7A	2.24	113.14	110.58
2	D	550	NAD	C4A-C5A-N7A	2.21	113.11	110.58
2	C	550	NAD	C6N-N1N-C2N	-2.17	120.03	121.88
2	C	550	NAD	O5D-C5D-C4D	2.15	116.31	108.99
2	D	550	NAD	C6A-C5A-C4A	2.09	120.03	117.18
2	C	550	NAD	O3D-C3D-C2D	2.07	118.47	111.82
2	B	550	NAD	C6A-C5A-C4A	2.07	120.00	117.18
2	B	550	NAD	C5N-C6N-N1N	2.05	123.18	120.38
2	A	550	NAD	O5D-C5D-C4D	2.04	115.94	108.99

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	550	NAD	C5B-O5B-PA-O1A
2	A	550	NAD	C5B-O5B-PA-O3
2	A	550	NAD	C5D-O5D-PN-O3
2	A	550	NAD	C5D-O5D-PN-O1N
2	B	550	NAD	C5B-O5B-PA-O1A
2	B	550	NAD	C5B-O5B-PA-O3
2	B	550	NAD	C5D-O5D-PN-O3
2	B	550	NAD	C5D-O5D-PN-O1N
2	C	550	NAD	C5B-O5B-PA-O1A
2	C	550	NAD	C5B-O5B-PA-O3
2	C	550	NAD	C5D-O5D-PN-O3
2	C	550	NAD	C5D-O5D-PN-O1N
2	D	550	NAD	C5B-O5B-PA-O1A
2	D	550	NAD	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
2	D	550	NAD	C5D-O5D-PN-O3
2	D	550	NAD	C5D-O5D-PN-O1N
2	C	550	NAD	PN-O3-PA-O1A
2	B	550	NAD	C2B-C1B-N9A-C8A
2	D	550	NAD	C2B-C1B-N9A-C8A
2	A	550	NAD	C2B-C1B-N9A-C8A
2	C	550	NAD	C2B-C1B-N9A-C8A
2	C	550	NAD	O4D-C4D-C5D-O5D
2	A	550	NAD	C5B-O5B-PA-O2A
2	A	550	NAD	C5D-O5D-PN-O2N
2	B	550	NAD	C5B-O5B-PA-O2A
2	C	550	NAD	C5B-O5B-PA-O2A
2	C	550	NAD	C5D-O5D-PN-O2N
2	D	550	NAD	C5B-O5B-PA-O2A
2	D	550	NAD	C5D-O5D-PN-O2N
2	A	550	NAD	PN-O3-PA-O1A
2	B	550	NAD	PN-O3-PA-O1A
2	D	550	NAD	PN-O3-PA-O1A
2	D	550	NAD	O4D-C4D-C5D-O5D
2	C	550	NAD	PN-O3-PA-O2A
2	D	550	NAD	PN-O3-PA-O2A
2	A	550	NAD	O4B-C1B-N9A-C8A
2	C	550	NAD	O4B-C1B-N9A-C8A
2	D	550	NAD	O4B-C1B-N9A-C8A
2	B	550	NAD	O4B-C1B-N9A-C8A
2	A	550	NAD	O4D-C4D-C5D-O5D
2	A	550	NAD	PN-O3-PA-O2A
2	B	550	NAD	O4D-C4D-C5D-O5D

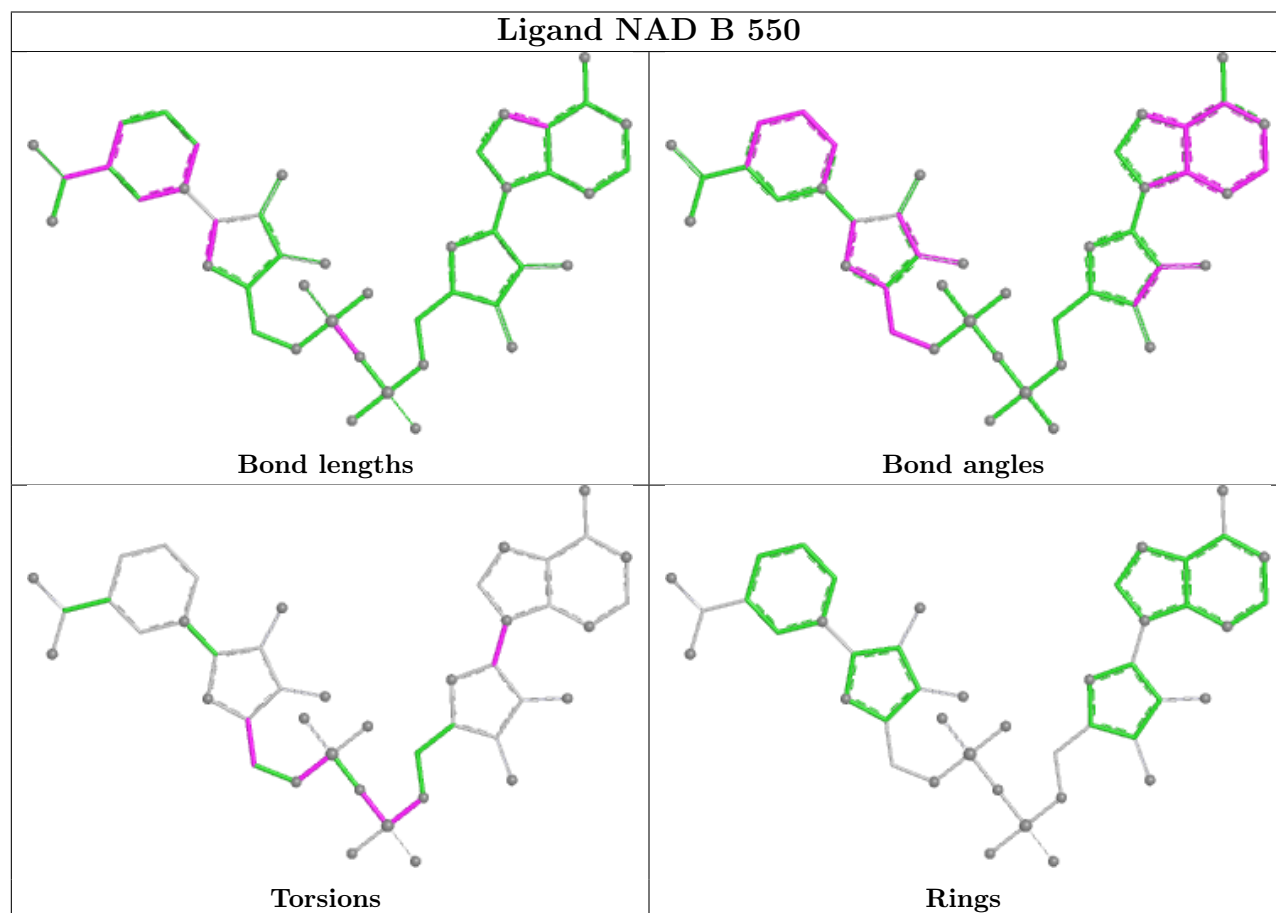
There are no ring outliers.

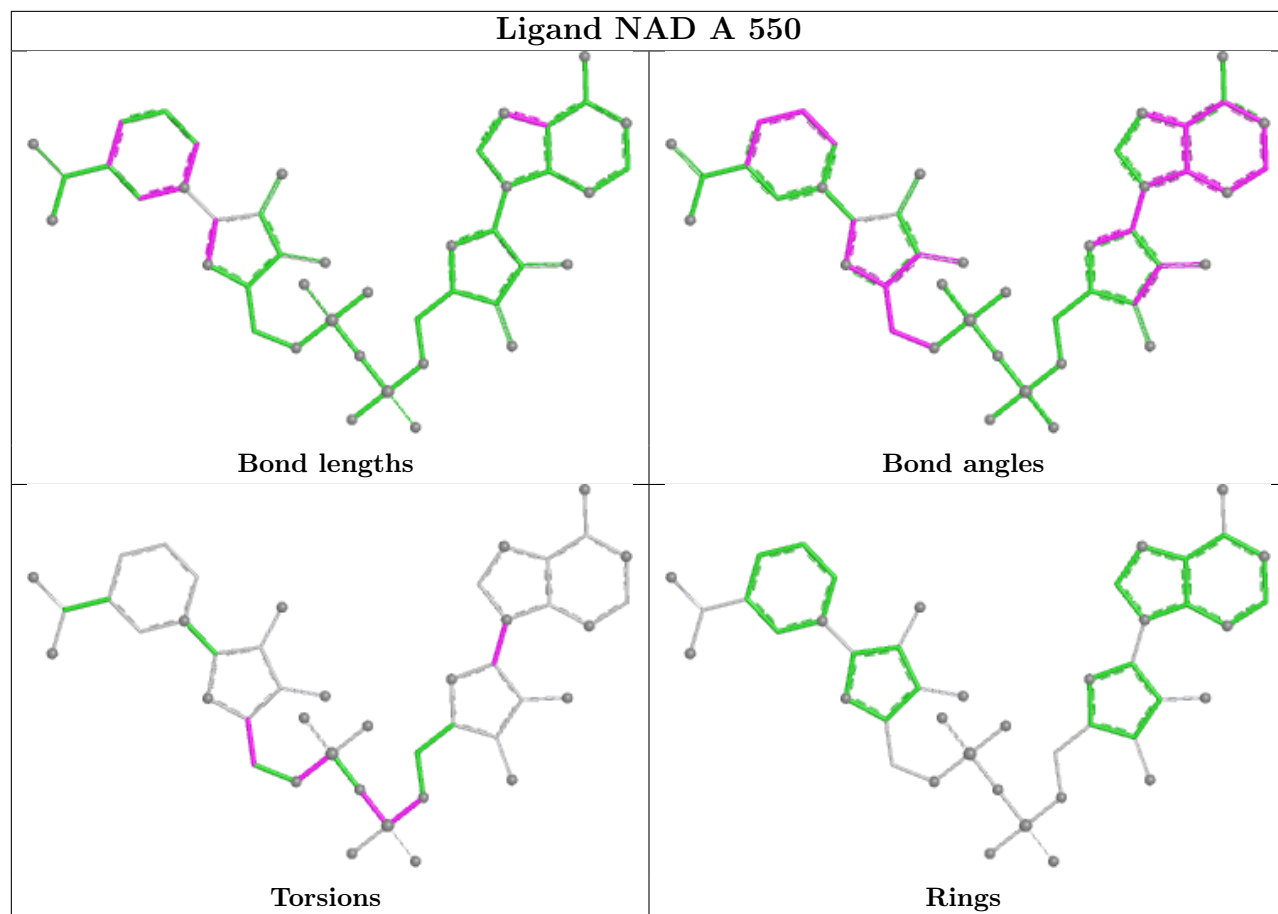
4 monomers are involved in 4 short contacts:

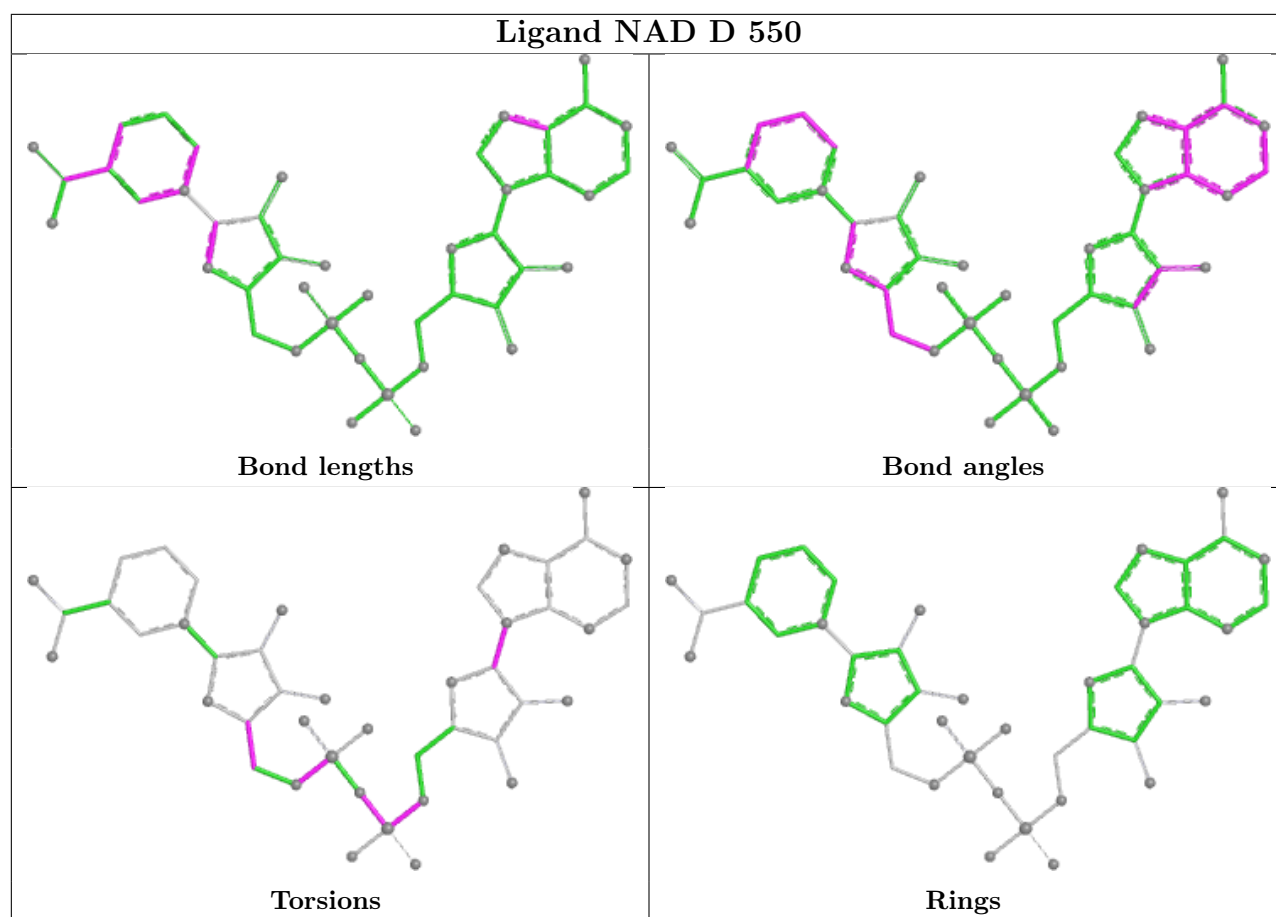
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	550	NAD	1	0
2	A	550	NAD	1	0
2	D	550	NAD	1	0
2	C	550	NAD	1	0

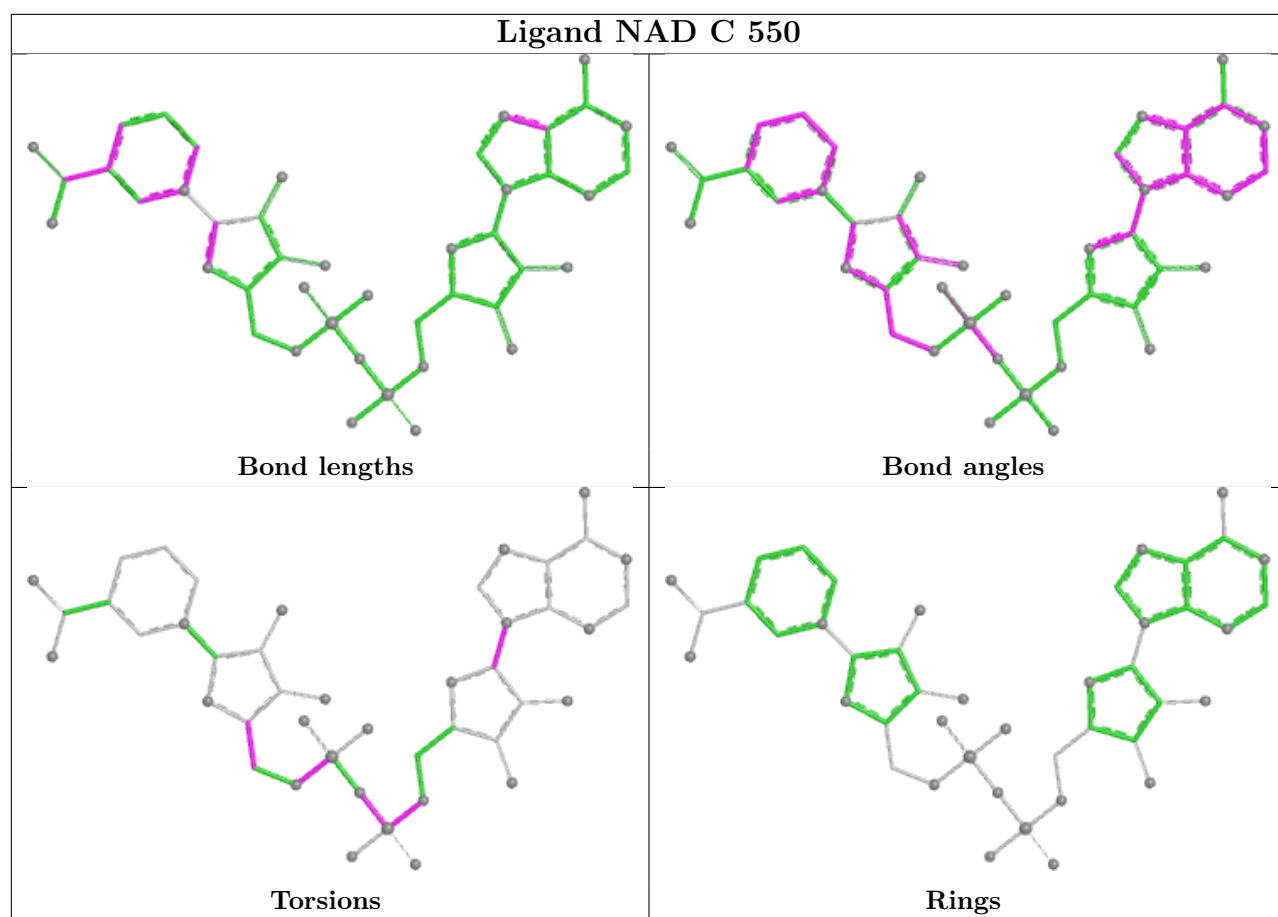
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

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	494/501 (98%)	0.30	11 (2%) 62 67	17, 28, 44, 60	0
1	B	494/501 (98%)	0.36	18 (3%) 46 52	18, 28, 44, 64	0
1	C	494/501 (98%)	0.35	21 (4%) 40 45	17, 26, 42, 58	0
1	D	494/501 (98%)	0.27	18 (3%) 46 52	17, 26, 41, 62	0
All	All	1976/2004 (98%)	0.32	68 (3%) 48 55	17, 27, 43, 64	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	14	ASN	5.2
1	D	14	ASN	4.6
1	D	379	TYR	4.4
1	B	376	ASN	3.9
1	B	379	TYR	3.8
1	C	369	CYS	3.8
1	D	261	ASN	3.7
1	A	379	TYR	3.7
1	D	15	LEU	3.5
1	C	15	LEU	3.4
1	C	8	VAL	3.4
1	D	317	GLU	3.4
1	B	14	ASN	3.4
1	B	7	ASP	3.3
1	D	7	ASP	3.3
1	C	7	ASP	3.2
1	B	15	LEU	3.1
1	D	377	LYS	3.0
1	C	283	LEU	3.0
1	D	8	VAL	2.9
1	A	369	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	7	ASP	2.9
1	D	415	ASP	2.9
1	C	366	LYS	2.8
1	D	13	THR	2.8
1	B	369	CYS	2.8
1	C	320	ARG	2.8
1	C	13	THR	2.7
1	C	321	ARG	2.6
1	D	369	CYS	2.6
1	B	483	HIS	2.6
1	C	483	HIS	2.6
1	D	483	HIS	2.6
1	A	14	ASN	2.6
1	C	261	ASN	2.6
1	A	15	LEU	2.6
1	B	12	LEU	2.6
1	B	8	VAL	2.5
1	C	415	ASP	2.5
1	B	366	LYS	2.5
1	B	415	ASP	2.5
1	B	403	PRO	2.5
1	B	261	ASN	2.4
1	C	414	ASP	2.4
1	C	361	LYS	2.4
1	C	480	TYR	2.3
1	B	365	ALA	2.3
1	D	294	VAL	2.3
1	B	480	TYR	2.3
1	A	261	ASN	2.3
1	D	434	ASN	2.2
1	B	374	TRP	2.2
1	D	349	GLN	2.2
1	A	376	ASN	2.2
1	C	379	TYR	2.2
1	B	375	GLY	2.2
1	C	392	ASP	2.2
1	C	313	SER	2.2
1	A	335	LEU	2.1
1	C	362	LYS	2.1
1	D	12	LEU	2.1
1	A	483	HIS	2.1
1	B	349	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	8	VAL	2.1
1	A	374	TRP	2.1
1	C	370	GLY	2.1
1	D	282	ASP	2.1
1	D	312	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

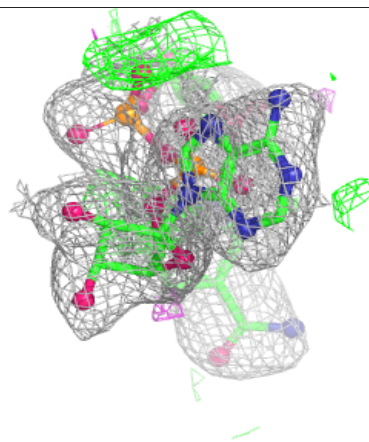
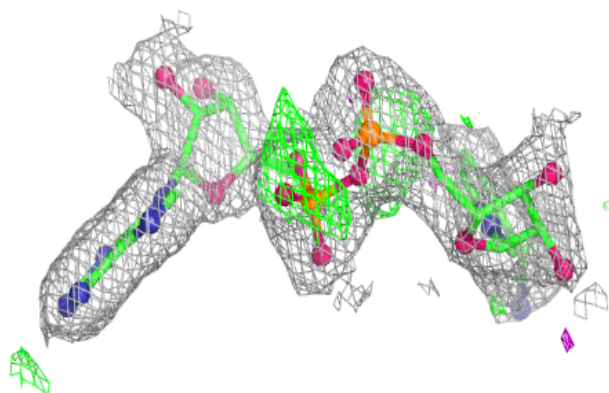
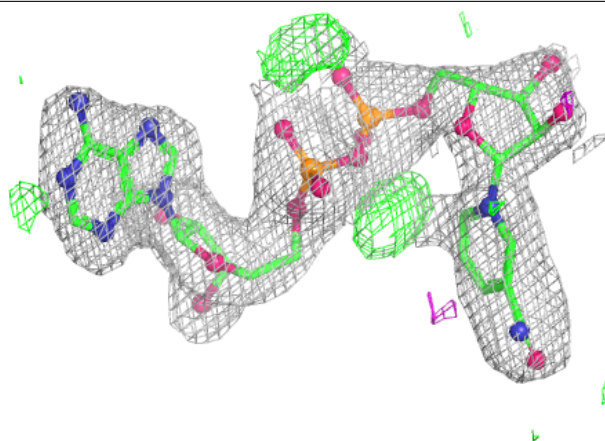
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	A	550	44/44	0.91	0.10	24,37,43,45	0
2	NAD	C	550	44/44	0.91	0.10	21,33,40,42	0
2	NAD	D	550	44/44	0.91	0.11	19,34,42,44	0
2	NAD	B	550	44/44	0.92	0.10	24,35,41,43	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.

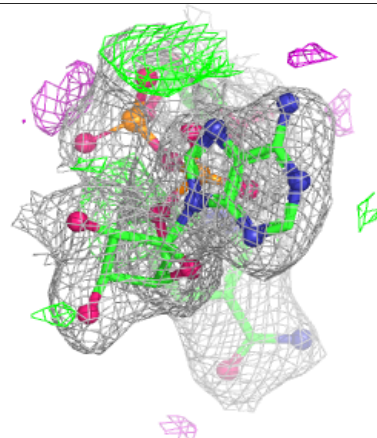
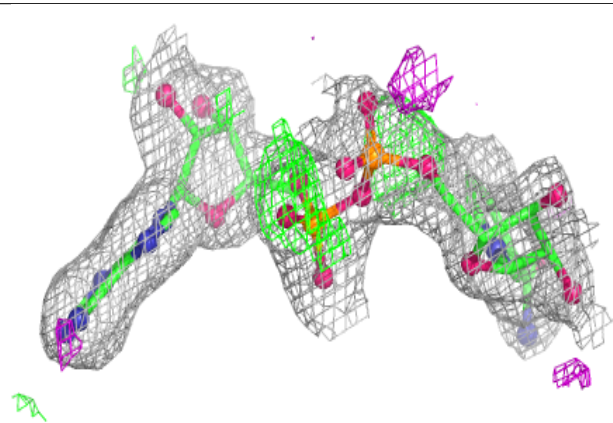
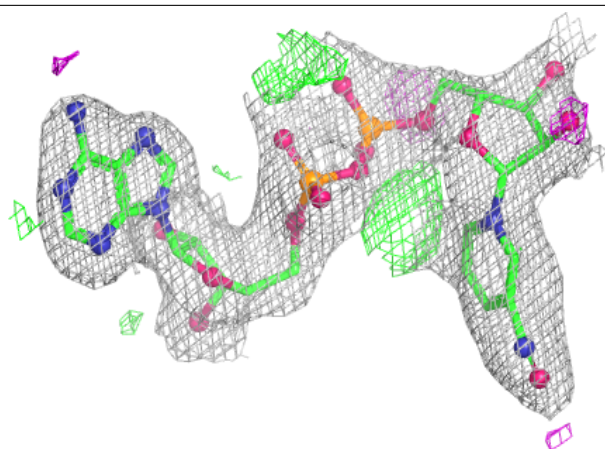
Electron density around NAD A 550:

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



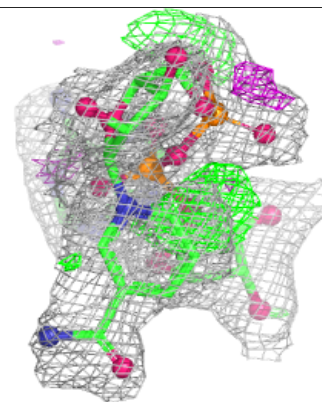
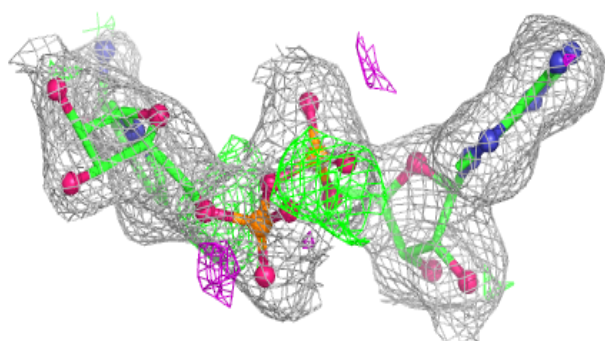
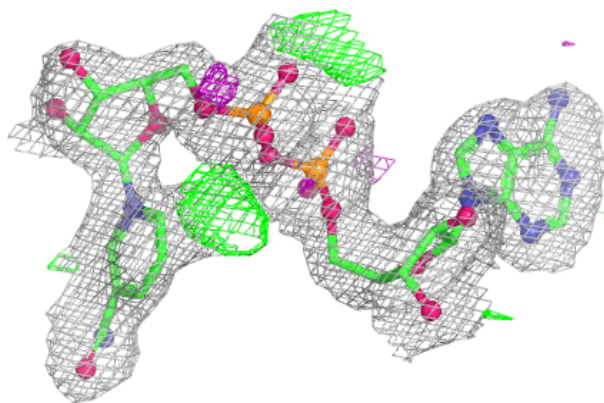
Electron density around NAD C 550:

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



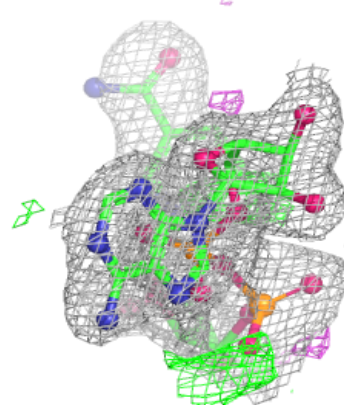
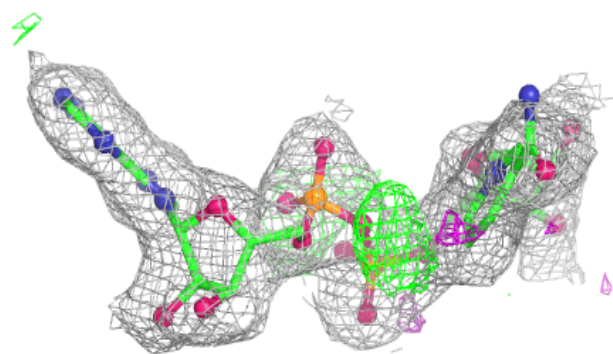
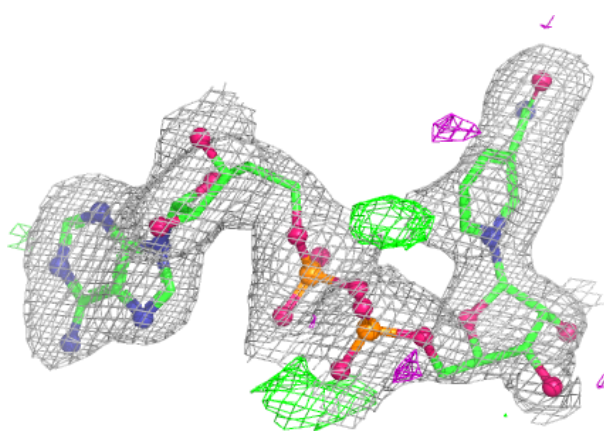
Electron density around NAD D 550:

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



Electron density around NAD B 550:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.