



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:15 PM UTC

PDB ID : 1EE2 / pdb_00001ee2
Title : THE STRUCTURE OF STEROID-ACTIVE ALCOHOL DEHYDROGE-
NASE AT 1.54 Å RESOLUTION
Authors : Adolph, H.W.
Deposited on : 2000-01-30
Resolution : 1.54 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

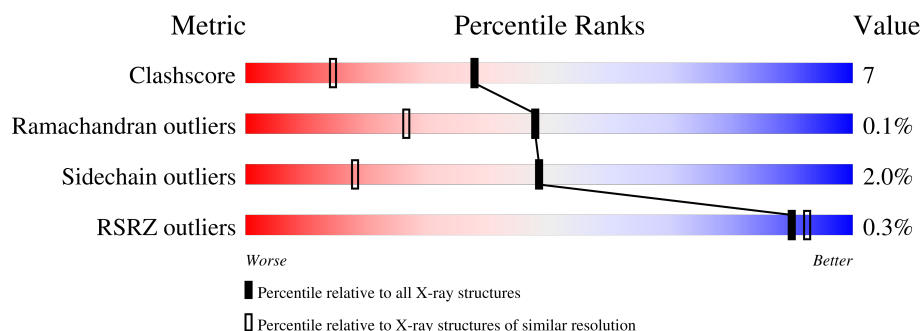
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	373	
1	B	373	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6939 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.

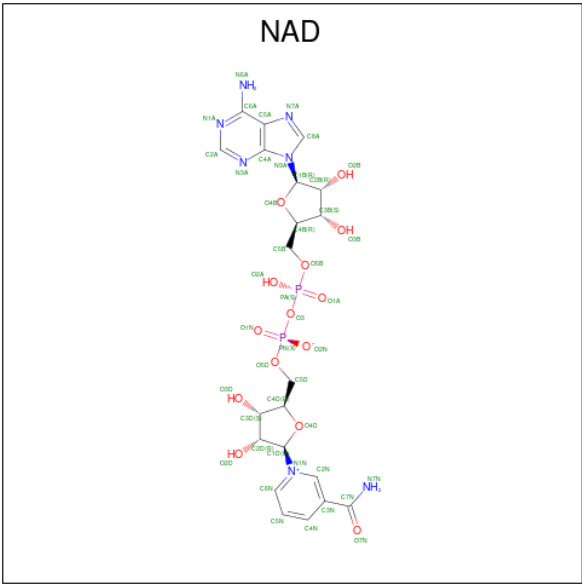
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	7	30	0
			2904	1854	490	535	25			
1	B	373	Total	C	N	O	S	0	27	0
			2875	1832	487	529	27			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

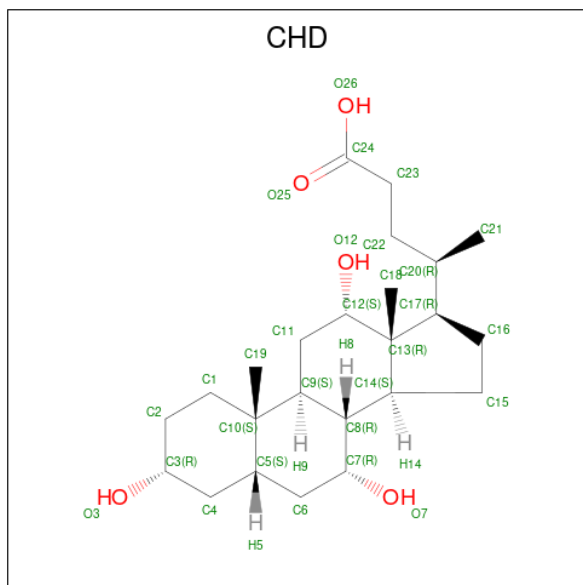
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			29	24	5		
4	B	1	Total	C	O	0	0
			29	24	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	505	Total	O	0	0
			505	505		
5	B	505	Total	O	0	0
			505	505		

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.

Chain A:

75% 22%

Residue	State
L300	Green
N303	Green
P304	Green
R311	Green
K312	Green
K313	Green
K314	Green
G315	Green
A316	Green
I317	Green
F321	Green
K322	Green
K323	Green
K324	Green
D325	Green
S326	Green
V327	Green
D333	Green
K337	Green
V348	Green
E352	Green
E356	Green
G357	Green
F358	Green
D359	Green
R362	Green
I367	Green
T372	Green
F373	Green
L165	Green
E166	Green
F175	Green
Q190	Green
T193	Green
G200	Green
G203	Green
G209	Green
G214	Green
A215	Green
A216	Green
R217	Green
G220	Green
N224	Green
F228	Green
E238	Green
G239	Green
V240	Green
N241	Green
P242	Green
Q243	Green
P248	Green
V252	Green
E255	Green
F265	Green
F266	Green
V267	Green
R270	Green
C281	Green
G286	Green
V289	Green
L290	Green
V291	Green
G292	Green
V293	Green
P294	Green
P295	Green
D296	Green
S297	Green
Q298	Green
N300	Green
S1	Red
T2	Red
A3	Yellow
E16	Yellow
K19	Yellow
P20	Yellow
I23	Yellow
E27	Yellow
K32	Yellow
A33	Yellow
H34	Yellow
E35	Yellow
V36	Yellow
M40	Yellow
V41	Yellow
A42	Yellow
A43	Yellow
R47	Yellow
T56	Yellow
E78	Yellow
R84	Yellow
K88	Yellow
V89	Yellow
I94	Yellow
G98	Yellow
K99	Yellow
E107	Yellow
G108	Yellow
M109	Yellow
L110	Yellow
C111	Yellow
M117	Yellow
P118	Yellow
R119	Yellow
R128	Yellow
F129	Yellow
T130	Yellow
P135	Yellow
T144	Yellow
S163	Yellow
D164	Yellow

Chain B:

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.03Å 73.16Å 92.49Å 90.00° 102.48° 90.00°	Depositor
Resolution (Å)	20.00 – 1.54 20.00 – 1.54	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.54) 98.2 (20.00-1.54)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.91 (at 1.54Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.145 , 0.183 0.143 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6939	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.10% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CHD, 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	1.36	6/3067 (0.2%)	2.06	112/4138 (2.7%)
1	B	1.29	5/3034 (0.2%)	2.00	90/4093 (2.2%)
All	All	1.32	11/6101 (0.2%)	2.03	202/8231 (2.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	0	1
All	All	1	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	ARG	NE-CZ	8.50	1.42	1.33
1	B	203	GLY	CA-C	5.58	1.58	1.52
1	B	53	VAL	C-O	5.56	1.30	1.24
1	B	163	SER	CA-C	-5.42	1.47	1.53
1	B	315	GLY	CA-C	-5.41	1.47	1.52
1	B	163	SER	CA-CB	5.35	1.61	1.53
1	A	291	VAL	CA-C	-5.34	1.47	1.52
1	A	47	ARG	NE-CZ	5.20	1.38	1.33
1	A	94[A]	ILE	CA-C	5.05	1.56	1.52
1	A	94[B]	ILE	CA-C	5.05	1.56	1.52
1	A	217	ARG	CZ-NH2	-5.02	1.26	1.33

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	GLU	CB-CG-CD	15.14	138.35	112.60
1	A	217	ARG	NE-CZ-NH2	15.00	132.70	119.20
1	A	217	ARG	NE-CZ-NH1	-14.34	107.16	121.50
1	B	134	LYS	CA-CB-CG	13.53	141.16	114.10
1	A	298	GLN	OE1-CD-NE2	13.16	135.76	122.60
1	A	325	ASP	CA-CB-CG	11.68	124.28	112.60
1	B	119[A]	ARG	CA-C-N	10.59	142.16	121.41
1	B	119[A]	ARG	C-N-CA	10.59	142.16	121.41
1	B	119[B]	ARG	CA-C-N	10.59	142.16	121.41
1	B	119[B]	ARG	C-N-CA	10.59	142.16	121.41
1	A	303	ASN	OD1-CG-ND2	10.03	132.63	122.60
1	B	323	SER	N-CA-C	9.96	121.90	111.14
1	A	1	SER	N-CA-CB	9.96	127.43	110.50
1	B	8	LYS	CB-CG-CD	9.79	133.82	111.30
1	A	323	SER	N-CA-C	9.13	122.07	111.11
1	A	1	SER	CB-CA-C	8.86	126.94	110.10
1	A	337	LYS	CD-CE-NZ	8.73	139.82	111.90
1	A	326	SER	N-CA-C	8.56	122.22	111.69
1	B	84[A]	ARG	O-C-N	-8.53	116.25	121.71
1	B	84[B]	ARG	O-C-N	-8.53	116.25	121.71
1	A	98	GLY	CA-C-O	-8.32	109.78	119.02
1	A	119[A]	ARG	CA-C-N	8.23	137.54	121.41
1	A	119[A]	ARG	C-N-CA	8.23	137.54	121.41
1	A	119[B]	ARG	CA-C-N	8.23	137.54	121.41
1	A	119[B]	ARG	C-N-CA	8.23	137.54	121.41
1	B	303	ASN	CA-C-N	8.22	127.95	119.56
1	B	303	ASN	C-N-CA	8.22	127.95	119.56
1	B	107[A]	GLU	CA-C-N	8.18	137.43	121.41
1	B	107[A]	GLU	C-N-CA	8.18	137.43	121.41
1	B	107[B]	GLU	CA-C-N	8.18	137.43	121.41
1	B	107[B]	GLU	C-N-CA	8.18	137.43	121.41
1	A	20	PRO	N-CA-CB	8.12	110.41	103.35
1	B	174	GLY	N-CA-C	8.08	121.87	112.50
1	B	327	VAL	O-C-N	7.91	125.48	120.42
1	A	220	GLY	O-C-N	-7.69	115.66	123.35
1	B	359	ASP	CA-CB-CG	7.58	120.18	112.60
1	B	134	LYS	CG-CD-CE	7.49	128.52	111.30
1	A	47	ARG	NE-CZ-NH2	-7.44	112.50	119.20
1	B	163	SER	CA-C-N	7.42	129.11	119.84
1	B	163	SER	C-N-CA	7.42	129.11	119.84
1	A	359	ASP	CA-CB-CG	-7.36	105.24	112.60
1	B	323	SER	CA-C-O	-7.34	113.14	120.70
1	B	322	LYS	N-CA-C	-7.28	99.03	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	PRO	N-CA-CB	7.19	109.61	103.35
1	B	134	LYS	O-C-N	7.14	126.95	121.88
1	A	292	GLY	CA-C-N	-7.11	117.47	122.59
1	A	292	GLY	C-N-CA	-7.11	117.47	122.59
1	A	20	PRO	CB-CA-C	-7.09	102.15	111.23
1	A	322	LYS	CA-C-O	6.94	128.44	120.60
1	B	8	LYS	CA-CB-CG	6.91	127.92	114.10
1	A	322	LYS	O-C-N	-6.91	113.84	122.82
1	A	94[A]	ILE	N-CA-C	-6.91	99.39	107.61
1	A	94[B]	ILE	N-CA-C	-6.91	99.39	107.61
1	B	107[A]	GLU	O-C-N	-6.88	113.14	122.36
1	B	107[B]	GLU	O-C-N	-6.88	113.14	122.36
1	A	238[A]	GLU	CA-C-O	-6.86	113.35	120.89
1	A	238[B]	GLU	CA-C-O	-6.86	113.35	120.89
1	B	160	ASP	CA-CB-CG	6.85	119.45	112.60
1	B	367	ILE	N-CA-C	-6.84	95.12	109.34
1	A	297	SER	CA-C-O	6.81	129.74	121.84
1	B	120	GLY	O-C-N	-6.70	116.47	122.57
1	A	323	SER	CA-C-O	-6.69	113.74	120.90
1	A	323	SER	O-C-N	6.67	129.03	122.09
1	A	300	LEU	N-CA-CB	-6.63	99.49	110.23
1	A	94[A]	ILE	CB-CA-C	6.59	116.52	110.13
1	A	94[B]	ILE	CB-CA-C	6.59	116.52	110.13
1	A	224	ASN	CA-CB-CG	-6.58	106.02	112.60
1	A	322	LYS	N-CA-C	-6.55	98.51	108.67
1	A	135	PRO	N-CA-CB	6.55	109.43	103.34
1	B	314	LYS	CA-C-N	-6.54	116.33	121.82
1	B	314	LYS	C-N-CA	-6.54	116.33	121.82
1	B	349	LEU	O-C-N	-6.47	117.57	121.71
1	B	365	LYS	N-CA-C	6.47	120.91	112.89
1	B	163	SER	N-CA-C	6.46	117.85	109.64
1	B	135	PRO	O-C-N	-6.45	115.12	123.06
1	B	119[A]	ARG	O-C-N	-6.41	114.44	122.83
1	B	119[B]	ARG	O-C-N	-6.41	114.44	122.83
1	A	311	ARG	NE-CZ-NH1	6.40	127.90	121.50
1	A	241	ASN	CA-C-N	6.36	126.85	119.47
1	A	241	ASN	C-N-CA	6.36	126.85	119.47
1	B	248	PRO	N-CA-CB	6.32	109.21	103.33
1	B	114	ASN	CA-C-O	6.28	128.10	121.19
1	A	228	PHE	N-CA-C	6.25	118.18	111.36
1	A	358	PHE	CA-C-O	-6.24	113.81	120.42
1	B	134	LYS	CD-CE-NZ	6.22	131.81	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	LYS	CA-C-N	6.21	126.18	119.78
1	A	19	LYS	C-N-CA	6.21	126.18	119.78
1	A	99	LYS	N-CA-CB	-6.20	102.33	110.88
1	B	327	VAL	CA-C-O	-6.19	114.54	118.69
1	A	88	LYS	CA-C-O	6.12	128.03	121.05
1	A	109	ASN	O-C-N	-6.08	115.60	122.23
1	A	200	GLY	O-C-N	-6.07	117.40	122.92
1	B	74	GLU	CA-C-O	-6.07	112.59	120.00
1	A	362	ARG	NE-CZ-NH2	-6.03	113.78	119.20
1	B	303	ASN	O-C-N	-6.02	116.35	121.23
1	B	155	SER	CA-C-N	-6.02	114.04	122.71
1	B	155	SER	C-N-CA	-6.02	114.04	122.71
1	B	203	GLY	O-C-N	5.99	127.94	122.19
1	B	175	PHE	CA-CB-CG	-5.99	107.81	113.80
1	A	200	GLY	CA-C-O	5.97	128.89	122.03
1	B	163	SER	O-C-N	-5.96	115.16	121.30
1	A	243	GLN	OE1-CD-NE2	-5.94	116.66	122.60
1	A	175	PHE	CA-CB-CG	-5.94	107.86	113.80
1	A	255	GLU	CA-CB-CG	5.91	125.92	114.10
1	B	323	SER	O-C-N	5.91	128.47	122.09
1	A	297	SER	N-CA-C	5.91	119.54	111.39
1	A	298	GLN	CG-CD-NE2	-5.85	107.62	116.40
1	A	304	PRO	N-CA-CB	5.84	109.32	103.48
1	B	189	THR	CA-C-O	5.84	128.78	121.66
1	A	34	HIS	CA-CB-CG	-5.81	107.99	113.80
1	A	296	ASP	O-C-N	5.79	129.99	122.87
1	B	303	ASN	OD1-CG-ND2	5.78	128.38	122.60
1	B	325	ASP	CB-CA-C	-5.78	101.02	110.85
1	A	89	VAL	CA-C-N	-5.78	118.31	123.33
1	A	89	VAL	C-N-CA	-5.78	118.31	123.33
1	B	314	LYS	CA-C-O	-5.77	115.09	121.33
1	B	361	LEU	O-C-N	5.75	127.99	122.07
1	A	315	GLY	O-C-N	5.74	128.59	123.60
1	A	228	PHE	CA-C-N	-5.72	112.61	120.28
1	A	228	PHE	C-N-CA	-5.72	112.61	120.28
1	A	128	ARG	CG-CD-NE	-5.70	99.45	112.00
1	A	291	VAL	N-CA-C	-5.70	107.28	111.90
1	B	217	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	B	335	MET	CA-C-O	-5.66	113.70	120.10
1	B	296	ASP	N-CA-C	5.64	118.19	110.24
1	B	164	PRO	N-CA-CB	5.63	109.16	103.25
1	A	36	VAL	CA-C-O	-5.62	114.41	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	GLU	CB-CA-C	-5.61	98.28	109.79
1	A	129	PHE	O-C-N	5.61	130.52	123.23
1	B	81	THR	CB-CA-C	-5.61	100.07	109.27
1	B	105	HIS	CE1-NE2-CD2	5.60	114.60	109.00
1	A	164	PRO	N-CA-CB	5.60	106.06	102.92
1	A	298	GLN	O-C-N	5.57	130.15	123.36
1	B	37	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	A	111	CYS	CA-C-O	-5.55	115.04	121.15
1	A	324	LYS	CA-C-O	-5.54	113.60	119.97
1	B	304	PRO	N-CA-CB	5.51	108.99	103.48
1	A	327	VAL	N-CA-CB	-5.51	107.03	110.50
1	B	283	GLU	CA-C-O	-5.50	113.88	120.10
1	B	145	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	238[A]	GLU	O-C-N	5.49	129.63	123.48
1	A	238[B]	GLU	O-C-N	5.49	129.63	123.48
1	A	321	PHE	CA-CB-CG	5.48	119.28	113.80
1	B	88	LYS	CA-C-N	-5.45	115.38	122.51
1	B	88	LYS	C-N-CA	-5.45	115.38	122.51
1	A	299[A]	ASN	CB-CG-ND2	5.43	124.55	116.40
1	A	299[B]	ASN	CB-CG-ND2	5.43	124.55	116.40
1	B	282	GLN	CB-CA-C	5.42	118.36	109.90
1	A	94[A]	ILE	N-CA-CB	5.41	118.11	112.37
1	A	94[B]	ILE	N-CA-CB	5.41	118.11	112.37
1	A	303	ASN	CB-CG-ND2	-5.40	108.30	116.40
1	A	293	VAL	O-C-N	5.39	126.26	121.57
1	B	297	SER	N-CA-C	5.39	119.02	111.90
1	A	98	GLY	N-CA-C	-5.39	108.19	115.36
1	B	313	TRP	O-C-N	-5.38	116.89	123.30
1	B	241	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	3	ALA	CA-C-O	-5.34	115.14	120.96
1	A	209	GLY	CA-C-O	-5.34	115.00	120.66
1	A	358	PHE	O-C-N	5.33	128.23	122.15
1	B	283	GLU	CB-CG-CD	5.33	121.65	112.60
1	B	238[A]	GLU	CA-C-O	-5.32	115.54	121.23
1	B	238[B]	GLU	CA-C-O	-5.32	115.54	121.23
1	A	163[A]	SER	CA-C-O	5.30	126.10	120.64
1	A	163[B]	SER	CA-C-O	5.30	126.10	120.64
1	B	150	VAL	O-C-N	5.30	128.92	123.20
1	A	238[A]	GLU	CG-CD-OE2	-5.29	106.24	118.40
1	A	238[B]	GLU	CG-CD-OE2	-5.29	106.24	118.40
1	A	1	SER	O-C-N	-5.26	114.59	123.00
1	B	2	THR	N-CA-CB	5.25	118.36	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	PRO	N-CA-CB	-5.25	97.98	103.08
1	B	94[A]	ILE	CB-CA-C	5.24	115.45	110.16
1	B	94[B]	ILE	CB-CA-C	5.24	115.45	110.16
1	B	197	PHE	CA-CB-CG	5.24	119.04	113.80
1	B	320	GLY	CA-C-O	-5.23	113.22	119.02
1	A	291	VAL	O-C-N	-5.22	116.64	122.07
1	A	333	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	326	SER	CA-C-N	-5.20	116.96	120.24
1	A	326	SER	C-N-CA	-5.20	116.96	120.24
1	B	182	ALA	O-C-N	5.19	128.45	122.17
1	A	56	THR	N-CA-C	-5.15	105.67	111.28
1	B	85	PRO	N-CA-CB	5.15	107.82	103.19
1	B	2	THR	N-CA-C	-5.14	107.06	113.38
1	A	298	GLN	CA-C-N	-5.13	113.91	122.64
1	A	298	GLN	C-N-CA	-5.13	113.91	122.64
1	B	217	ARG	CA-C-O	-5.12	114.63	120.32
1	A	47	ARG	CD-NE-CZ	-5.12	117.23	124.40
1	A	352	GLU	O-C-N	5.10	129.02	122.39
1	B	24	GLU	CA-CB-CG	5.08	124.26	114.10
1	A	203	GLY	O-C-N	5.08	127.06	122.19
1	A	217	ARG	CA-C-O	-5.07	114.04	120.28
1	A	216	ALA	CA-C-O	5.07	125.77	119.79
1	B	163	SER	CB-CA-C	-5.05	101.53	109.52
1	A	313	TRP	O-C-N	-5.05	117.29	123.30
1	A	84[A]	ARG	CA-C-N	5.05	125.33	119.93
1	A	84[A]	ARG	C-N-CA	5.05	125.33	119.93
1	A	84[B]	ARG	CA-C-N	5.05	125.33	119.93
1	A	84[B]	ARG	C-N-CA	5.05	125.33	119.93
1	B	38	ILE	N-CA-C	5.04	115.17	108.11
1	B	37	ARG	CD-NE-CZ	-5.03	117.36	124.40
1	A	144	THR	CA-C-N	-5.00	114.58	122.08
1	A	144	THR	C-N-CA	-5.00	114.58	122.08
1	A	240	VAL	O-C-N	-5.00	117.75	123.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	SER	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	SER	Mainchain
1	A	107[B]	GLU	Mainchain
1	B	107[B]	GLU	Mainchain

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	2904	0	3002	44	0
1	B	2875	0	2966	40	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	26	1	0
3	B	44	0	26	0	0
4	A	29	0	39	1	0
4	B	29	0	39	0	0
5	A	505	0	0	16	0
5	B	505	0	0	15	0
All	All	6939	0	6098	85	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 7.

All (85) 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:190[B]:GLN:HE21	1:A:214:GLY:HA3	1.21	1.00
1:A:16[A]:GLU:HG3	1:A:19:LYS:HG3	1.45	0.99
1:A:193:THR:HB	5:A:1795:HOH:O	1.62	0.97
1:A:348[A]:VAL:HG13	5:A:1461:HOH:O	1.66	0.95
1:A:372[A]:THR:HG23	5:A:1461:HOH:O	1.78	0.83
1:A:265:PHE:CD2	1:A:289[B]:VAL:CG1	2.62	0.82
1:B:151[A]:VAL:CG2	1:B:156[A]:VAL:HG12	2.09	0.82
1:B:15:TRP:HZ3	1:B:134:LYS:HE3	1.44	0.81
1:A:190[B]:GLN:NE2	1:A:214:GLY:HA3	1.96	0.80
1:B:372[A]:THR:HG22	5:B:1451:HOH:O	1.81	0.79
1:A:193:THR:HG23	5:A:1456:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372[A]:THR:HG22	5:A:1801:HOH:O	1.84	0.77
1:B:15:TRP:CZ3	1:B:134:LYS:HE3	2.21	0.75
1:A:130[B]:THR:HG23	5:A:1359:HOH:O	1.87	0.74
1:A:16[A]:GLU:HG3	1:A:19:LYS:CG	2.17	0.73
1:B:282:GLN:NE2	1:B:284:ALA:H	1.87	0.72
1:A:16[A]:GLU:CG	1:A:19:LYS:HG3	2.20	0.71
1:A:270[A]:ARG:HH22	1:A:295:PRO:HB3	1.55	0.70
1:B:151[A]:VAL:HG21	1:B:156[A]:VAL:HG12	1.72	0.70
1:A:193:THR:HG21	5:A:1574:HOH:O	1.91	0.70
1:B:151[A]:VAL:HG23	1:B:156[A]:VAL:HG12	1.73	0.69
1:B:105:HIS:ND1	1:B:107[B]:GLU:O	2.26	0.68
1:B:282:GLN:HE22	1:B:284:ALA:H	1.42	0.67
1:B:372[A]:THR:HG23	5:B:1402:HOH:O	1.96	0.66
1:A:265:PHE:CD2	1:A:289[B]:VAL:HG12	2.32	0.65
1:B:151[A]:VAL:HG23	1:B:156[A]:VAL:CG1	2.27	0.65
1:A:94[B]:ILE:HD11	1:A:317:ILE:HG21	1.80	0.63
1:A:265:PHE:HD2	1:A:289[B]:VAL:CG1	2.12	0.62
1:A:270[A]:ARG:NH2	1:A:295:PRO:HG3	2.16	0.61
1:A:265:PHE:CD2	1:A:289[B]:VAL:HG11	2.38	0.58
1:A:193:THR:HG22	1:A:217:ARG:HB2	1.85	0.58
1:A:130[B]:THR:HG22	5:A:1620:HOH:O	2.03	0.58
1:B:329[A]:LYS:HD2	5:B:1658:HOH:O	2.03	0.57
1:B:350:PRO:HD2	1:B:353:LYS:HD2	1.87	0.56
1:B:151[A]:VAL:CG2	1:B:156[A]:VAL:CG1	2.81	0.55
1:B:3:ALA:O	1:B:5:LYS:HD2	2.07	0.55
1:A:32:LYS:HE3	5:A:1580:HOH:O	2.07	0.54
1:A:270[A]:ARG:NH2	1:A:295:PRO:CG	2.71	0.54
1:B:303:ASN:C	1:B:303:ASN:HD22	2.15	0.54
1:B:281[B]:CYS:HB3	1:B:286:GLY:HA3	1.91	0.53
1:B:104[A]:LYS:NZ	5:B:1384:HOH:O	2.37	0.52
1:A:166[B]:GLU:HG3	5:A:1801:HOH:O	2.09	0.52
1:B:43:ALA:HB1	5:B:1523:HOH:O	2.09	0.52
1:A:43:ALA:HB1	5:A:1486:HOH:O	2.10	0.51
1:A:130[B]:THR:HG21	5:A:1712:HOH:O	2.11	0.51
1:B:270[A]:ARG:NE	5:B:1432:HOH:O	2.44	0.51
1:B:84[B]:ARG:NH2	5:B:1744:HOH:O	2.44	0.49
1:B:117[B]:MET:CE	1:B:140:LEU:HD21	2.43	0.49
1:B:303:ASN:ND2	1:B:305:MET:H	2.11	0.48
1:B:356[B]:GLU:HG3	5:B:1435:HOH:O	2.12	0.48
1:A:270[A]:ARG:HH22	1:A:295:PRO:CB	2.23	0.48
1:B:83:VAL:HG12	1:B:158[A]:LYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:VAL:O	1:A:255:GLU:HG3	2.13	0.47
1:A:356[B]:GLU:HG3	5:A:1642:HOH:O	2.16	0.46
1:A:281[B]:CYS:HB3	1:A:286:GLY:HA3	1.97	0.46
1:B:39:LYS:HE2	5:B:1644:HOH:O	2.15	0.46
1:B:59:ALA:HB2	1:B:117[A]:MET:CE	2.46	0.46
1:B:282:GLN:HE22	1:B:284:ALA:HB3	1.81	0.45
1:B:365:LYS:HG3	5:B:1713:HOH:O	2.17	0.45
1:B:99[B]:LYS:HE3	5:B:1807:HOH:O	2.16	0.45
1:A:23[A]:ILE:HG22	5:A:1796:HOH:O	2.17	0.45
1:B:10:LYS:HG3	5:B:1626:HOH:O	2.17	0.45
1:A:16[A]:GLU:CD	1:A:19:LYS:HG3	2.42	0.44
4:A:1150:CHD:H211	4:A:1150:CHD:H231	1.72	0.44
1:B:270[A]:ARG:NH2	5:B:1389:HOH:O	2.51	0.43
1:B:282:GLN:HE22	1:B:284:ALA:N	2.14	0.43
1:B:117[B]:MET:HB2	1:B:118:PRO:HD3	2.01	0.43
1:A:27:GLU:HB2	1:A:130[B]:THR:OG1	2.19	0.43
1:B:303:ASN:C	1:B:303:ASN:ND2	2.77	0.42
1:A:117:MET:HB2	1:A:118:PRO:HD3	2.02	0.42
1:A:291:VAL:O	3:A:1100:NAD:H2N	2.20	0.42
1:B:40[B]:MET:HE3	1:B:149:THR:HG22	2.02	0.42
1:A:84[A]:ARG:NH2	5:A:1544:HOH:O	2.52	0.41
1:B:105:HIS:CE1	1:B:107[B]:GLU:O	2.73	0.41
1:A:42:ALA:HB2	5:A:1801:HOH:O	2.20	0.41
1:B:84[A]:ARG:NH2	5:B:1741:HOH:O	2.52	0.41
1:B:87:ASP:OD2	1:B:158[A]:LYS:HD3	2.21	0.41
1:B:119[A]:ARG:HG3	5:B:1377:HOH:O	2.20	0.41

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	401/373 (108%)	389 (97%)	11 (3%)	1 (0%)	43	25
1	B	398/373 (107%)	384 (96%)	14 (4%)	0	100	100
All	All	799/746 (107%)	773 (97%)	25 (3%)	1 (0%)	48	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ILE

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	334/304 (110%)	325 (97%)	9 (3%)	39	10
1	B	331/304 (109%)	322 (97%)	9 (3%)	39	10
All	All	665/608 (109%)	647 (97%)	18 (3%)	48	10

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	40[A]	MET
1	A	40[B]	MET
1	A	78	GLU
1	A	190[A]	GLN
1	A	190[B]	GLN
1	A	238[A]	GLU
1	A	238[B]	GLU
1	A	267	VAL
1	B	8	LYS
1	B	156[A]	VAL
1	B	156[B]	VAL
1	B	238[A]	GLU
1	B	238[B]	GLU
1	B	267	VAL

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Mol	Chain	Res	Type
1	B	270[A]	ARG
1	B	270[B]	ARG
1	B	303	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	HIS
1	B	243	GLN
1	B	258	ASN
1	B	282	GLN
1	B	298	GLN
1	B	299	ASN
1	B	303	ASN

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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
4	CHD	A	1150	2	32,32,32	1.53	7 (21%)	51,51,51	1.89	11 (21%)
3	NAD	B	1200	-	46,48,48	2.24	15 (32%)	64,73,73	2.18	17 (26%)
4	CHD	B	1250	2	32,32,32	1.39	2 (6%)	51,51,51	2.15	13 (25%)
3	NAD	A	1100	-	46,48,48	2.18	11 (23%)	64,73,73	2.39	18 (28%)

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	CHD	A	1150	2	-	2/9/74/74	0/4/4/4
3	NAD	B	1200	-	-	4/30/62/62	0/5/5/5
4	CHD	B	1250	2	-	1/9/74/74	0/4/4/4
3	NAD	A	1100	-	-	4/30/62/62	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1200	NAD	PN-O3	6.45	1.66	1.59
3	A	1100	NAD	C4N-C3N	6.34	1.49	1.39
3	B	1200	NAD	C2N-N1N	6.16	1.41	1.35
3	A	1100	NAD	O7N-C7N	5.05	1.33	1.24
3	A	1100	NAD	PA-O3	-4.64	1.54	1.59
4	A	1150	CHD	O25-C24	4.55	1.37	1.22
3	A	1100	NAD	C2A-N3A	4.26	1.41	1.33
3	B	1200	NAD	C4N-C3N	4.08	1.45	1.39
4	B	1250	CHD	O25-C24	3.82	1.34	1.22
3	A	1100	NAD	C5A-C4A	3.69	1.45	1.39
4	B	1250	CHD	O12-C12	3.44	1.49	1.43
3	A	1100	NAD	C3N-C7N	-3.43	1.45	1.50
3	B	1200	NAD	C5A-N7A	-3.40	1.32	1.39
3	B	1200	NAD	C2A-N3A	3.40	1.40	1.33
3	B	1200	NAD	C5A-C4A	3.32	1.45	1.39
3	A	1100	NAD	C5A-C6A	3.29	1.50	1.41
3	A	1100	NAD	PN-O3	3.29	1.63	1.59
3	A	1100	NAD	C5A-N7A	-3.26	1.33	1.39
3	B	1200	NAD	O4D-C4D	3.20	1.52	1.45
3	A	1100	NAD	O4D-C1D	3.20	1.45	1.40
3	B	1200	NAD	C3N-C7N	3.14	1.55	1.50
3	B	1200	NAD	O4D-C1D	2.98	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1150	CHD	O26-C24	-2.75	1.21	1.30
3	B	1200	NAD	C2N-C3N	-2.72	1.34	1.39
4	A	1150	CHD	C16-C17	2.38	1.59	1.54
4	A	1150	CHD	O12-C12	2.34	1.47	1.43
3	B	1200	NAD	C7N-N7N	2.27	1.37	1.33
4	A	1150	CHD	C10-C5	-2.24	1.51	1.55
3	B	1200	NAD	PN-O1N	-2.17	1.43	1.50
3	A	1100	NAD	O4D-C4D	2.17	1.49	1.45
4	A	1150	CHD	O7-C7	2.08	1.47	1.43
3	B	1200	NAD	C4A-N9A	2.07	1.42	1.37
3	B	1200	NAD	C3B-C4B	2.06	1.58	1.53
4	A	1150	CHD	C6-C5	2.02	1.57	1.53
3	B	1200	NAD	C5A-C6A	2.02	1.46	1.41

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1200	NAD	C2N-C3N-C4N	7.36	126.82	118.26
3	B	1200	NAD	C5N-C4N-C3N	-7.21	113.28	120.36
3	A	1100	NAD	C2A-N1A-C6A	7.12	130.43	118.73
3	A	1100	NAD	N3A-C2A-N1A	-6.88	118.16	128.58
3	A	1100	NAD	C6N-N1N-C2N	6.65	127.53	121.88
3	A	1100	NAD	C3N-C7N-N7N	6.64	125.91	117.74
3	B	1200	NAD	N3A-C2A-N1A	-5.75	119.87	128.58
3	A	1100	NAD	O7N-C7N-N7N	-5.51	114.66	122.62
4	B	1250	CHD	C15-C14-C8	-5.45	110.89	118.36
3	B	1200	NAD	C2A-N1A-C6A	5.13	127.16	118.73
4	A	1150	CHD	O12-C12-C13	-4.86	102.81	111.02
3	A	1100	NAD	N6A-C6A-N1A	4.85	129.17	118.38
3	A	1100	NAD	C5N-C4N-C3N	-4.83	115.61	120.36
4	B	1250	CHD	O12-C12-C13	-4.72	103.06	111.02
4	B	1250	CHD	C18-C13-C12	-4.67	104.38	109.06
4	B	1250	CHD	O26-C24-O25	-4.55	111.63	123.33
4	A	1150	CHD	O26-C24-C23	4.24	127.40	114.00
4	A	1150	CHD	C17-C13-C12	3.81	121.10	117.67
4	B	1250	CHD	C1-C2-C3	-3.80	105.45	110.48
4	A	1150	CHD	C9-C8-C7	-3.77	107.11	111.86
4	B	1250	CHD	C23-C22-C20	3.71	121.39	114.46
4	B	1250	CHD	C19-C10-C1	-3.70	102.42	108.31
3	B	1200	NAD	C6N-N1N-C2N	3.51	124.87	121.88
3	B	1200	NAD	C6N-C5N-C4N	3.49	124.48	119.45
3	A	1100	NAD	C2N-C3N-C4N	3.40	122.22	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1200	NAD	C5A-N7A-C8A	3.22	108.51	103.45
4	A	1150	CHD	C11-C9-C10	-3.17	110.48	113.70
4	B	1250	CHD	C9-C8-C7	-3.15	107.90	111.86
4	A	1150	CHD	C17-C13-C14	3.11	103.23	100.11
3	A	1100	NAD	C2N-N1N-C1D	-3.07	112.35	119.13
4	A	1150	CHD	C1-C10-C5	3.04	112.11	107.75
3	A	1100	NAD	C5A-C6A-N6A	-2.94	116.00	123.29
4	A	1150	CHD	O25-C24-C23	-2.93	113.79	123.09
3	B	1200	NAD	C6A-C5A-N7A	2.89	137.66	132.09
3	B	1200	NAD	C1B-N9A-C8A	2.89	133.51	127.09
4	B	1250	CHD	C14-C13-C12	-2.79	104.86	107.42
4	A	1150	CHD	C18-C13-C12	-2.76	106.29	109.06
4	A	1150	CHD	C15-C14-C8	-2.69	114.67	118.36
3	B	1200	NAD	O7N-C7N-C3N	-2.60	116.41	119.60
3	A	1100	NAD	C3B-C2B-C1B	-2.60	96.55	101.46
3	B	1200	NAD	N6A-C6A-N1A	2.57	124.10	118.38
4	A	1150	CHD	C19-C10-C1	-2.55	104.25	108.31
3	B	1200	NAD	C4A-N9A-C8A	-2.52	103.09	105.74
4	B	1250	CHD	C4-C5-C10	-2.48	110.02	112.66
3	B	1200	NAD	C2N-C3N-C7N	-2.43	112.46	119.46
3	B	1200	NAD	C5N-C6N-N1N	-2.42	117.08	120.38
3	A	1100	NAD	C6N-C5N-C4N	2.38	122.88	119.45
3	B	1200	NAD	C6A-C5A-C4A	-2.38	113.93	117.18
3	A	1100	NAD	C6A-C5A-C4A	-2.35	113.96	117.18
4	B	1250	CHD	C6-C5-C10	-2.35	110.16	112.66
4	B	1250	CHD	C6-C7-C8	-2.29	109.00	111.50
3	A	1100	NAD	C5N-C6N-N1N	-2.21	117.37	120.38
3	A	1100	NAD	O3B-C3B-C2B	2.16	118.75	111.82
3	A	1100	NAD	C2B-C3B-C4B	2.12	106.70	102.61
3	A	1100	NAD	C4B-O4B-C1B	-2.08	104.87	109.47
4	B	1250	CHD	O26-C24-C23	2.07	120.53	114.00
3	A	1100	NAD	O4B-C4B-C5B	-2.06	102.74	109.33
3	B	1200	NAD	O2A-PA-O3	2.03	112.76	107.27
3	B	1200	NAD	C5A-C6A-N6A	-2.02	118.28	123.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1100	NAD	O4D-C1D-N1N-C2N
3	A	1100	NAD	O4D-C1D-N1N-C6N
3	A	1100	NAD	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	A	1100	NAD	C2D-C1D-N1N-C6N
3	B	1200	NAD	O4D-C1D-N1N-C2N
3	B	1200	NAD	O4D-C1D-N1N-C6N
3	B	1200	NAD	C2D-C1D-N1N-C2N
3	B	1200	NAD	C2D-C1D-N1N-C6N
4	A	1150	CHD	C21-C20-C22-C23
4	A	1150	CHD	C20-C22-C23-C24
4	B	1250	CHD	C22-C23-C24-O26

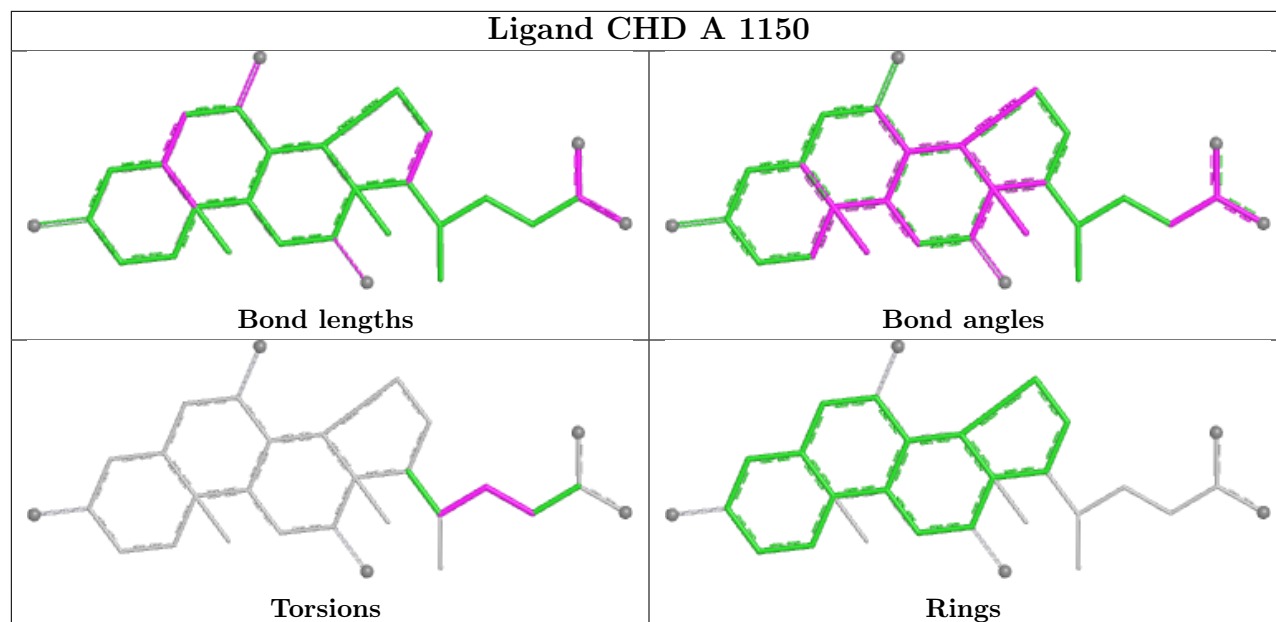
There are no ring outliers.

2 monomers are involved in 2 short contacts:

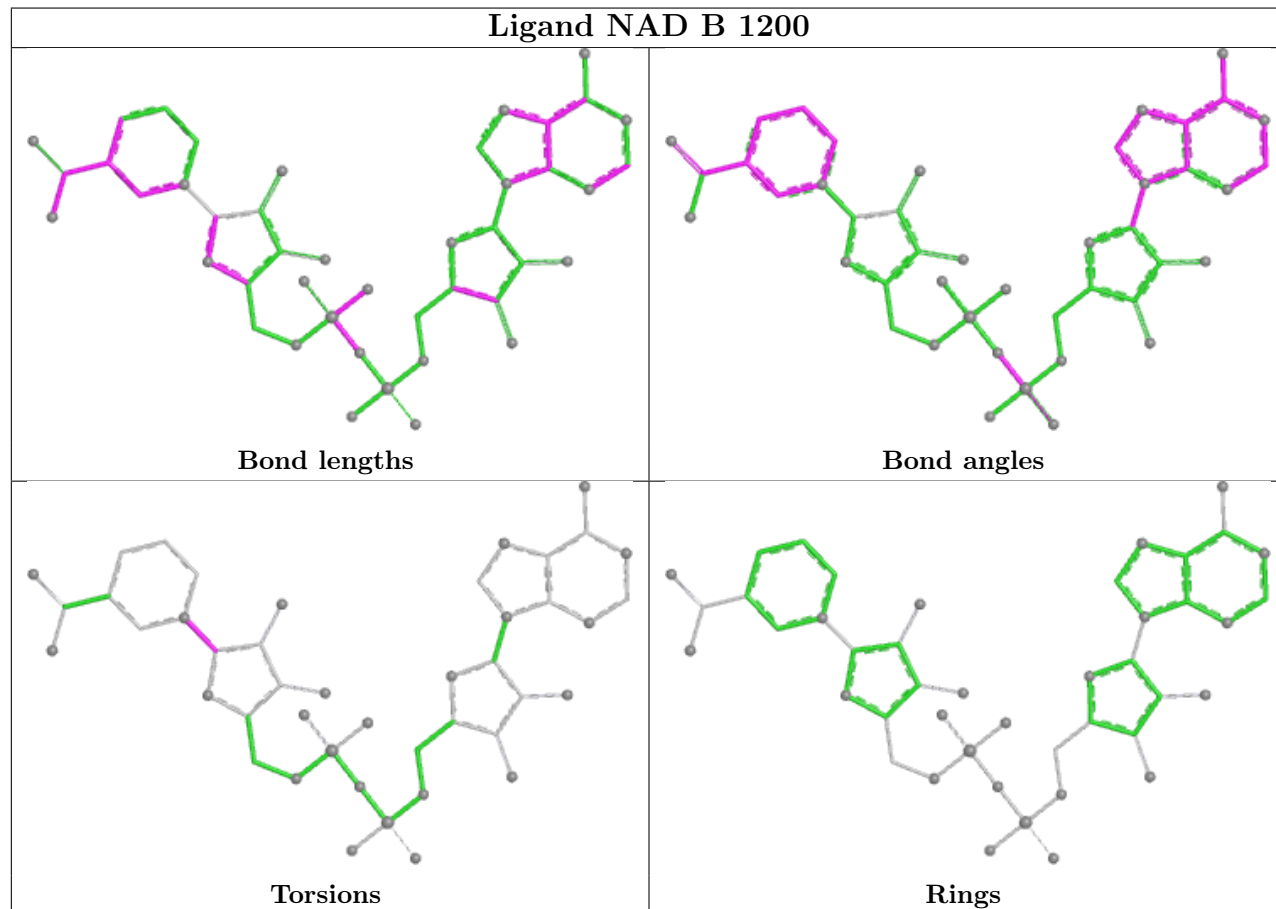
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1150	CHD	1	0
3	A	1100	NAD	1	0

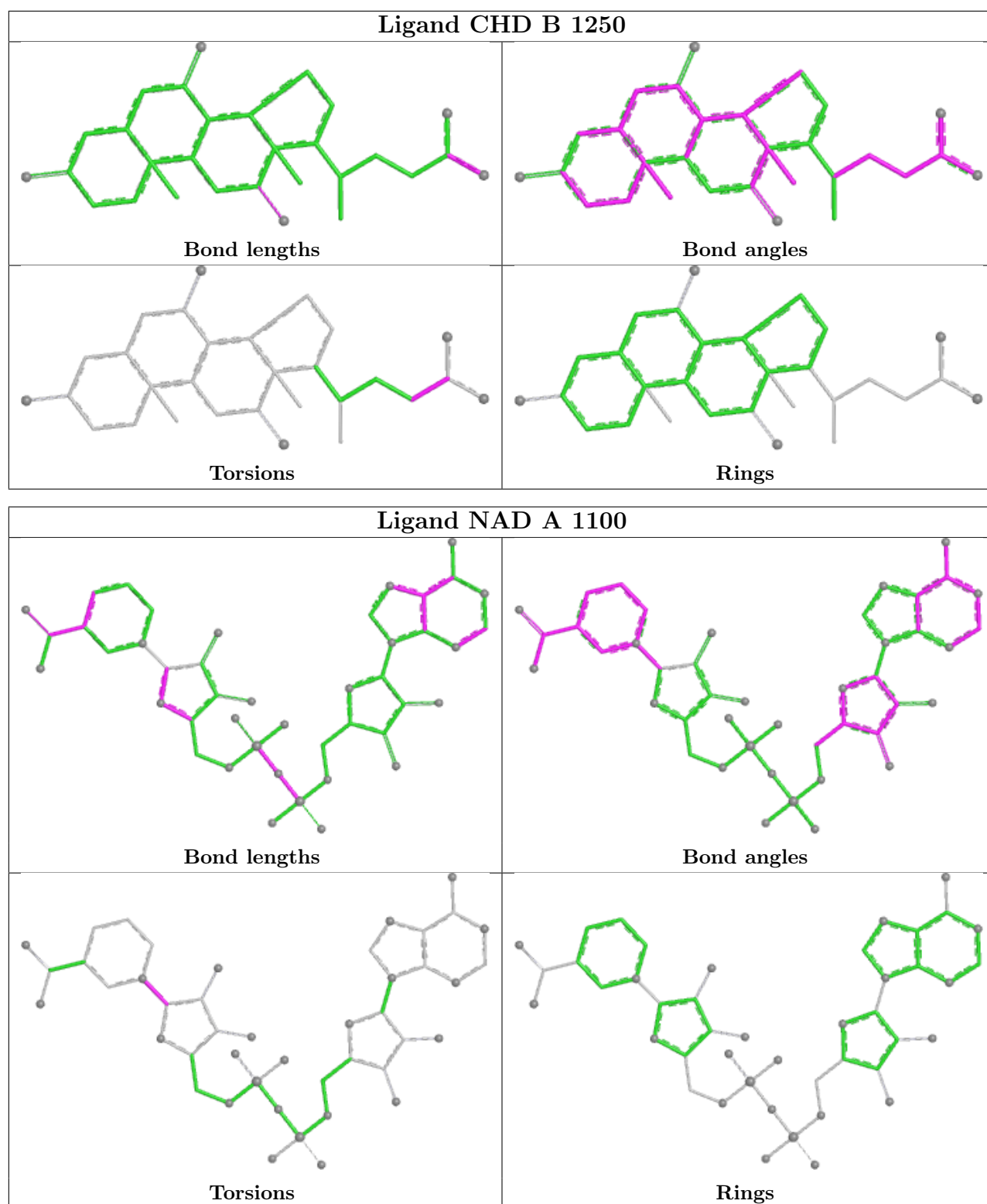
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand CHD A 1150



Ligand NAD B 1200





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	373/373 (100%)	-0.59	1 (0%) 90 92	7, 12, 19, 37	35 (9%)
1	B	373/373 (100%)	-0.43	1 (0%) 90 92	7, 13, 24, 44	27 (7%)
All	All	746/746 (100%)	-0.51	2 (0%) 90 92	7, 12, 21, 44	62 (8%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107[A]	GLU	3.3
1	A	255	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(Å ²)	Q<0.9
4	CHD	A	1150	29/29	0.94	0.06	12,15,21,28	0
4	CHD	B	1250	29/29	0.95	0.07	11,14,22,28	0
3	NAD	A	1100	44/44	0.99	0.04	7,9,14,18	0

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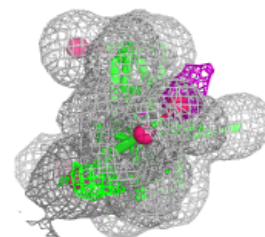
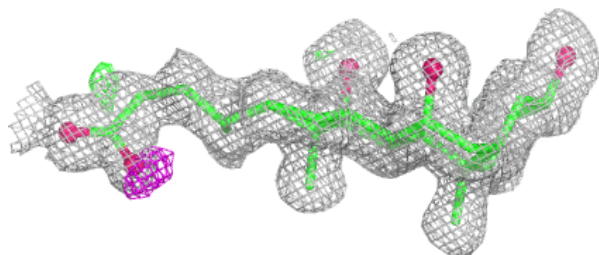
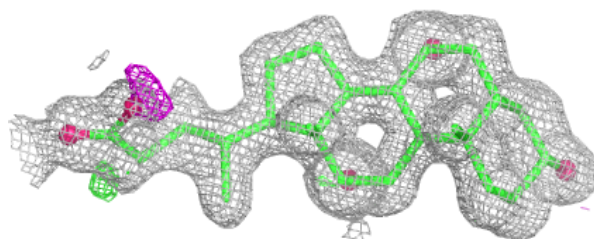
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAD	B	1200	44/44	0.99	0.04	8,10,13,20	0
2	ZN	A	1300	1/1	1.00	0.01	10,10,10,10	0
2	ZN	A	1301	1/1	1.00	0.01	12,12,12,12	0
2	ZN	B	1302	1/1	1.00	0.01	11,11,11,11	0
2	ZN	B	1303	1/1	1.00	0.01	11,11,11,11	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.

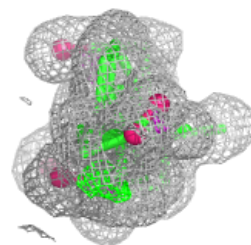
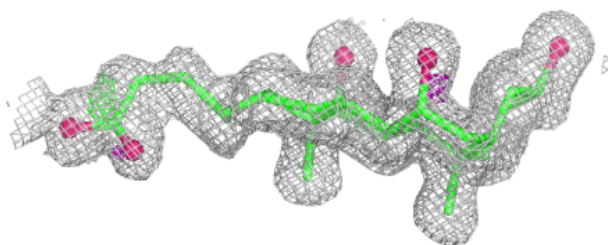
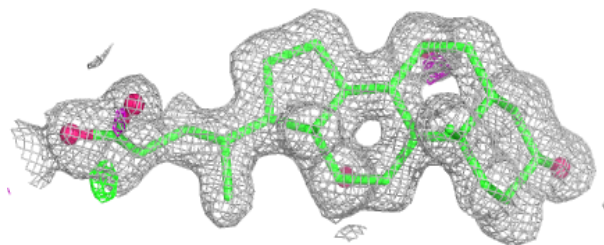
Electron density around CHD A 1150:

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

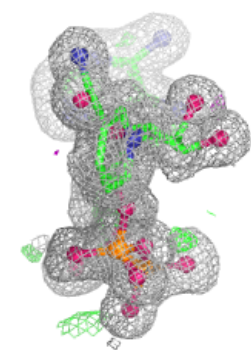
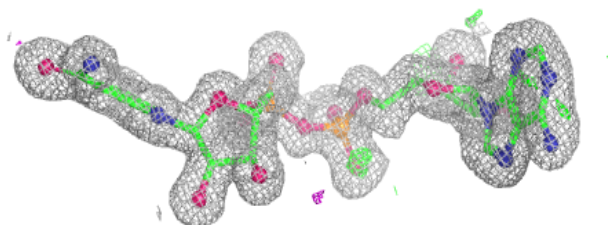
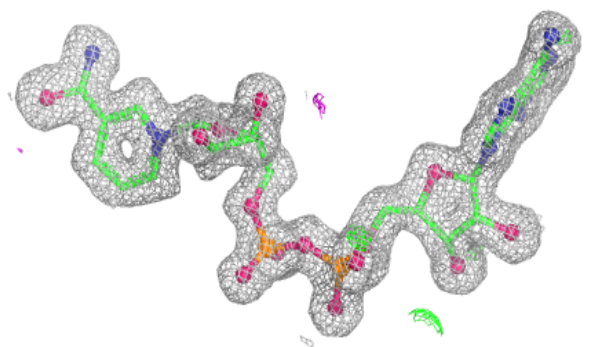


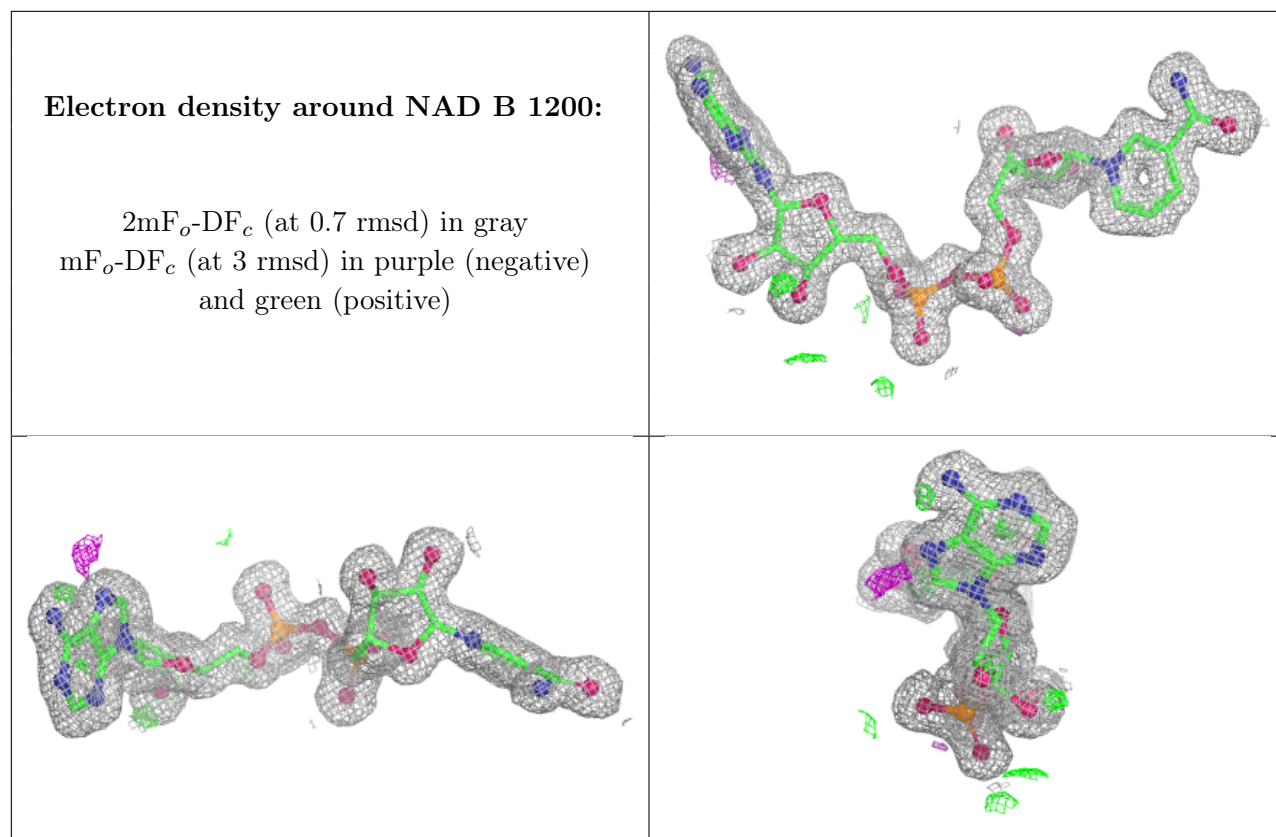
Electron density around CHD B 1250:

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

**Electron density around NAD A 1100:**

$2mF_o-DF_c$ (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.