



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:18 AM UTC

PDB ID : 3GVP / pdb_00003gvp
Title : Human SAHH-like domain of human adenosylhomocysteinase 3
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Deposited on : 2009-03-31
Resolution : 2.25 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

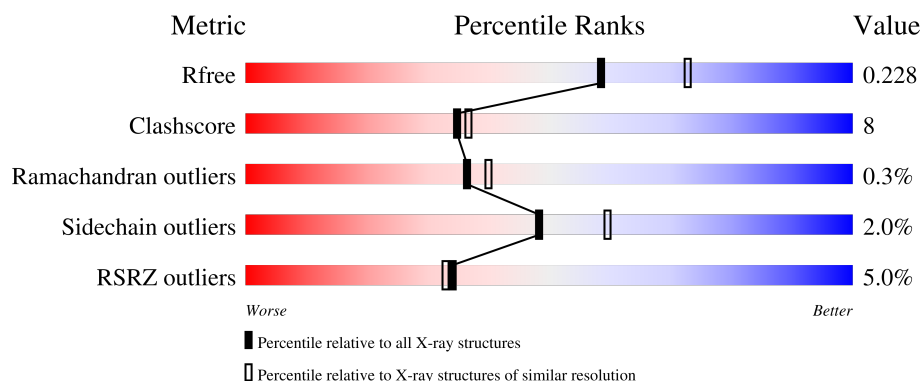
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	435	% 88% 11%
1	B	435	2% 90% 10%
1	C	435	2% 89% 9%

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	435	14% 83% 14% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14173 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 Adenosylhomocysteinase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	2	0
			3368	2126	584	626	32			
1	B	432	Total	C	N	O	S	0	1	0
			3337	2107	574	624	32			
1	C	432	Total	C	N	O	S	0	1	0
			3367	2125	584	627	31			
1	D	431	Total	C	N	O	S	0	3	0
			3343	2114	574	624	31			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q96HN2
A	-1	MET	-	expression tag	UNP Q96HN2
B	-2	SER	-	expression tag	UNP Q96HN2
B	-1	MET	-	expression tag	UNP Q96HN2
C	173	SER	-	expression tag	UNP Q96HN2
C	174	MET	-	expression tag	UNP Q96HN2
D	173	SER	-	expression tag	UNP Q96HN2
D	174	MET	-	expression tag	UNP Q96HN2

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

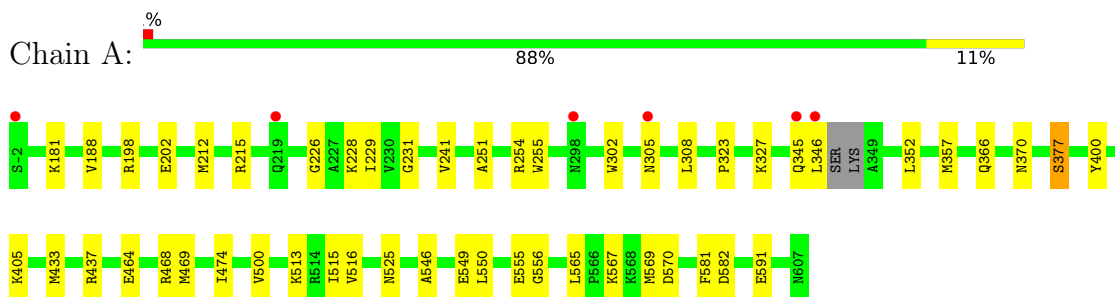
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	157	Total	O	0	0
			157	157		
3	B	117	Total	O	0	0
			117	117		
3	C	181	Total	O	0	0
			181	181		
3	D	127	Total	O	0	0
			127	127		

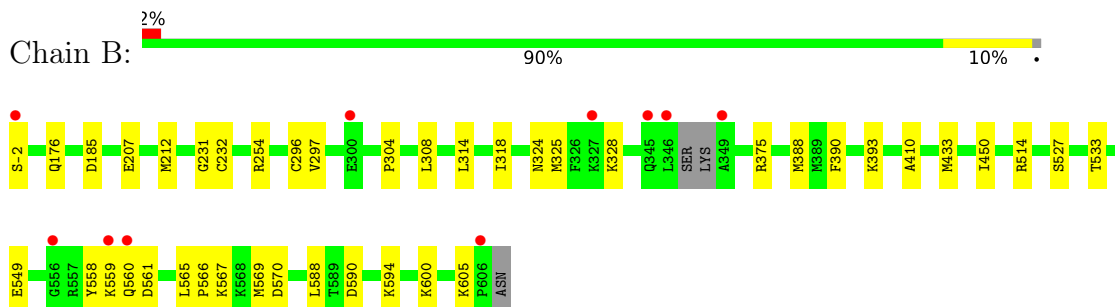
3 Residue-property plots [i](#)

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.

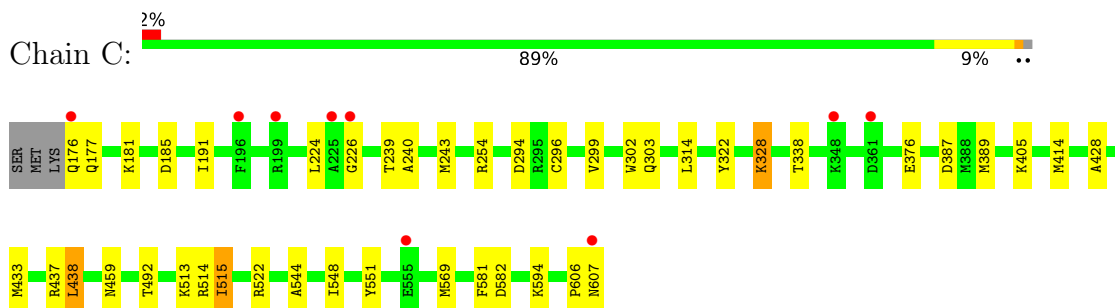
- Molecule 1: Adenosylhomocysteinase 3



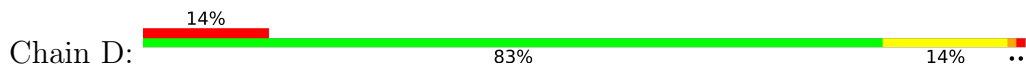
- Molecule 1: Adenosylhomocysteinase 3

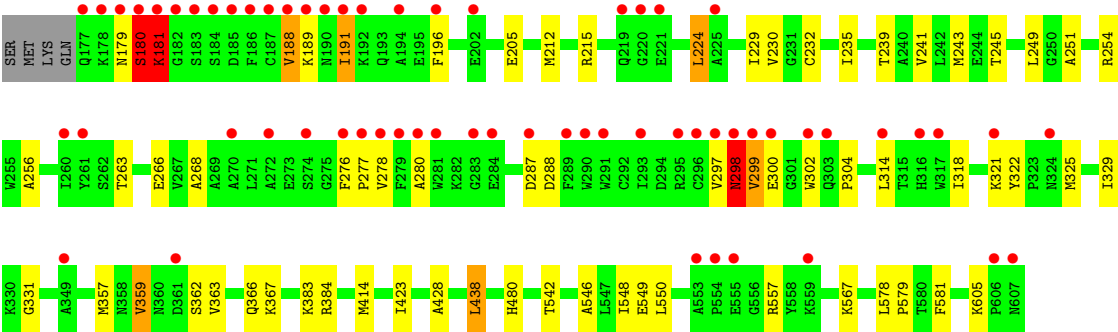


- Molecule 1: Adenosylhomocysteinase 3



- Molecule 1: Adenosylhomocysteinase 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	164.19Å 164.19Å 184.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.25 19.91 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.91-2.25) 99.8 (19.91-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.65 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.226 0.187 , 0.228	Depositor DCC
R_{free} test set	1204 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14173	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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	0.88	0/3435	0.92	1/4647 (0.0%)
1	B	0.79	0/3401	0.84	0/4607
1	C	0.91	0/3429	0.91	0/4638
1	D	0.81	0/3415	0.89	3/4625 (0.1%)
All	All	0.85	0/13680	0.89	4/18517 (0.0%)

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	D	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	557	ARG	N-CA-C	6.69	118.23	111.07
1	A	377	SER	CB-CA-C	-5.67	101.97	110.88
1	D	298	ASN	CA-C-N	5.19	131.04	121.70
1	D	298	ASN	C-N-CA	5.19	131.04	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	180	SER	Peptide
1	D	298	ASN	Peptide

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	3368	0	3371	54	0
1	B	3337	0	3320	38	0
1	C	3367	0	3380	49	0
1	D	3343	0	3335	84	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	157	0	0	8	0
3	B	117	0	0	2	0
3	C	181	0	0	7	0
3	D	127	0	0	5	0
All	All	14173	0	13510	204	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 8.

All (204) 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:D:363:VAL:CG1	1:D:367:LYS:HZ2	1.47	1.28
1:D:363:VAL:CG1	1:D:367:LYS:NZ	2.02	1.23
1:D:245:THR:O	1:D:249:LEU:HD23	1.41	1.20
1:C:239:THR:HG22	1:C:243:MET:CE	1.72	1.18
1:C:239:THR:CG2	1:C:243:MET:HE2	1.76	1.16
1:D:363:VAL:HG12	1:D:367:LYS:HZ2	1.09	1.16
1:A:468[A]:ARG:NH2	3:A:730:HOH:O	1.80	1.14
1:A:569:MET:HE1	3:A:662:HOH:O	1.44	1.13
1:C:176:GLN:CB	1:C:191:ILE:HG22	1.79	1.12
1:D:239:THR:HG22	1:D:243:MET:HE3	1.18	1.11
1:D:239:THR:HG22	1:D:243:MET:CE	1.85	1.05
1:C:338:THR:HG21	3:C:655:HOH:O	1.55	1.04
1:A:468[A]:ARG:NH1	3:A:731:HOH:O	1.90	1.02
1:D:297:VAL:CG1	1:D:325:MET:HE1	1.89	1.02
1:B:565:LEU:HD11	1:B:569:MET:HE3	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:THR:O	1:D:249:LEU:CD2	2.08	1.00
1:D:205:GLU:HG2	1:D:212:MET:CE	1.98	0.94
1:A:591:GLU:OE1	3:A:720:HOH:O	1.85	0.94
1:D:205:GLU:CB	1:D:212:MET:HE3	1.99	0.92
1:A:581:PHE:CZ	1:C:433:MET:HE3	2.03	0.92
1:B:566:PRO:HD2	1:B:569:MET:HE2	1.51	0.91
1:D:363:VAL:HG13	1:D:367:LYS:NZ	1.87	0.90
1:A:581:PHE:CZ	1:C:433:MET:CE	2.60	0.84
1:B:565:LEU:CD1	1:B:569:MET:HE3	2.06	0.84
1:A:581:PHE:CE1	1:C:433:MET:CE	2.61	0.83
1:A:469:MET:O	1:A:513:LYS:HE3	1.78	0.83
1:B:212:MET:HA	1:B:212:MET:HE2	1.59	0.83
1:D:363:VAL:CG1	1:D:367:LYS:HZ1	1.89	0.83
1:A:212:MET:HA	1:A:212:MET:HE2	1.61	0.82
1:A:357:MET:HE3	1:A:546:ALA:HB1	1.61	0.82
1:D:205:GLU:CG	1:D:212:MET:HE3	2.10	0.81
1:C:239:THR:HG22	1:C:243:MET:HE2	0.86	0.81
1:D:297:VAL:HG11	1:D:325:MET:HE1	1.63	0.80
1:C:389:MET:CE	3:D:751:HOH:O	2.29	0.79
1:D:188:VAL:HG11	1:D:268:ALA:HB3	1.64	0.79
1:D:205:GLU:HB3	1:D:212:MET:HE3	1.62	0.79
1:D:363:VAL:HG11	1:D:367:LYS:NZ	1.98	0.78
1:A:357:MET:HE3	1:A:546:ALA:CB	2.14	0.78
1:C:176:GLN:CB	1:C:191:ILE:CG2	2.61	0.77
1:D:357:MET:HE2	1:D:550:LEU:HG	1.66	0.77
1:A:581:PHE:CE1	1:C:433:MET:HE1	2.20	0.77
1:B:433:MET:HE3	1:D:581:PHE:CZ	2.20	0.76
1:B:559:LYS:O	1:B:561:ASP:N	2.17	0.76
1:A:357:MET:HE3	1:A:546:ALA:CA	2.16	0.76
1:D:205:GLU:HG2	1:D:212:MET:HE1	1.68	0.75
1:B:527:SER:OG	3:B:701:HOH:O	2.00	0.74
1:A:582:ASP:HB3	3:A:728:HOH:O	1.87	0.73
1:D:299:VAL:CG1	1:D:302:TRP:HB3	2.19	0.72
1:D:239:THR:CG2	1:D:243:MET:CE	2.66	0.72
1:A:345:GLN:HA	1:A:346:LEU:C	2.15	0.71
1:C:387:ASP:OD2	3:C:714:HOH:O	2.09	0.71
1:B:565:LEU:HD11	1:B:569:MET:CE	2.20	0.71
1:D:363:VAL:HG13	1:D:367:LYS:HZ1	1.52	0.70
1:B:433:MET:CE	1:D:581:PHE:CE1	2.75	0.69
1:A:357:MET:HE2	1:A:550:LEU:HG	1.74	0.69
1:A:433:MET:HE1	1:C:581:PHE:CE1	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:ILE:HG23	1:D:325:MET:HE3	1.74	0.69
1:A:433:MET:CE	1:C:581:PHE:CE1	2.76	0.69
1:D:205:GLU:HG2	1:D:212:MET:HE3	1.70	0.68
1:D:179:ASN:HA	1:D:191:ILE:HD12	1.76	0.67
1:A:212:MET:HE1	1:A:215:ARG:CZ	2.26	0.66
1:B:433:MET:HE1	1:D:581:PHE:CE1	2.31	0.66
1:B:565:LEU:CD1	1:B:569:MET:CE	2.73	0.66
1:A:433:MET:HE3	1:C:581:PHE:CZ	2.32	0.65
1:D:180:SER:HB2	1:D:181:LYS:HB2	1.78	0.65
1:A:346:LEU:HD13	1:A:352:LEU:HB3	1.79	0.65
1:A:437:ARG:HH12	1:C:582:ASP:HB2	1.61	0.65
1:D:188:VAL:HG11	1:D:268:ALA:CB	2.27	0.65
1:D:318:ILE:HG23	1:D:325:MET:CE	2.27	0.65
1:A:198:ARG:O	1:A:202:GLU:HG3	1.97	0.64
1:D:179:ASN:O	1:D:180:SER:C	2.40	0.64
1:C:459:ASN:HB2	3:C:707:HOH:O	1.97	0.64
1:A:357:MET:HE3	1:A:546:ALA:HA	1.79	0.62
1:B:433:MET:CE	1:D:581:PHE:CZ	2.84	0.61
1:C:224:LEU:HD21	1:C:548:ILE:HD13	1.82	0.61
1:D:196:PHE:CD1	1:D:266:GLU:HG2	2.35	0.60
1:C:303:GLN:OE1	1:C:328:LYS:NZ	2.33	0.60
1:D:297:VAL:HG13	1:D:325:MET:HE1	1.83	0.60
1:A:212:MET:HE1	1:A:215:ARG:NH2	2.17	0.59
1:D:180:SER:CB	1:D:181:LYS:HB2	2.33	0.59
1:D:359:VAL:HG22	1:D:542:THR:HG22	1.83	0.58
1:A:549:GLU:HB2	1:A:569:MET:CE	2.34	0.58
1:B:185:ASP:OD2	1:B:254:ARG:NH2	2.36	0.57
1:D:205:GLU:CG	1:D:212:MET:CE	2.69	0.57
1:C:240:ALA:HA	1:C:243:MET:HE3	1.88	0.56
1:D:179:ASN:HA	1:D:191:ILE:CD1	2.35	0.56
1:D:276:PHE:HB3	1:D:278:VAL:HG23	1.86	0.55
1:B:588:LEU:HD21	1:D:423:ILE:HD13	1.89	0.55
1:D:298:ASN:N	1:D:299:VAL:HG23	2.22	0.55
1:D:188:VAL:HG13	1:D:280:ALA:O	2.07	0.55
1:A:581:PHE:HE1	1:C:433:MET:HE1	1.70	0.54
1:B:388:MET:HE2	1:B:390:PHE:CD1	2.43	0.54
1:A:229:ILE:HD12	1:A:251:ALA:HB1	1.89	0.54
1:C:226:GLY:HA3	1:C:551:TYR:OH	2.08	0.53
1:C:185:ASP:OD2	1:C:254:ARG:NH2	2.42	0.53
1:B:232:CYS:HB2	1:B:314:LEU:HD13	1.91	0.53
1:C:254:ARG:HD3	1:C:296:CYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:MET:HE2	1:B:390:PHE:HA	1.91	0.52
1:D:249:LEU:HD22	1:D:249:LEU:N	2.25	0.52
1:A:228:LYS:H	1:A:305:ASN:HB2	1.75	0.52
1:C:513:LYS:HE3	1:C:515:ILE:HD13	1.90	0.52
1:D:215:ARG:HG3	1:D:245:THR:HG23	1.90	0.52
1:D:229:ILE:HD12	1:D:251:ALA:HB1	1.90	0.52
1:D:254:ARG:HD3	1:D:302:TRP:CZ3	2.45	0.52
1:A:433:MET:HE1	1:C:581:PHE:HE1	1.75	0.51
1:D:239:THR:CG2	1:D:243:MET:HE2	2.41	0.51
1:B:375:ARG:HG3	1:B:410:ALA:HB2	1.93	0.51
1:A:469:MET:O	1:A:513:LYS:CE	2.55	0.51
1:D:298:ASN:HA	1:D:299:VAL:HB	1.93	0.51
1:D:357:MET:HE3	1:D:546:ALA:HB1	1.93	0.51
1:C:389:MET:HE3	3:D:751:HOH:O	2.02	0.50
1:A:474:ILE:HD12	1:A:516:VAL:HB	1.93	0.50
1:C:254:ARG:NH2	1:C:299:VAL:HG21	2.26	0.50
1:D:357:MET:HE3	1:D:546:ALA:CA	2.42	0.50
1:A:582:ASP:HB2	1:C:437:ARG:HH12	1.77	0.49
1:B:304:PRO:HD2	1:B:325:MET:HE2	1.94	0.49
1:A:212:MET:HE3	1:A:241:VAL:CG1	2.42	0.49
1:A:433:MET:CE	1:C:581:PHE:CZ	2.95	0.49
1:D:428:ALA:HA	1:D:438:LEU:HD13	1.95	0.49
1:D:299:VAL:HG11	1:D:302:TRP:HB3	1.94	0.49
1:C:176:GLN:N	1:C:191:ILE:H	2.11	0.49
1:C:569:MET:HE1	3:C:724:HOH:O	2.13	0.49
1:D:212:MET:HE2	1:D:241:VAL:HG13	1.95	0.48
1:B:433:MET:HA	1:B:433:MET:HE2	1.95	0.48
1:C:405:LYS:NZ	3:C:690:HOH:O	2.46	0.48
1:C:414:MET:HA	1:C:414:MET:HE2	1.94	0.48
1:A:357:MET:CE	1:A:546:ALA:HA	2.43	0.48
1:D:363:VAL:HG21	1:D:567:LYS:NZ	2.29	0.48
1:A:229:ILE:HD12	1:A:251:ALA:CB	2.44	0.47
1:D:322:TYR:HB2	1:D:325:MET:HE2	1.95	0.47
1:C:544:ALA:O	1:C:548:ILE:HG12	2.15	0.47
1:B:433:MET:HE1	1:D:581:PHE:HE1	1.77	0.47
1:B:549:GLU:OE2	1:B:558:TYR:OH	2.22	0.47
1:C:514:ARG:HD3	3:D:623:HOH:O	2.14	0.47
1:A:581:PHE:CZ	1:C:433:MET:HE1	2.42	0.46
1:A:323:PRO:O	1:A:327:LYS:HG3	2.15	0.46
1:A:366:GLN:OE1	1:A:370:ASN:ND2	2.48	0.46
1:B:185:ASP:CG	1:B:254:ARG:HH22	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:VAL:HG12	1:D:367:LYS:NZ	1.92	0.46
1:A:474:ILE:CD1	1:A:516:VAL:HB	2.46	0.46
1:B:567:LYS:CD	1:B:605:LYS:O	2.63	0.46
1:A:377:SER:HB3	1:A:525:ASN:HB3	1.98	0.46
1:B:388:MET:HE1	1:B:450:ILE:HD11	1.98	0.45
1:D:235:ILE:HB	1:D:263:THR:HG23	1.97	0.45
1:A:226:GLY:O	1:A:305:ASN:ND2	2.49	0.45
1:D:329:ILE:HG22	1:D:331:GLY:H	1.82	0.45
1:D:414:MET:HA	1:D:414:MET:HE2	1.98	0.45
1:D:318:ILE:CG2	1:D:325:MET:HE3	2.43	0.45
1:C:606:PRO:O	1:C:607:ASN:HB2	2.16	0.45
1:D:578:LEU:N	1:D:579:PRO:CD	2.80	0.45
1:B:231:GLY:HA2	1:B:308:LEU:O	2.17	0.45
1:D:298:ASN:C	1:D:299:VAL:HG23	2.42	0.45
1:D:299:VAL:HG11	1:D:302:TRP:HE3	1.81	0.45
1:B:588:LEU:O	1:B:600:LYS:HE3	2.17	0.45
1:C:338:THR:HB	3:C:686:HOH:O	2.16	0.45
1:B:207:GLU:HB2	1:B:533:THR:HG21	1.99	0.45
1:B:297:VAL:HG11	1:B:318:ILE:HG12	1.99	0.45
1:B:254:ARG:HD3	1:B:296:CYS:O	2.17	0.45
1:D:363:VAL:HG11	1:D:367:LYS:HZ1	1.73	0.44
1:A:549:GLU:HB2	1:A:569:MET:HE2	2.00	0.44
1:C:224:LEU:CD2	1:C:548:ILE:HD13	2.48	0.44
1:A:231:GLY:HA2	1:A:308:LEU:O	2.17	0.44
1:C:522:ARG:NH2	3:C:752:HOH:O	2.51	0.44
1:D:188:VAL:HG12	1:D:189:LYS:H	1.82	0.44
1:D:322:TYR:CB	1:D:325:MET:HE2	2.47	0.44
1:B:-2:SER:OG	1:B:176:GLN:HG3	2.18	0.44
1:B:212:MET:HA	1:B:212:MET:CE	2.40	0.44
1:A:567:LYS:NZ	3:A:705:HOH:O	2.45	0.43
1:C:389:MET:HE2	3:D:751:HOH:O	2.10	0.43
1:A:400:TYR:O	1:A:405:LYS:NZ	2.51	0.43
1:B:590:ASP:O	1:B:594:LYS:HG3	2.19	0.43
1:D:224:LEU:HD13	1:D:548:ILE:HG12	1.99	0.43
1:D:230:VAL:HG13	1:D:304:PRO:HB3	1.99	0.43
1:D:230:VAL:HG23	1:D:314:LEU:HD21	2.00	0.43
1:D:180:SER:CB	1:D:181:LYS:CB	2.97	0.43
1:A:254[A]:ARG:HG2	1:A:302:TRP:CH2	2.54	0.43
1:A:464:GLU:O	1:A:468[A]:ARG:HG2	2.19	0.42
1:C:226:GLY:CA	1:C:551:TYR:OH	2.67	0.42
1:C:299:VAL:HG13	1:C:302:TRP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:MET:HE3	1:D:546:ALA:HA	2.02	0.42
1:B:324:ASN:O	1:B:328:LYS:HG2	2.19	0.42
1:A:582:ASP:CB	3:A:728:HOH:O	2.58	0.42
1:A:565:LEU:HG	1:A:569:MET:HB2	2.02	0.42
1:D:384:ARG:HB2	3:D:720:HOH:O	2.19	0.42
1:D:229:ILE:HD12	1:D:251:ALA:CB	2.50	0.42
1:D:212:MET:HE2	1:D:241:VAL:CG1	2.50	0.41
1:D:245:THR:O	1:D:249:LEU:HD22	2.09	0.41
3:B:742:HOH:O	1:D:605:LYS:HE3	2.20	0.41
1:A:555:GLU:HA	1:A:556:GLY:HA2	1.80	0.41
1:D:232:CYS:HA	1:D:256:ALA:O	2.20	0.41
1:A:474:ILE:HD11	3:A:624:HOH:O	2.19	0.41
1:A:357:MET:CE	1:A:546:ALA:O	2.69	0.41
1:C:294:ASP:OD1	1:C:322:TYR:OH	2.36	0.41
1:C:513:LYS:HE3	1:C:515:ILE:CD1	2.49	0.41
1:D:357:MET:HE3	1:D:546:ALA:CB	2.51	0.41
1:D:357:MET:HE1	1:D:549:GLU:HB3	2.02	0.41
1:D:363:VAL:HG21	1:D:567:LYS:HZ1	1.86	0.41
1:B:212:MET:HE2	1:B:212:MET:CA	2.39	0.40
1:B:433:MET:HE3	1:D:581:PHE:CE1	2.46	0.40
1:B:565:LEU:HD12	1:B:569:MET:CE	2.51	0.40
1:C:376:GLU:OE1	1:D:383:LYS:NZ	2.55	0.40
1:B:388:MET:CE	1:B:393:LYS:HG3	2.51	0.40
1:C:239:THR:C	1:C:243:MET:HE3	2.47	0.40
1:C:428:ALA:HA	1:C:438:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/435 (99%)	415 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	429/435 (99%)	419 (98%)	9 (2%)	1 (0%)	43	50
1	C	431/435 (99%)	421 (98%)	10 (2%)	0	100	100
1	D	432/435 (99%)	413 (96%)	14 (3%)	5 (1%)	10	7
All	All	1723/1740 (99%)	1668 (97%)	49 (3%)	6 (0%)	36	40

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	560	GLN
1	D	299	VAL
1	D	300	GLU
1	D	180	SER
1	D	181	LYS
1	D	277	PRO

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	364/370 (98%)	358 (98%)	6 (2%)	55	66
1	B	360/370 (97%)	358 (99%)	2 (1%)	78	84
1	C	366/370 (99%)	358 (98%)	8 (2%)	45	56
1	D	362/370 (98%)	349 (96%)	13 (4%)	31	39
All	All	1452/1480 (98%)	1423 (98%)	29 (2%)	48	59

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	LYS
1	A	188	VAL
1	A	255	TRP
1	A	500	VAL
1	A	515	ILE

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Mol	Chain	Res	Type
1	A	570	ASP
1	B	514	ARG
1	B	570	ASP
1	C	177	GLN
1	C	181	LYS
1	C	314	LEU
1	C	328	LYS
1	C	438	LEU
1	C	492	THR
1	C	515	ILE
1	C	594	LYS
1	D	180	SER
1	D	181	LYS
1	D	188	VAL
1	D	191	ILE
1	D	224	LEU
1	D	287	ASP
1	D	288	ASP
1	D	321	LYS
1	D	359	VAL
1	D	362	SER
1	D	366	GLN
1	D	438	LEU
1	D	480	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	GLN
1	B	303	GLN
1	B	360	ASN
1	B	366	GLN
1	B	447	GLN
1	B	543	GLN
1	C	219	GLN
1	C	345	GLN
1	C	394	GLN
1	C	447	GLN
1	D	298	ASN
1	D	366	GLN
1	D	447	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	608	-	46,48,48	1.67	4 (8%)	64,73,73	1.56	9 (14%)
2	NAD	D	608	-	46,48,48	1.79	5 (10%)	64,73,73	2.16	20 (31%)
2	NAD	C	608	-	46,48,48	1.55	2 (4%)	64,73,73	1.58	13 (20%)
2	NAD	B	608	-	46,48,48	1.69	6 (13%)	64,73,73	1.62	12 (18%)

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	A	608	-	-	4/30/62/62	0/5/5/5
2	NAD	D	608	-	-	9/30/62/62	0/5/5/5
2	NAD	C	608	-	-	6/30/62/62	0/5/5/5
2	NAD	B	608	-	-	4/30/62/62	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	608	NAD	O7N-C7N	9.17	1.41	1.24
2	A	608	NAD	O7N-C7N	8.79	1.40	1.24
2	B	608	NAD	O7N-C7N	8.38	1.39	1.24
2	C	608	NAD	O7N-C7N	7.66	1.38	1.24
2	D	608	NAD	O4D-C1D	3.39	1.45	1.40
2	D	608	NAD	C2N-N1N	3.11	1.38	1.35
2	A	608	NAD	C2A-N1A	3.01	1.39	1.33
2	B	608	NAD	PN-O3	2.79	1.62	1.59
2	A	608	NAD	O4D-C1D	2.58	1.44	1.40
2	D	608	NAD	PN-O3	2.54	1.62	1.59
2	B	608	NAD	C2N-N1N	2.31	1.37	1.35
2	C	608	NAD	C2N-N1N	2.21	1.37	1.35
2	B	608	NAD	O4D-C1D	2.16	1.43	1.40
2	A	608	NAD	C8A-N7A	2.15	1.35	1.31
2	D	608	NAD	O5B-C5B	2.12	1.52	1.44
2	B	608	NAD	C5A-N7A	-2.05	1.35	1.39
2	B	608	NAD	C2A-N1A	2.02	1.37	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	608	NAD	O2A-PA-O5B	-6.11	79.88	107.57
2	A	608	NAD	N3A-C2A-N1A	-5.52	120.23	128.58
2	B	608	NAD	N3A-C2A-N1A	-5.31	120.55	128.58
2	D	608	NAD	N3A-C2A-N1A	-4.70	121.47	128.58
2	D	608	NAD	C5A-N7A-C8A	4.57	110.63	103.45
2	D	608	NAD	C5A-C4A-N3A	-4.48	120.55	126.72
2	D	608	NAD	N9A-C8A-N7A	-4.40	107.69	113.94
2	D	608	NAD	O5B-PA-O1A	4.32	126.07	108.94
2	B	608	NAD	N9A-C8A-N7A	-4.32	107.81	113.94
2	C	608	NAD	O7N-C7N-C3N	-4.19	114.47	119.60
2	C	608	NAD	N3A-C2A-N1A	-4.19	122.24	128.58
2	A	608	NAD	N9A-C8A-N7A	-4.02	108.23	113.94
2	A	608	NAD	O2A-PA-O3	3.94	117.93	107.27
2	D	608	NAD	C4A-C5A-N7A	-3.84	106.19	110.58
2	C	608	NAD	N9A-C8A-N7A	-3.83	108.50	113.94
2	D	608	NAD	O3-PA-O1A	3.83	122.22	110.70
2	B	608	NAD	C5A-N7A-C8A	3.75	109.35	103.45
2	C	608	NAD	C3N-C7N-N7N	3.37	121.89	117.74
2	D	608	NAD	O2A-PA-O3	-3.34	98.23	107.27
2	B	608	NAD	C5A-C4A-N3A	-3.33	122.12	126.72
2	D	608	NAD	O5B-C5B-C4B	3.31	120.27	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	608	NAD	C5A-C4A-N3A	-3.28	122.20	126.72
2	D	608	NAD	O2A-PA-O1A	-3.20	97.55	112.44
2	B	608	NAD	O2N-PN-O3	3.17	115.85	107.27
2	D	608	NAD	C2A-N3A-C4A	3.15	119.52	111.83
2	A	608	NAD	C5A-C4A-N3A	-3.10	122.44	126.72
2	D	608	NAD	C3N-C7N-N7N	3.03	121.47	117.74
2	B	608	NAD	O7N-C7N-C3N	-2.97	115.97	119.60
2	C	608	NAD	C5A-N7A-C8A	2.87	107.96	103.45
2	A	608	NAD	C2A-N3A-C4A	2.86	118.83	111.83
2	C	608	NAD	C4A-N9A-C8A	2.81	108.69	105.74
2	A	608	NAD	O7N-C7N-C3N	-2.71	116.28	119.60
2	A	608	NAD	C5A-N7A-C8A	2.70	107.70	103.45
2	B	608	NAD	C3N-C7N-N7N	2.69	121.06	117.74
2	C	608	NAD	C4D-O4D-C1D	-2.64	107.51	109.92
2	B	608	NAD	C2A-N3A-C4A	2.62	118.22	111.83
2	D	608	NAD	O2N-PN-O3	2.61	114.32	107.27
2	D	608	NAD	C2B-C3B-C4B	2.51	107.47	102.61
2	C	608	NAD	C4A-C5A-N7A	-2.47	107.75	110.58
2	A	608	NAD	C3N-C7N-N7N	2.47	120.78	117.74
2	C	608	NAD	O2N-PN-O1N	2.44	123.78	112.44
2	D	608	NAD	PA-O5B-C5B	-2.43	107.42	121.35
2	D	608	NAD	N3A-C4A-N9A	2.42	131.28	127.17
2	B	608	NAD	C4A-N9A-C8A	2.42	108.28	105.74
2	D	608	NAD	O7N-C7N-C3N	-2.39	116.67	119.60
2	B	608	NAD	C4A-C5A-N7A	-2.36	107.88	110.58
2	B	608	NAD	N3A-C4A-N9A	2.36	131.18	127.17
2	B	608	NAD	O2A-PA-O3	2.32	113.55	107.27
2	C	608	NAD	C2A-N3A-C4A	2.22	117.26	111.83
2	C	608	NAD	O2N-PN-O3	2.18	113.17	107.27
2	D	608	NAD	O4B-C1B-N9A	2.15	112.22	108.09
2	C	608	NAD	N3A-C4A-N9A	2.08	130.71	127.17
2	D	608	NAD	C5A-C4A-N9A	2.08	108.08	105.81
2	A	608	NAD	C4A-N9A-C8A	2.03	107.87	105.74

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	608	NAD	O4D-C1D-N1N-C2N
2	A	608	NAD	O4D-C1D-N1N-C6N
2	A	608	NAD	C2D-C1D-N1N-C2N
2	A	608	NAD	C2D-C1D-N1N-C6N

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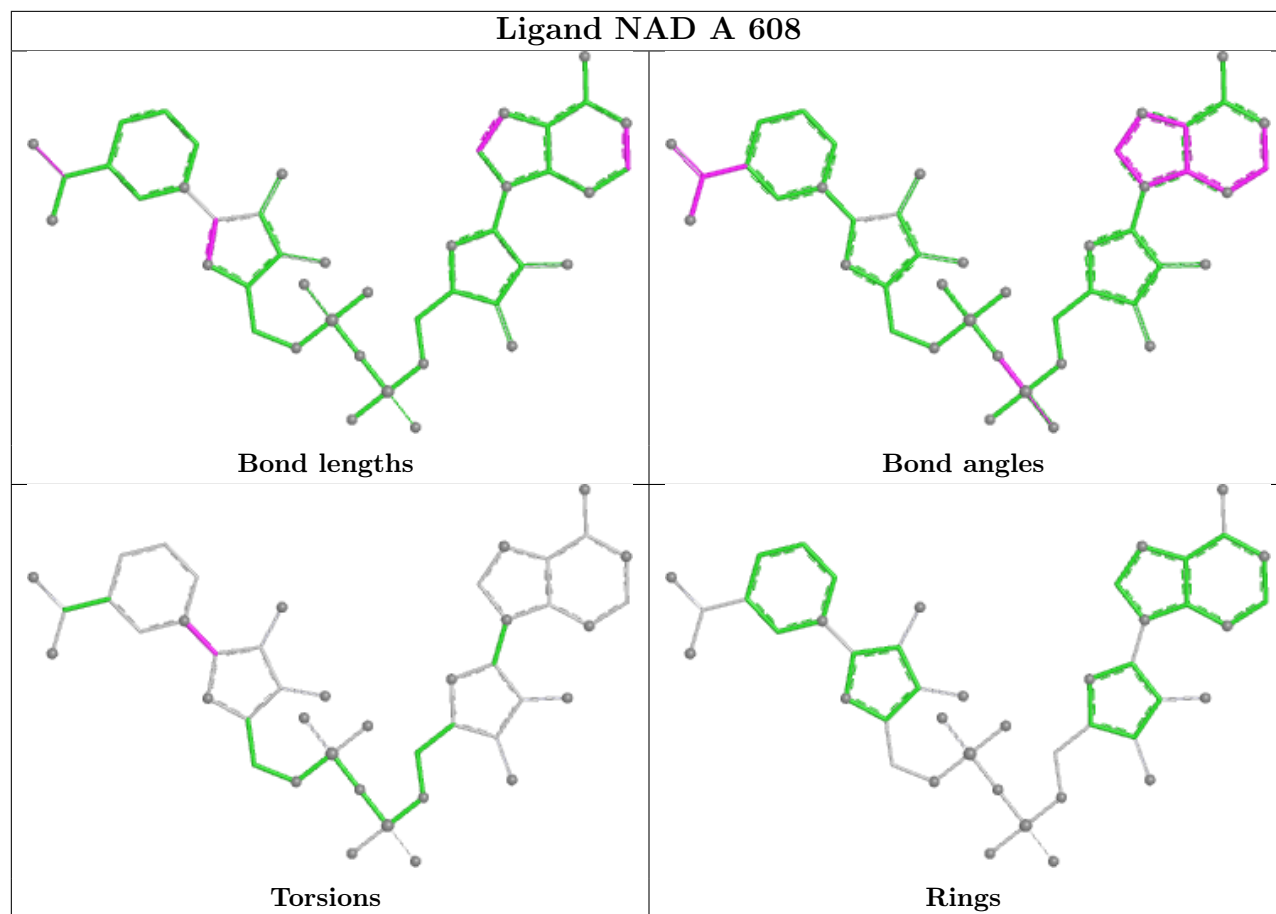
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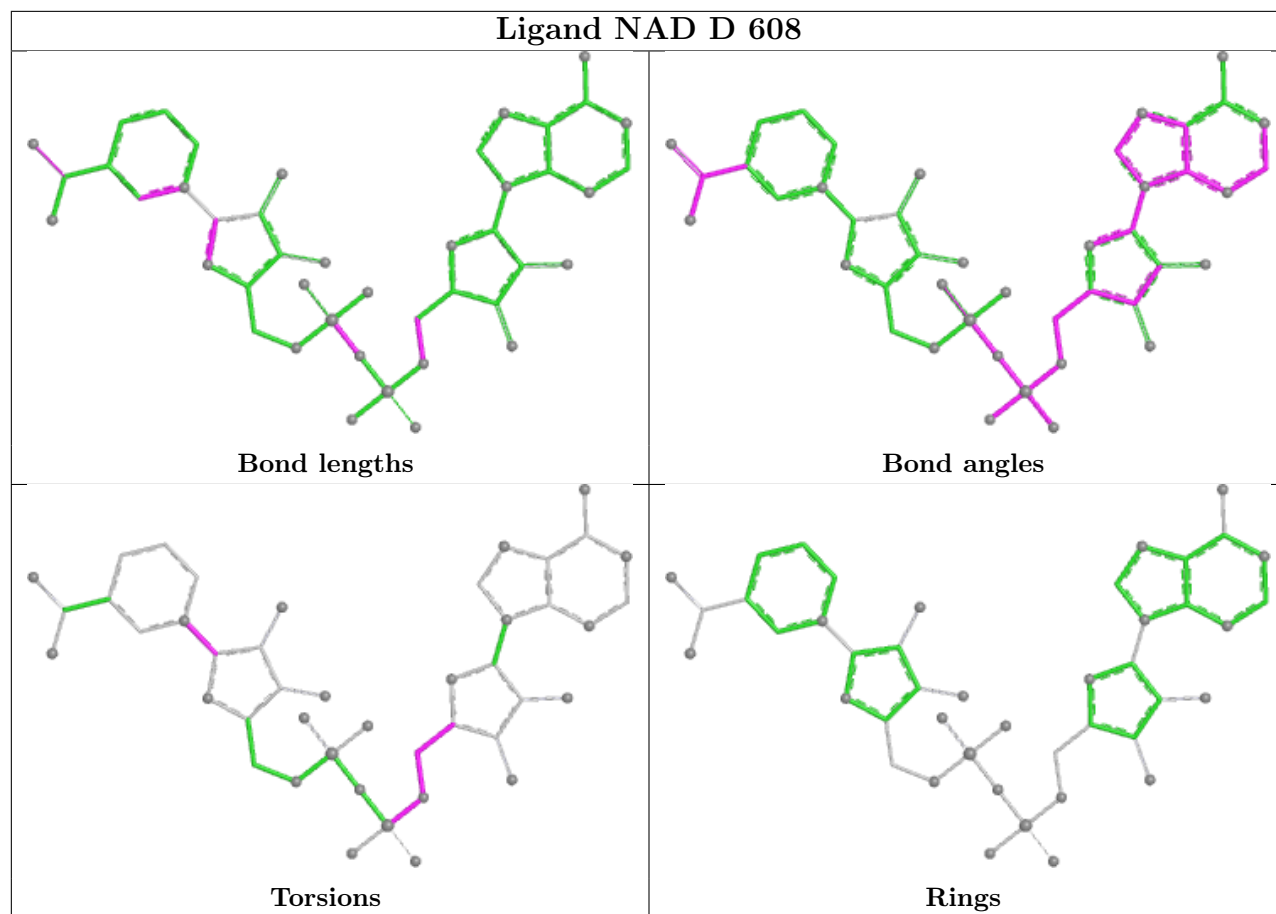
Mol	Chain	Res	Type	Atoms
2	B	608	NAD	O4D-C1D-N1N-C2N
2	B	608	NAD	O4D-C1D-N1N-C6N
2	B	608	NAD	C2D-C1D-N1N-C2N
2	B	608	NAD	C2D-C1D-N1N-C6N
2	C	608	NAD	O4D-C1D-N1N-C2N
2	C	608	NAD	O4D-C1D-N1N-C6N
2	C	608	NAD	C2D-C1D-N1N-C2N
2	C	608	NAD	C2D-C1D-N1N-C6N
2	D	608	NAD	C5B-O5B-PA-O1A
2	D	608	NAD	C5B-O5B-PA-O2A
2	D	608	NAD	O4D-C1D-N1N-C2N
2	D	608	NAD	O4D-C1D-N1N-C6N
2	D	608	NAD	C2D-C1D-N1N-C2N
2	D	608	NAD	C2D-C1D-N1N-C6N
2	D	608	NAD	O4B-C4B-C5B-O5B
2	D	608	NAD	C3B-C4B-C5B-O5B
2	D	608	NAD	C4B-C5B-O5B-PA
2	C	608	NAD	PA-O3-PN-O1N
2	C	608	NAD	C2B-C1B-N9A-C8A

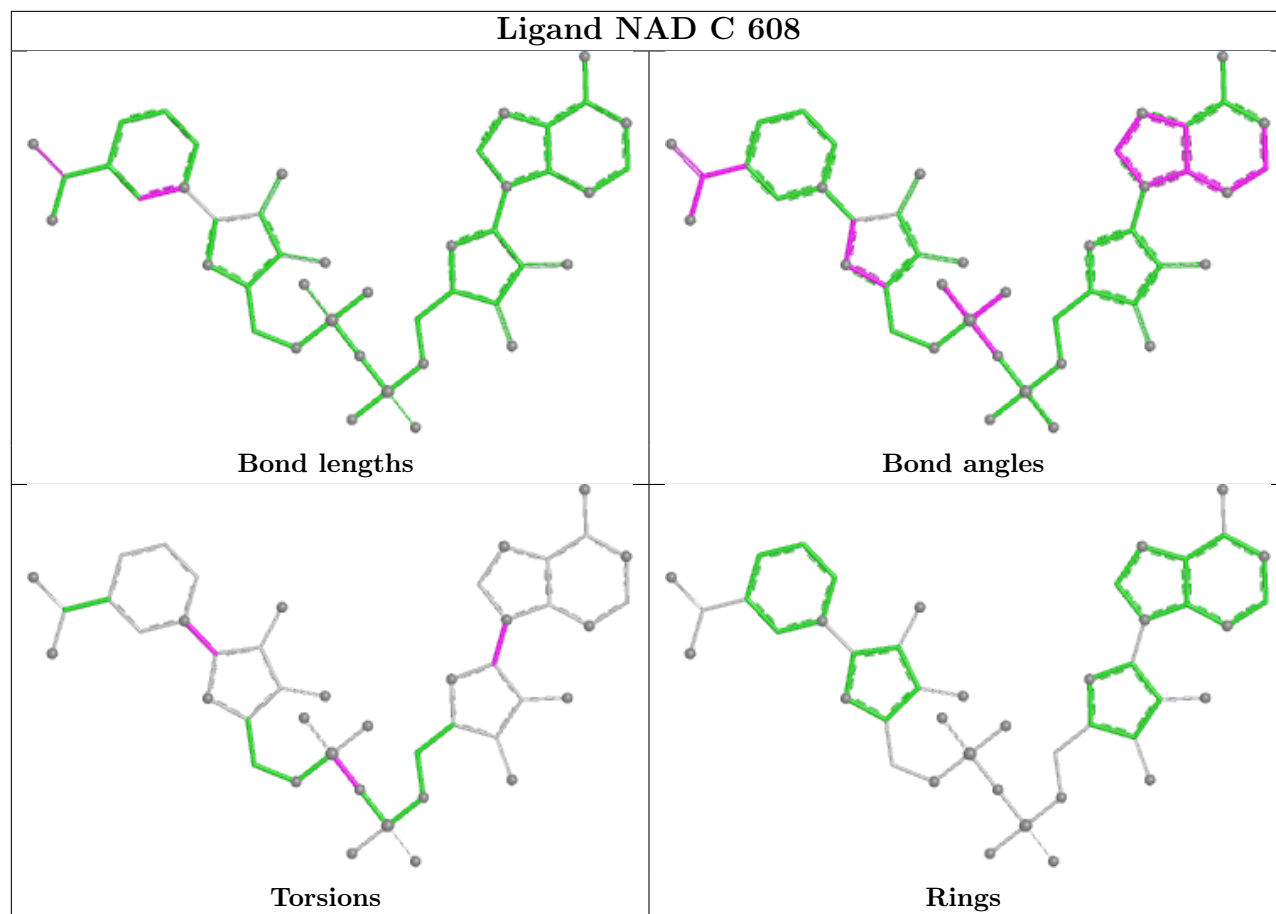
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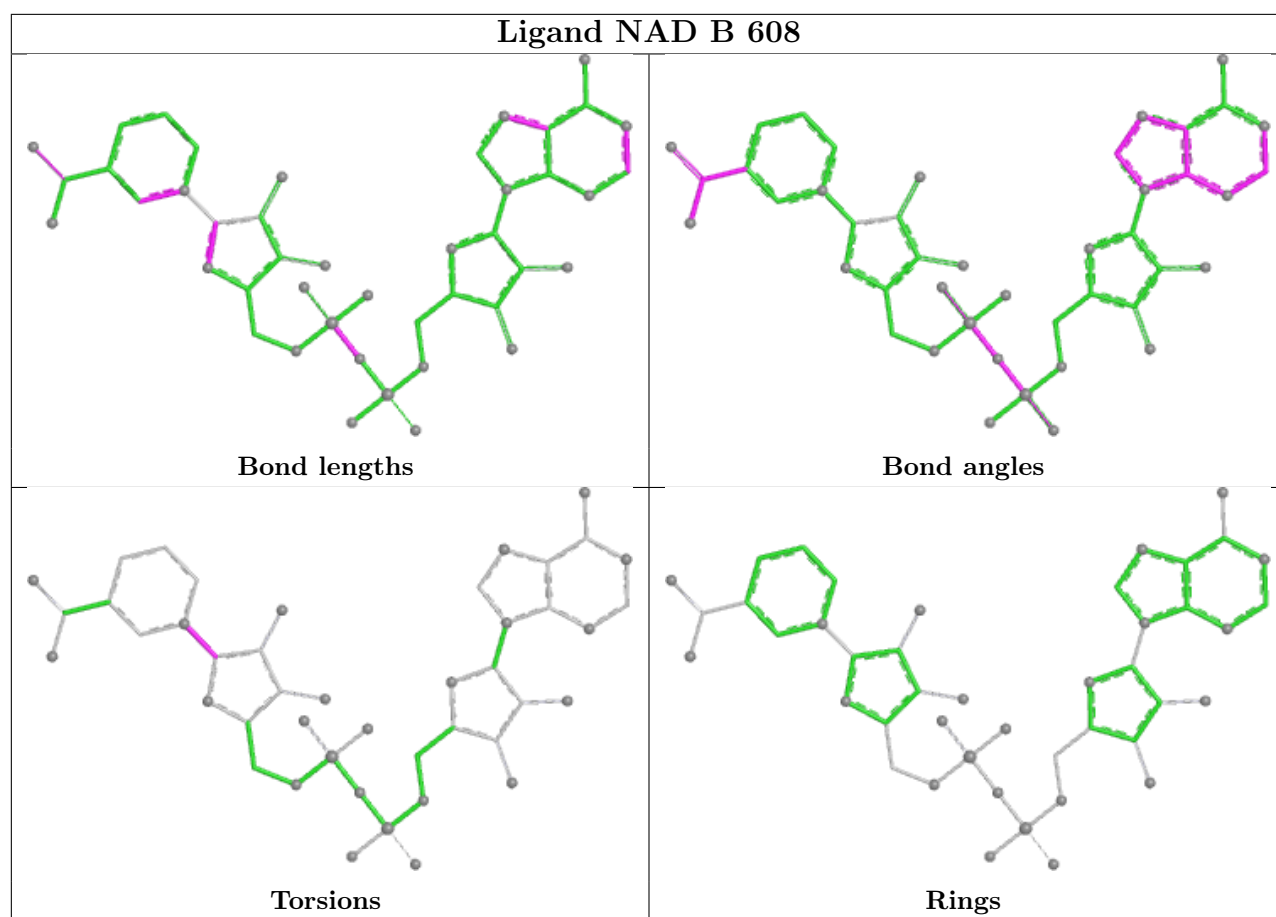
No monomer is involved in short contacts.

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, 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	433/435 (99%)	-0.07	6 (1%) 73 74	14, 36, 56, 71	2 (0%)
1	B	432/435 (99%)	0.08	10 (2%) 61 61	24, 40, 60, 67	1 (0%)
1	C	432/435 (99%)	-0.14	9 (2%) 63 64	17, 34, 51, 60	1 (0%)
1	D	431/435 (99%)	0.52	62 (14%) 6 5	16, 44, 76, 92	3 (0%)
All	All	1728/1740 (99%)	0.10	87 (5%) 34 33	14, 37, 64, 92	7 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	188	VAL	6.1
1	D	299	VAL	5.0
1	A	346	LEU	4.4
1	D	302	TRP	4.2
1	D	220	GLY	4.1
1	D	296	CYS	4.1
1	D	297	VAL	4.0
1	D	177	GLN	3.9
1	D	291	TRP	3.9
1	D	287	ASP	3.8
1	A	-2	SER	3.7
1	D	261	TYR	3.7
1	D	283	GLY	3.5
1	D	290	TRP	3.5
1	C	176	GLN	3.4
1	D	303	GLN	3.4
1	C	607	ASN	3.4
1	D	281	TRP	3.3
1	D	280	ALA	3.3
1	D	221	GLU	3.3
1	D	279	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	560	GLN	3.3
1	B	346	LEU	3.2
1	D	196	PHE	3.1
1	B	606	PRO	3.1
1	C	225	ALA	3.1
1	D	186	PHE	3.0
1	D	554	PRO	3.0
1	B	349	ALA	2.9
1	D	260	ILE	2.9
1	D	289	PHE	2.9
1	D	225	ALA	2.8
1	D	182	GLY	2.8
1	C	196	PHE	2.8
1	A	219	GLN	2.8
1	D	187	CYS	2.8
1	D	607	ASN	2.7
1	D	349	ALA	2.7
1	B	345	GLN	2.7
1	D	298	ASN	2.7
1	D	276	PHE	2.7
1	C	348	LYS	2.6
1	D	185	ASP	2.6
1	D	295	ARG	2.6
1	D	181	LYS	2.6
1	C	361	ASP	2.5
1	D	553	ALA	2.5
1	D	317	TRP	2.5
1	D	293	ILE	2.5
1	D	555	GLU	2.5
1	D	189	LYS	2.5
1	D	316	HIS	2.4
1	D	284	GLU	2.4
1	B	556	GLY	2.4
1	D	178	LYS	2.4
1	D	278	VAL	2.3
1	A	345	GLN	2.3
1	B	-2	SER	2.3
1	D	191	ILE	2.3
1	D	300	GLU	2.3
1	D	321	LYS	2.3
1	D	606	PRO	2.2
1	C	226	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	194	ALA	2.2
1	D	270	ALA	2.2
1	D	274	SER	2.2
1	D	559	LYS	2.2
1	C	199	ARG	2.2
1	C	555	GLU	2.2
1	B	327	LYS	2.2
1	D	180	SER	2.2
1	D	190	ASN	2.2
1	D	361	ASP	2.1
1	D	277	PRO	2.1
1	D	183	SER	2.1
1	D	314	LEU	2.1
1	A	298	ASN	2.1
1	A	305	ASN	2.1
1	D	219	GLN	2.1
1	D	272	ALA	2.1
1	B	300	GLU	2.1
1	D	324	ASN	2.0
1	D	192	LYS	2.0
1	D	184	SER	2.0
1	D	202	GLU	2.0
1	D	179	ASN	2.0
1	B	559	LYS	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](#)

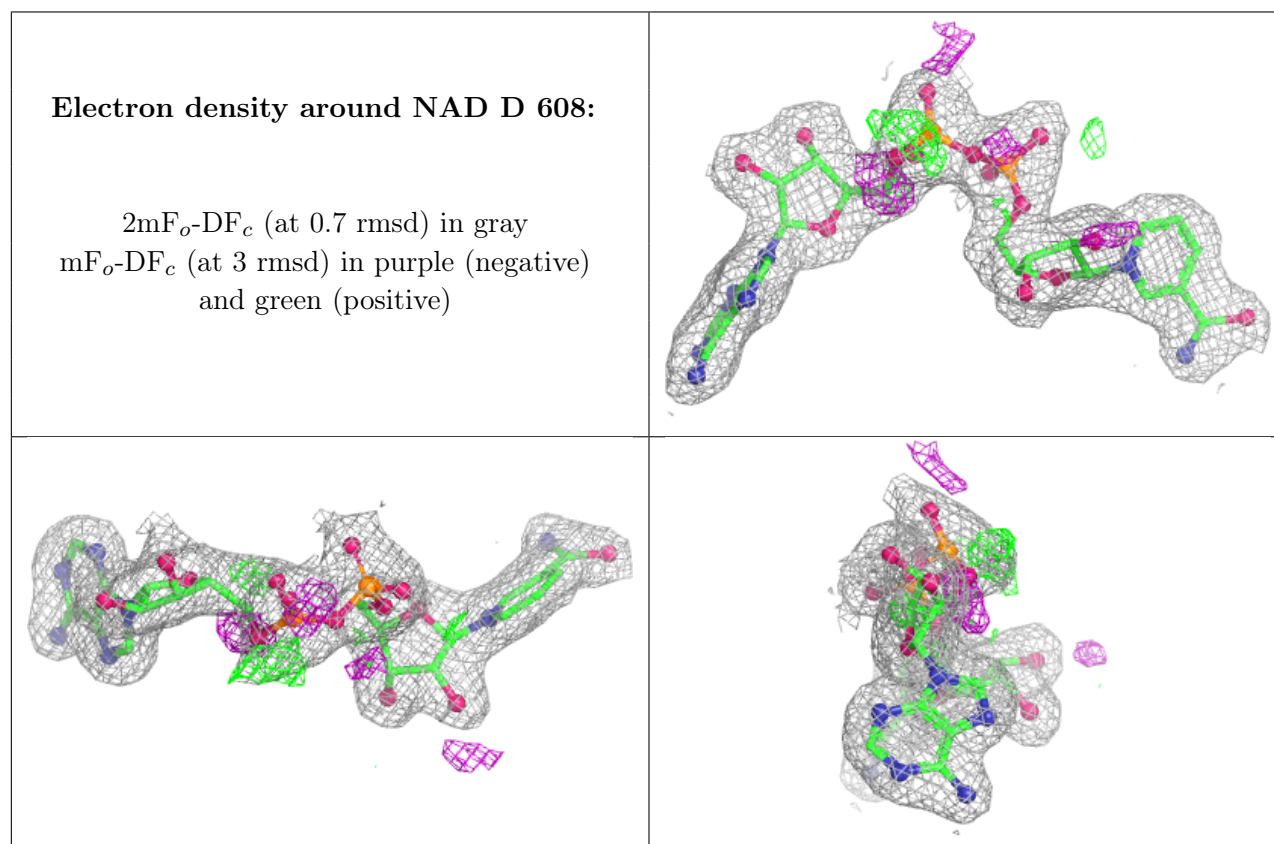
There are no oligosaccharides in this entry.

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.

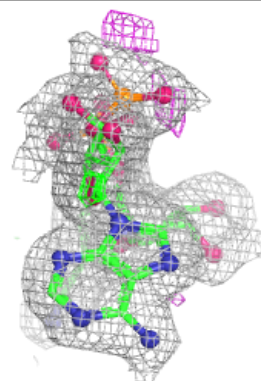
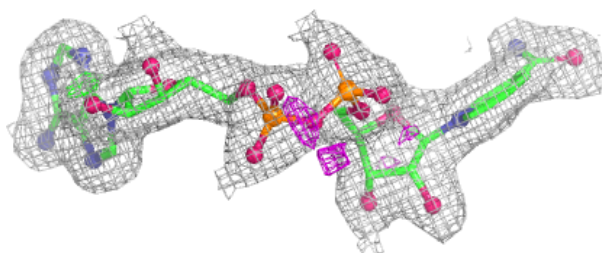
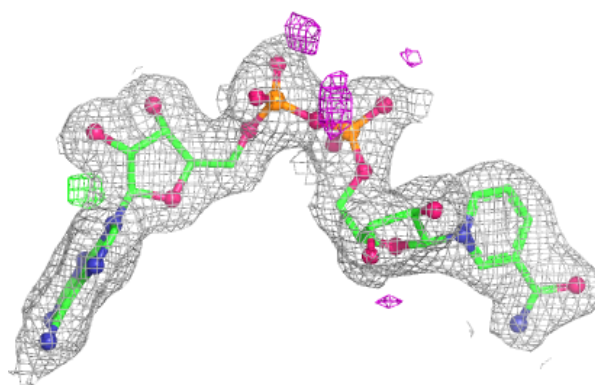
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	D	608	44/44	0.96	0.07	22,30,36,40	0
2	NAD	C	608	44/44	0.98	0.05	18,24,29,36	0
2	NAD	B	608	44/44	0.98	0.06	24,30,35,38	0
2	NAD	A	608	44/44	0.99	0.04	19,26,36,40	0

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.

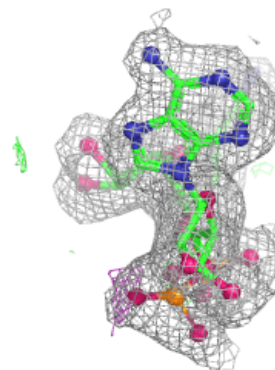
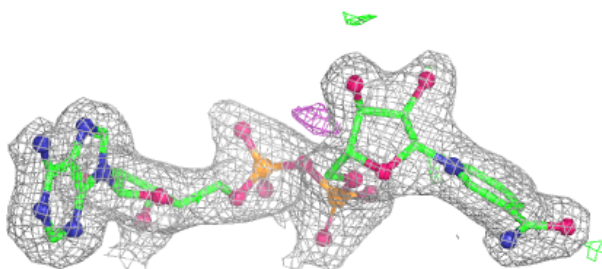
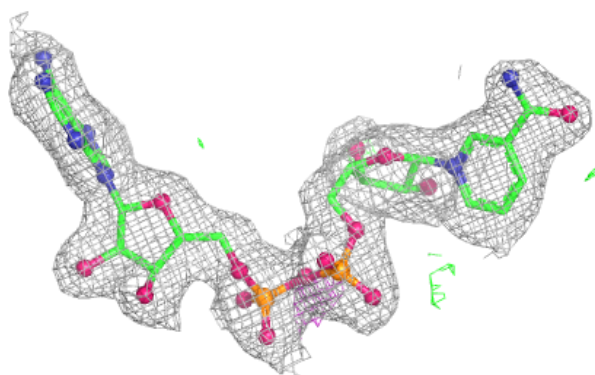


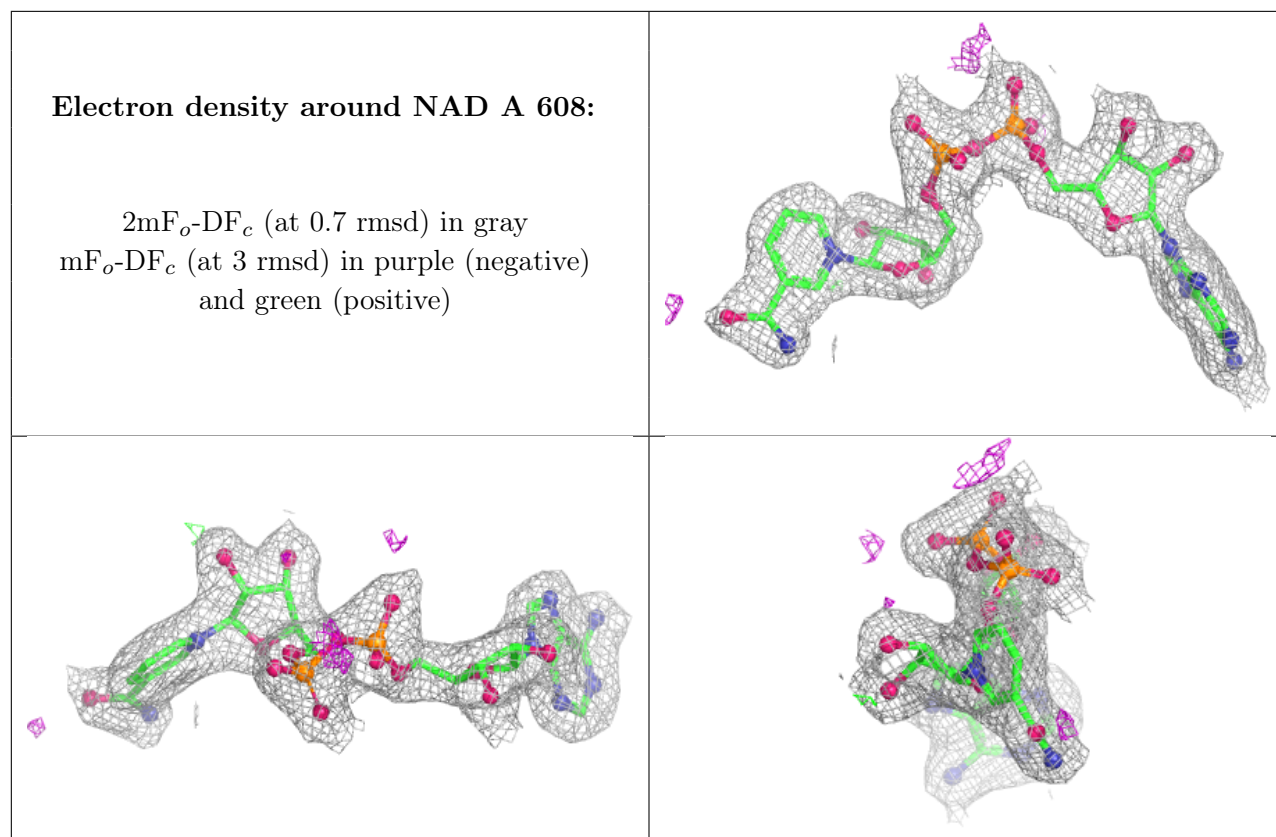
Electron density around NAD C 608:

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

**Electron density around NAD B 608:**

$2mF_o-DF_c$ (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.