Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 10:02 AM EDT

PDB ID	:	3GVP
Title	:	Human SAHH-like domain of human adenosylhomocysteinase 3
Authors	:	Siponen, M.I.; Wisniewska, M.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Karlberg, T.; Kotenyova, T.; Lehtio, L.; Moche, M.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Schutz, P.; Thorsell, A.G.; Tresaugues, L.; Van Den Berg, S.; Weigelt, J.; Welin, M.; Schueler, H.
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 (i) 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 (i)) were used in the production of this report:

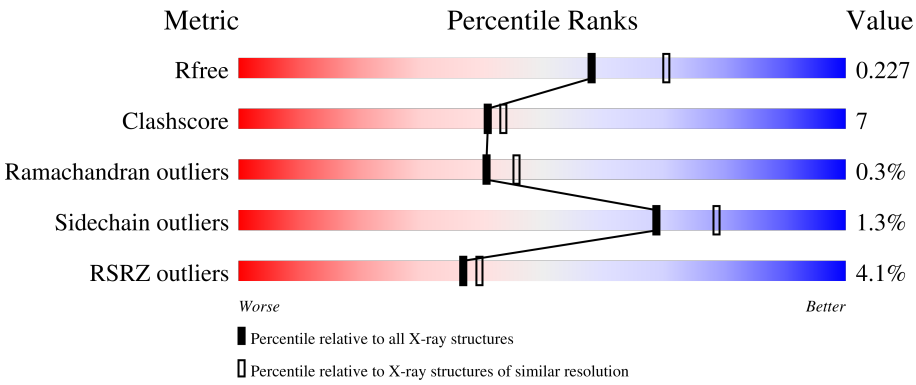
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

1 Overall quality at a glance (i)

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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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 <=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	.% 89% 11%
1	B	435	4% 90% 9% •
1	C	435	2% 90% 9% •

Continued on next page...

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	D	435	10% 84% 13%

2 Entry composition (i)

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.

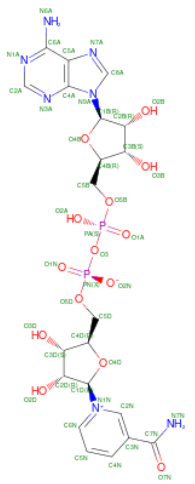
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	433	3368	2126	584	626	32	0	2	0
1	B	432	3337	2107	574	624	32	0	1	0
1	C	432	3367	2125	584	627	31	0	1	0
1	D	431	3343	2114	574	624	31	0	3	0

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 (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

NAD



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

- Molecule 3 is water.

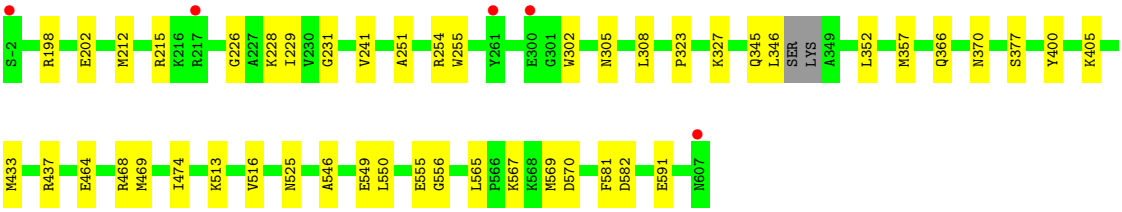
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	157	157	157	0	0
3	B	117	117	117	0	0
3	C	181	181	181	0	0
3	D	127	127	127	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

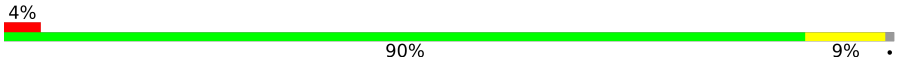
• Molecule 1: Adenosylhomocysteinase 3

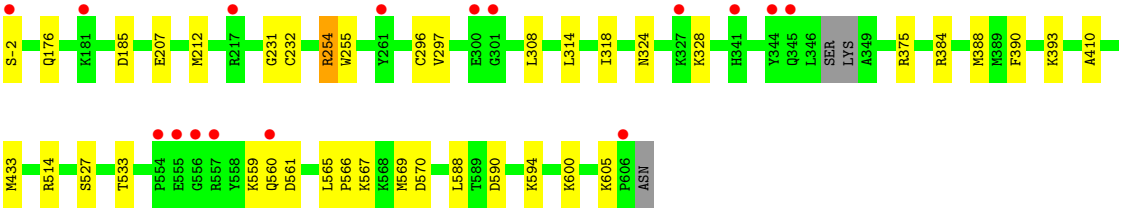
Chain A:



• Molecule 1: Adenosylhomocysteinase 3

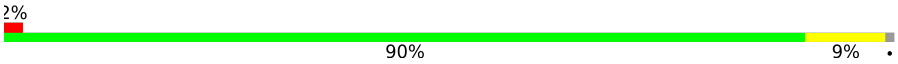
Chain B:

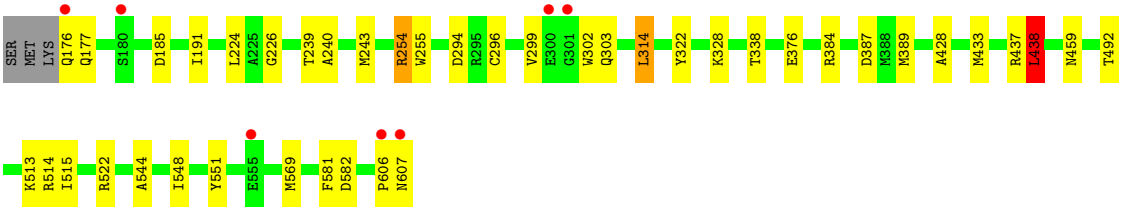




• Molecule 1: Adenosylhomocysteinase 3

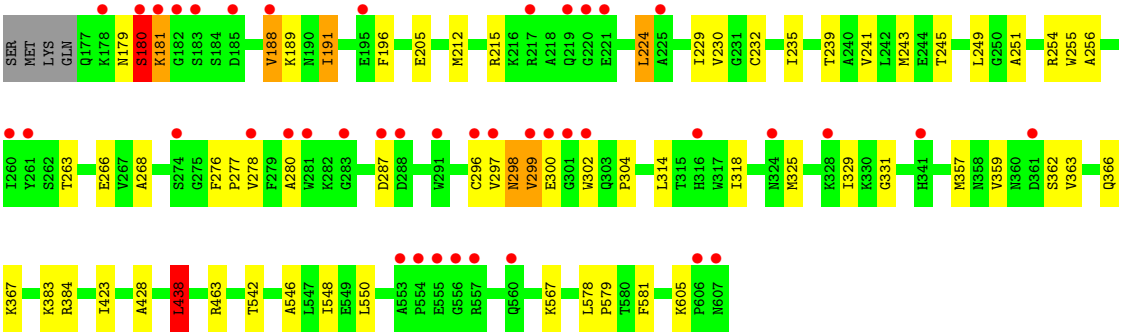
Chain C:





• Molecule 1: Adenosylhomocysteinase 3

Chain D:


SER MET LYS GLN Q177 K178 N179 S180 K181 G182 S183 S184 D185 V188 K189 N190 I191 E195 F196 E205 M212 R215 K216 R217 A218 Q219 G220 E221 L224 A225 I229 V230 G231 C232 I235 T239 A240 V241 L242 M243 E244 T245 L249 G250 A251 R254 W255 A256
I260 Y261 S262 T263 E266 V267 A268 S274 G275 F276 P277 V278 F279 A280 W281 K282 G283 D287 D288 W291 C296 V297 N298 V299 E300 G301 W302 Q303 P304 L314 T315 H316 W317 I318 M324 M325 K328 I329 K330 G331 H341 M357 N358 V359 N360 D361 S362 V363 Q366
K367 K383 R384 I423 A428 L438 R463 T542 A546 L547 I548 E549 L550 A553 P554 E555 G556 R557 Q560 K567 L578 P579 T580 F581 K605 P606 M607

4 Data and refinement statistics (i)

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) 100.0 (19.91-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	7.65 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.226 0.187 , 0.227	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)	0.35 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.72	0/3435	0.74	0/4647
1	B	0.64	0/3401	0.70	3/4607 (0.1%)
1	C	0.75	0/3429	0.75	5/4638 (0.1%)
1	D	0.67	1/3415 (0.0%)	0.72	2/4625 (0.0%)
All	All	0.70	1/13680 (0.0%)	0.73	10/18517 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	296	CYS	CB-SG	-5.32	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	254	ARG	NE-CZ-NH2	-10.57	115.01	120.30
1	C	254	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	B	254	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	C	254	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	B	384	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	C	384	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	314	LEU	CA-CB-CG	5.58	128.13	115.30
1	D	463	ARG	NE-CZ-NH1	5.13	122.86	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	438	LEU	CA-CB-CG	-5.12	103.53	115.30
1	C	438	LEU	CA-CB-CG	-5.07	103.63	115.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3368	0	3371	51	0
1	B	3337	0	3320	35	0
1	C	3367	0	3380	47	0
1	D	3343	0	3335	78	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	6	0
3	D	127	0	0	5	0
All	All	14173	0	13510	191	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 (191) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:569:MET:HE1	3:A:662:HOH:O	1.38	1.17
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:C:176:GLN:CB	1:C:191:ILE:HG22	1.79	1.12
1:D:239:THR:HG22	1:D:243:MET:HE3	1.29	1.12
1:D:239:THR:HG22	1:D:243:MET:CE	1.85	1.05
1:C:239:THR:HG22	1:C:243:MET:HE2	1.06	1.04
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:245:THR:O	1:D:249:LEU:CD2	2.08	1.00
1:D:205:GLU:CG	1:D:212:MET:HE3	1.94	0.98
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:A:357:MET:HE3	1:A:546:ALA:HA	1.50	0.94
1:D:205:GLU:HG2	1:D:212:MET:HE3	1.52	0.90
1:D:363:VAL:HG13	1:D:367:LYS:NZ	1.87	0.90
1:C:239:THR:CG2	1:C:243:MET:HE2	2.00	0.88
1:A:581:PHE:CZ	1:C:433:MET:CE	2.60	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:D:205:GLU:CB	1:D:212:MET:HE3	2.09	0.83
1:D:363:VAL:CG1	1:D:367:LYS:HZ1	1.89	0.83
1:A:581:PHE:CE1	1:C:433:MET:HE1	2.16	0.81
1:A:581:PHE:CZ	1:C:433:MET:HE1	2.17	0.79
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:363:VAL:HG11	1:D:367:LYS:NZ	1.98	0.78
1:C:176:GLN:CB	1:C:191:ILE:CG2	2.61	0.77
1:B:433:MET:HE1	1:D:581:PHE:CE1	2.18	0.77
1:B:559:LYS:O	1:B:561:ASP:N	2.17	0.76
1:A:357:MET:HE3	1:A:546:ALA:CA	2.17	0.74
1:B:527:SER:OG	3:B:701:HOH:O	2.00	0.74
1:A:433:MET:HE1	1:C:581:PHE:CE1	2.23	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:318:ILE:HG23	1:D:325:MET:HE2	1.71	0.72
1:D:239:THR:CG2	1:D:243:MET:CE	2.66	0.72
1:B:565:LEU:HD11	1:B:569:MET:CE	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:ASP:OD2	3:C:714:HOH:O	2.09	0.71
1:A:581:PHE:CZ	1:C:433:MET:HE3	2.25	0.71
1:B:565:LEU:CD1	1:B:569:MET:HE2	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:433:MET:CE	1:C:581:PHE:CE1	2.76	0.69
1:D:205:GLU:HB3	1:D:212:MET:HE3	1.75	0.68
1:D:179:ASN:HA	1:D:191:ILE:HD12	1.76	0.67
1:B:565:LEU:HD11	1:B:569:MET:HE2	1.75	0.67
1:A:345:GLN:HA	1:A:346:LEU:C	2.15	0.66
1:D:239:THR:HG22	1:D:243:MET:HE2	1.75	0.66
1:B:565:LEU:CD1	1:B:569:MET:CE	2.73	0.66
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:C:239:THR:HG22	1:C:243:MET:HE1	1.76	0.64
1:C:459:ASN:HB2	3:C:707:HOH:O	1.97	0.64
1:D:239:THR:CG2	1:D:243:MET:HE2	2.29	0.62
1:D:297:VAL:CG1	1:D:325:MET:CE	2.78	0.61
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:357:MET:HE3	1:D:546:ALA:HA	1.82	0.60
1:D:179:ASN:O	1:D:180:SER:C	2.40	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:179:ASN:HA	1:D:191:ILE:CD1	2.35	0.56
1:A:433:MET:HE3	1:C:581:PHE:CZ	2.41	0.56
1:D:276:PHE:HB3	1:D:278:VAL:HG23	1.86	0.55
1:A:357:MET:HE1	1:A:550:LEU:HG	1.87	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:B:433:MET:HE1	1:D:581:PHE:CZ	2.41	0.55
1:D:188:VAL:HG13	1:D:280:ALA:O	2.07	0.55
1:D:205:GLU:HG2	1:D:212:MET:HE1	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:MET:HE1	1:C:581:PHE:HE1	1.72	0.54
1:A:229:ILE:HD12	1:A:251:ALA:HB1	1.89	0.54
1:B:433:MET:HE3	1:D:581:PHE:CZ	2.42	0.53
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:B:565:LEU:HD11	1:B:569:MET:HE3	1.90	0.53
1:C:254:ARG:HD3	1:C:296:CYS:O	2.09	0.53
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:B:212:MET:HA	1:B:212:MET:HE2	1.92	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:D:212:MET:HE1	1:D:241:VAL:HG13	1.92	0.51
1:D:357:MET:HE1	1:D:550:LEU:HG	1.93	0.51
1:B:212:MET:HA	1:B:212:MET:CE	2.40	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:297:VAL:HG13	1:D:325:MET:HE3	1.93	0.50
1:C:389:MET:HE3	3:D:751:HOH:O	2.03	0.50
1:C:239:THR:CG2	1:C:243:MET:CE	2.66	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:A:582:ASP:HB2	1:C:437:ARG:HH12	1.77	0.49
1:B:433:MET:HE1	1:D:581:PHE:HE1	1.73	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:A:212:MET:HE1	1:A:215:ARG:NH2	2.28	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:297:VAL:CG1	1:D:325:MET:HE1	2.42	0.49
1:A:212:MET:HA	1:A:212:MET:CE	2.44	0.48
1:D:363:VAL:HG21	1:D:567:LYS:NZ	2.29	0.48
1:B:566:PRO:HD2	1:B:569:MET:CE	2.44	0.48
1:A:229:ILE:HD12	1:A:251:ALA:CB	2.44	0.47
1:C:240:ALA:HA	1:C:243:MET:HE3	1.96	0.47
1:A:212:MET:HA	1:A:212:MET:HE2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:ALA:O	1:C:548:ILE:HG12	2.15	0.47
1:C:514:ARG:HD3	3:D:623:HOH:O	2.14	0.47
1:D:297:VAL:CG1	1:D:325:MET:HE3	2.44	0.47
1:B:566:PRO:HD2	1:B:569:MET:HE1	1.96	0.46
1:A:323:PRO:O	1:A:327:LYS:HG3	2.15	0.46
1:B:388:MET:HE2	1:B:390:PHE:HA	1.97	0.46
1:A:366:GLN:OE1	1:A:370:ASN:ND2	2.48	0.46
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:C:389:MET:HE2	3:D:751:HOH:O	2.08	0.46
1:A:549:GLU:HB2	1:A:569:MET:HE2	1.97	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: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: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:357:MET:CE	1:D:550:LEU:HG	2.46	0.44
1:D:363:VAL:HG11	1:D:367:LYS:HZ1	1.73	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:B:-2:SER:OG	1:B:176:GLN:HG3	2.18	0.44
1:A:357:MET:HE2	1:A:546:ALA:HB1	1.98	0.43
1:A:400:TYR:O	1:A:405:LYS:NZ	2.51	0.43
1:A:212:MET:HE1	1:A:241:VAL:HG13	2.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:567:LYS:NZ	3:A:705:HOH:O	2.45	0.41
1:B:185:ASP:CG	1:B:254:ARG:HH22	2.24	0.41
1:D:245:THR:O	1:D:249:LEU:HD22	2.09	0.41
1:D:363:VAL:HG21	1:D:567:LYS:HZ1	1.86	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:B:433:MET:HA	1:B:433:MET:HE2	2.01	0.40
1:D:298:ASN:C	1:D:299:VAL:HG23	2.42	0.40
1:D:357:MET:HE3	1:D:546:ALA:CA	2.48	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:428:ALA:HA	1:C:438:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/435 (99%)	415 (96%)	16 (4%)	0	100	100
1	B	429/435 (99%)	419 (98%)	9 (2%)	1 (0%)	47	55
1	C	431/435 (99%)	421 (98%)	10 (2%)	0	100	100
1	D	432/435 (99%)	413 (96%)	14 (3%)	5 (1%)	13	9
All	All	1723/1740 (99%)	1668 (97%)	49 (3%)	6 (0%)	41	46

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 (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	364/370 (98%)	362 (100%)	2 (0%)	88	92
1	B	360/370 (97%)	357 (99%)	3 (1%)	81	88
1	C	366/370 (99%)	361 (99%)	5 (1%)	67	76
1	D	362/370 (98%)	353 (98%)	9 (2%)	47	56
All	All	1452/1480 (98%)	1433 (99%)	19 (1%)	69	79

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	TRP
1	A	570	ASP
1	B	255	TRP
1	B	514	ARG
1	B	570	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	177	GLN
1	C	255	TRP
1	C	314	LEU
1	C	438	LEU
1	C	492	THR
1	D	180	SER
1	D	188	VAL
1	D	191	ILE
1	D	224	LEU
1	D	255	TRP
1	D	287	ASP
1	D	362	SER
1	D	366	GLN
1	D	438	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	608	-	42,48,48	1.67	3 (7%)	50,73,73	1.31	3 (6%)
2	NAD	A	608	-	42,48,48	1.70	4 (9%)	50,73,73	1.26	5 (10%)
2	NAD	C	608	-	42,48,48	1.62	4 (9%)	50,73,73	1.49	8 (16%)
2	NAD	D	608	-	42,48,48	1.80	5 (11%)	50,73,73	1.92	12 (24%)

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	608	-	-	5/26/62/62	0/5/5/5
2	NAD	A	608	-	-	5/26/62/62	0/5/5/5
2	NAD	C	608	-	-	6/26/62/62	0/5/5/5
2	NAD	D	608	-	-	9/26/62/62	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	608	NAD	O7N-C7N	8.91	1.41	1.24
2	A	608	NAD	O7N-C7N	8.54	1.40	1.24
2	B	608	NAD	O7N-C7N	8.14	1.39	1.24
2	C	608	NAD	O7N-C7N	7.44	1.38	1.24
2	D	608	NAD	O4D-C1D	3.05	1.45	1.41
2	C	608	NAD	C2A-N3A	3.01	1.36	1.32
2	A	608	NAD	C2A-N3A	2.99	1.36	1.32
2	B	608	NAD	C2A-N3A	2.94	1.36	1.32
2	A	608	NAD	C2A-N1A	2.89	1.39	1.33
2	D	608	NAD	C2A-N3A	2.88	1.36	1.32
2	D	608	NAD	C2N-N1N	2.83	1.38	1.35
2	C	608	NAD	C2D-C1D	-2.34	1.50	1.53
2	A	608	NAD	O4D-C1D	2.29	1.44	1.41
2	B	608	NAD	C2N-N1N	2.11	1.37	1.35
2	D	608	NAD	O5B-C5B	2.04	1.52	1.44
2	C	608	NAD	C2N-N1N	2.02	1.37	1.35

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	608	NAD	O2A-PA-O5B	-6.00	79.88	107.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	608	NAD	N3A-C2A-N1A	-5.40	120.23	128.68
2	B	608	NAD	N3A-C2A-N1A	-5.20	120.55	128.68
2	D	608	NAD	N3A-C2A-N1A	-4.61	121.47	128.68
2	D	608	NAD	O5B-PA-O1A	4.35	126.07	109.07
2	C	608	NAD	O7N-C7N-C3N	-4.31	114.47	119.63
2	C	608	NAD	N3A-C2A-N1A	-4.12	122.24	128.68
2	C	608	NAD	C3N-C7N-N7N	3.45	121.89	117.75
2	D	608	NAD	C5A-C6A-N6A	3.40	125.52	120.35
2	D	608	NAD	O5B-C5B-C4B	3.28	120.27	108.99
2	D	608	NAD	O4D-C1D-C2D	-3.27	102.14	106.93
2	D	608	NAD	C3N-C7N-N7N	3.10	121.47	117.75
2	D	608	NAD	C4A-C5A-N7A	-3.08	106.19	109.40
2	B	608	NAD	O7N-C7N-C3N	-3.06	115.97	119.63
2	D	608	NAD	O2A-PA-O1A	-2.97	97.55	112.24
2	C	608	NAD	C5A-C6A-N6A	2.84	124.67	120.35
2	A	608	NAD	O7N-C7N-C3N	-2.80	116.28	119.63
2	B	608	NAD	C3N-C7N-N7N	2.75	121.06	117.75
2	C	608	NAD	O4B-C1B-C2B	-2.59	103.14	106.93
2	A	608	NAD	C3N-C7N-N7N	2.53	120.78	117.75
2	D	608	NAD	C2B-C3B-C4B	2.48	107.47	102.64
2	D	608	NAD	O7N-C7N-C3N	-2.47	116.67	119.63
2	D	608	NAD	PA-O5B-C5B	-2.43	107.42	121.68
2	C	608	NAD	O2N-PN-O1N	2.33	123.78	112.24
2	A	608	NAD	C2N-C3N-C4N	2.04	120.56	118.26
2	A	608	NAD	O4D-C1D-C2D	-2.03	103.96	106.93
2	C	608	NAD	O4D-C1D-C2D	-2.01	103.98	106.93
2	C	608	NAD	C3N-C2N-N1N	-2.01	118.46	120.43

There are no chirality outliers.

All (25) 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
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

Continued on next page...

Continued from previous page...

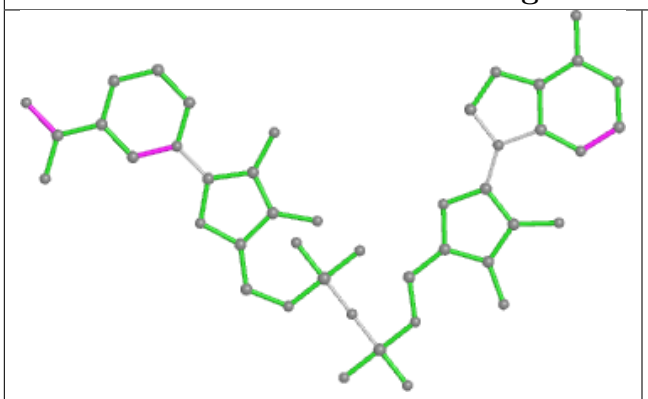
Mol	Chain	Res	Type	Atoms
2	C	608	NAD	C2D-C1D-N1N-C2N
2	C	608	NAD	C2D-C1D-N1N-C6N
2	D	608	NAD	C5B-O5B-PA-O1A
2	D	608	NAD	C5B-O5B-PA-O2A
2	D	608	NAD	O4D-C1D-N1N-C2N
2	D	608	NAD	O4D-C1D-N1N-C6N
2	D	608	NAD	C2D-C1D-N1N-C2N
2	D	608	NAD	C2D-C1D-N1N-C6N
2	D	608	NAD	O4B-C4B-C5B-O5B
2	D	608	NAD	C3B-C4B-C5B-O5B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

There are no ring outliers.

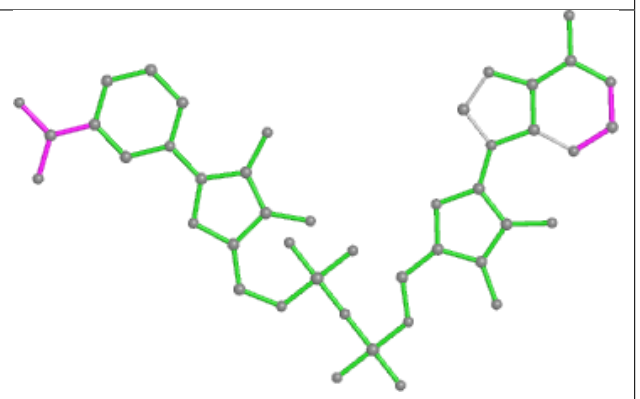
No monomer is involved in short contacts.

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

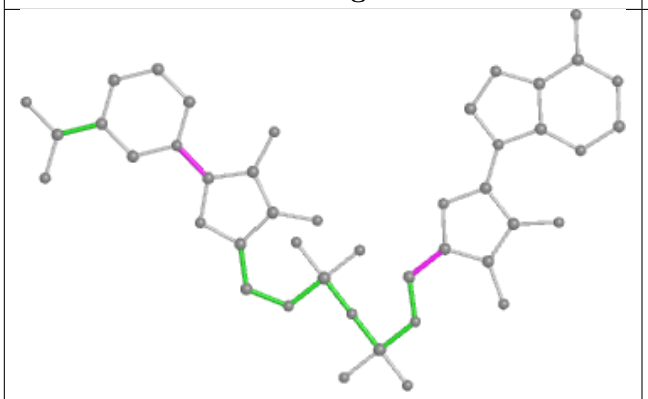
Ligand NAD B 608



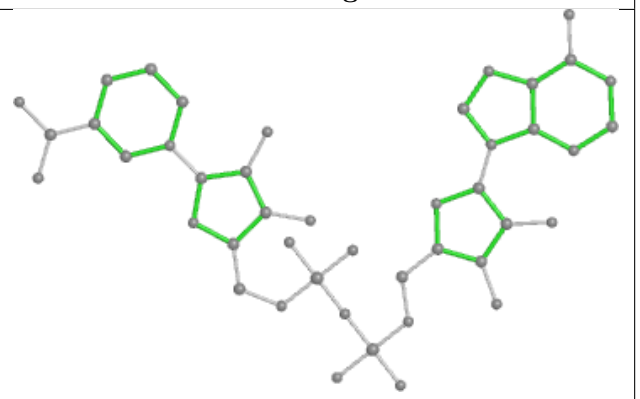
Bond lengths



Bond angles

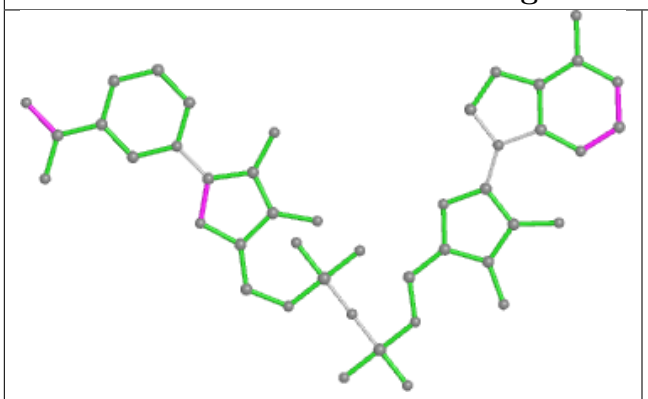


Torsions

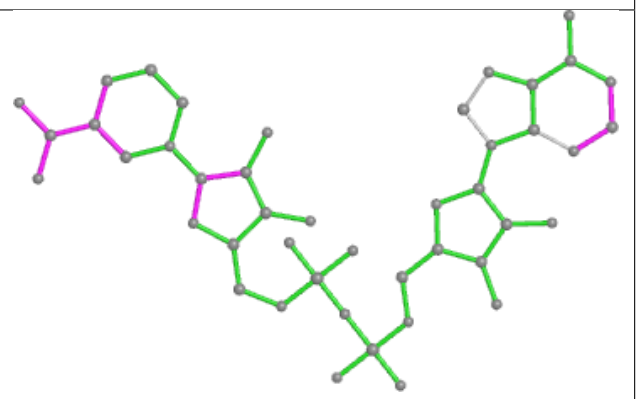


Rings

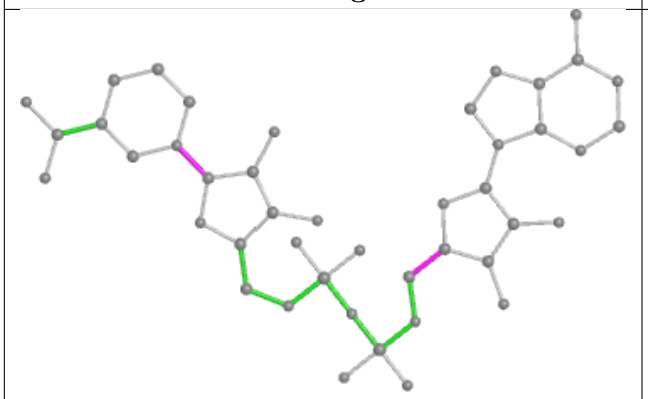
Ligand NAD A 608



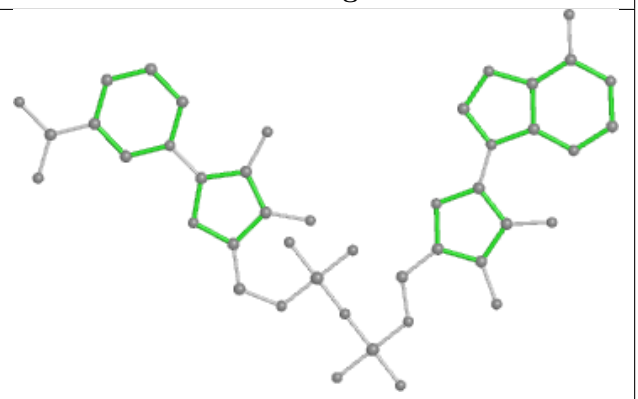
Bond lengths



Bond angles

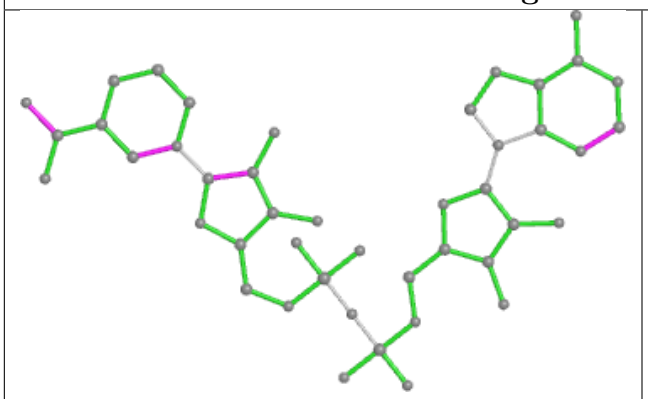


Torsions

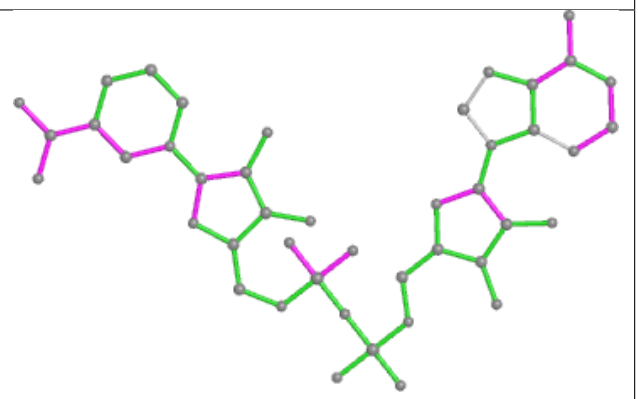


Rings

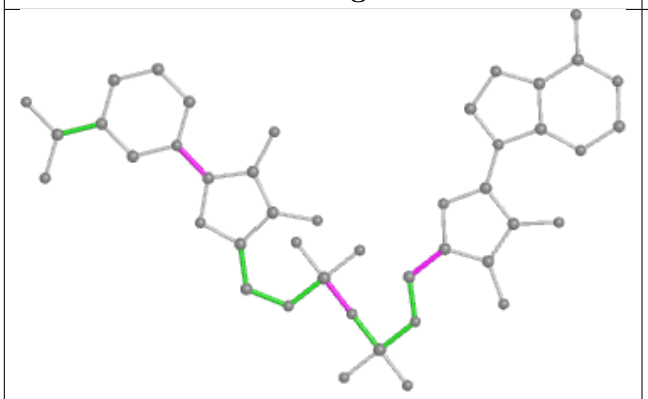
Ligand NAD C 608



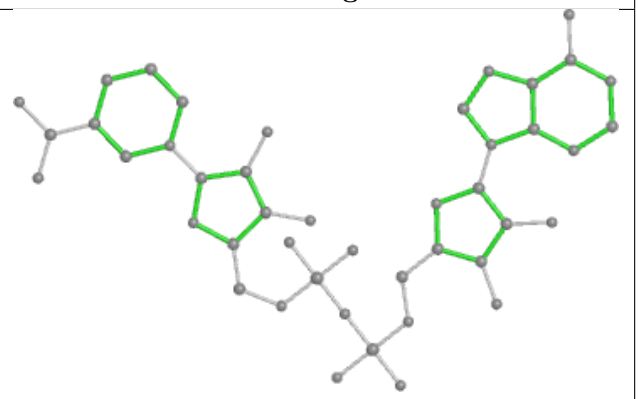
Bond lengths



Bond angles

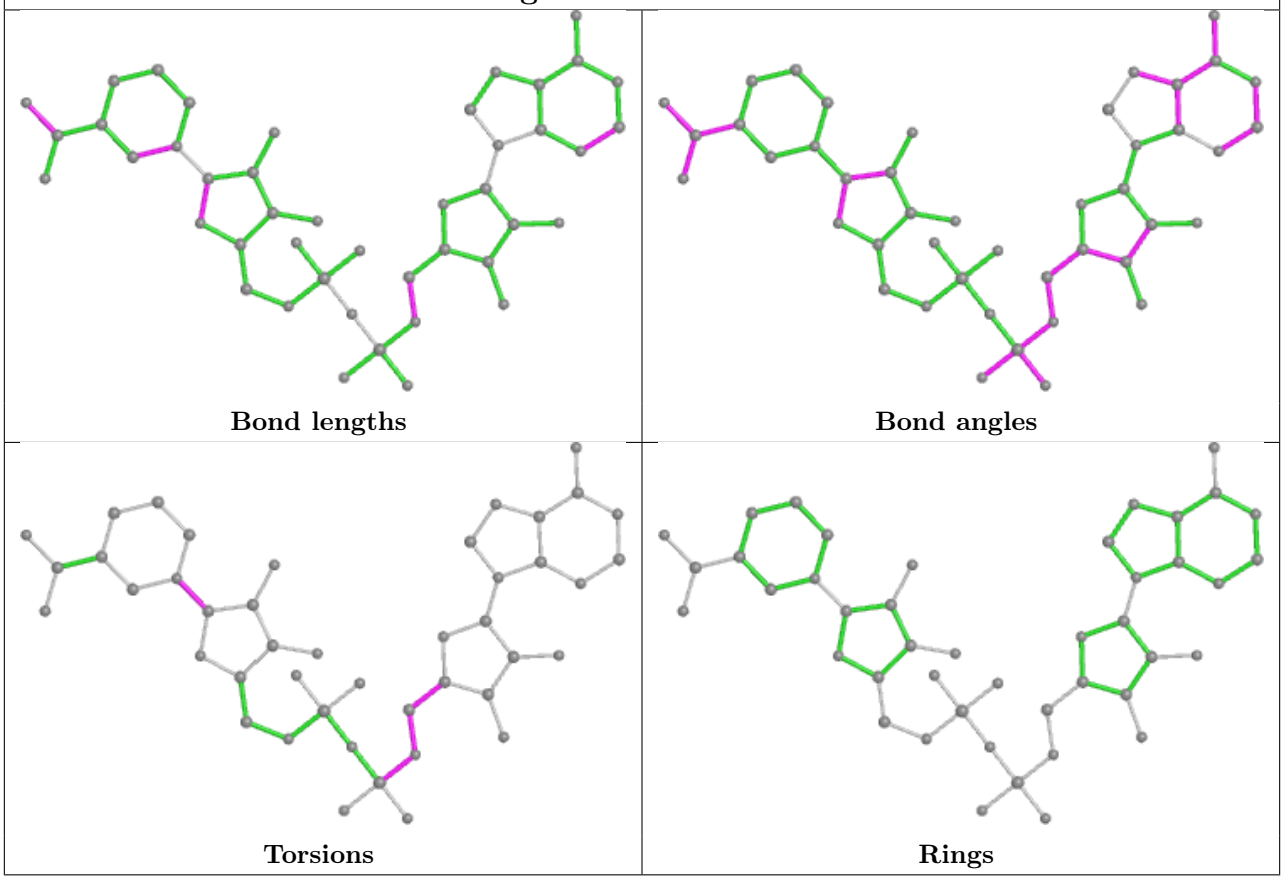


Torsions



Rings

Ligand NAD D 608



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	433/435 (99%)	-0.18	5 (1%) 79 81	22, 36, 56, 71	0
1	B	432/435 (99%)	-0.08	16 (3%) 41 44	27, 40, 60, 67	0
1	C	432/435 (99%)	-0.20	7 (1%) 72 74	22, 34, 51, 60	0
1	D	431/435 (99%)	0.29	42 (9%) 7 8	23, 44, 76, 92	0
All	All	1728/1740 (99%)	-0.04	70 (4%) 37 40	22, 37, 64, 92	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	TYR	6.5
1	D	607	ASN	5.4
1	D	554	PRO	5.3
1	C	607	ASN	5.3
1	B	606	PRO	5.2
1	D	299	VAL	4.8
1	D	287	ASP	4.7
1	B	556	GLY	4.6
1	D	260	ILE	4.4
1	D	300	GLU	4.4
1	D	188	VAL	4.2
1	D	291	TRP	4.1
1	D	181	LYS	4.0
1	D	180	SER	4.0
1	D	302	TRP	4.0
1	D	221	GLU	4.0
1	B	301	GLY	3.9
1	D	182	GLY	3.8
1	D	553	ALA	3.8
1	D	301	GLY	3.8
1	C	555	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	556	GLY	3.3
1	D	606	PRO	3.3
1	D	324	ASN	3.2
1	A	-2	SER	3.2
1	D	278	VAL	3.2
1	B	327	LYS	3.2
1	B	554	PRO	3.1
1	D	361	ASP	3.0
1	B	300	GLU	3.0
1	D	178	LYS	3.0
1	D	555	GLU	2.9
1	D	183	SER	2.9
1	B	341	HIS	2.9
1	C	300	GLU	2.9
1	D	220	GLY	2.9
1	A	607	ASN	2.9
1	D	185	ASP	2.9
1	D	328	LYS	2.8
1	C	176	GLN	2.8
1	B	345	GLN	2.8
1	A	261	TYR	2.8
1	C	606	PRO	2.7
1	A	300	GLU	2.7
1	D	280	ALA	2.7
1	D	195	GLU	2.6
1	D	341	HIS	2.6
1	B	-2	SER	2.6
1	D	274	SER	2.6
1	B	344	TYR	2.6
1	D	281	TRP	2.5
1	B	261	TYR	2.5
1	D	219	GLN	2.5
1	D	217	ARG	2.4
1	C	180	SER	2.4
1	B	555	GLU	2.4
1	D	297	VAL	2.3
1	A	217	ARG	2.3
1	D	316	HIS	2.2
1	D	296	CYS	2.2
1	D	288	ASP	2.2
1	D	560	GLN	2.2
1	B	557	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	557	ARG	2.1
1	B	217	ARG	2.1
1	B	181	LYS	2.1
1	D	225	ALA	2.1
1	C	301	GLY	2.1
1	D	283	GLY	2.1
1	B	560	GLN	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

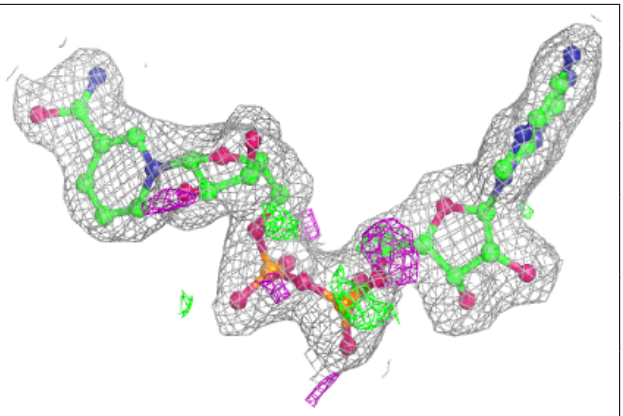
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

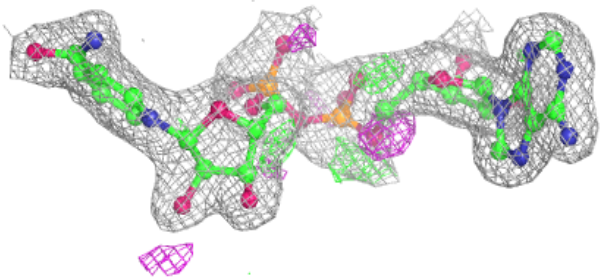
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	D	608	44/44	0.95	0.10	22,30,36,40	0
2	NAD	C	608	44/44	0.97	0.09	18,24,29,36	0
2	NAD	B	608	44/44	0.97	0.08	24,30,35,38	0
2	NAD	A	608	44/44	0.98	0.08	19,26,36,40	0

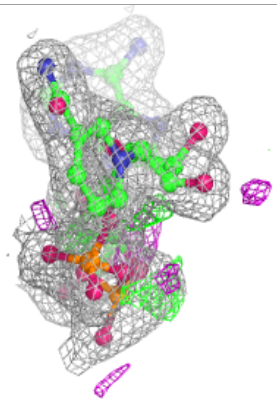
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 608:

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

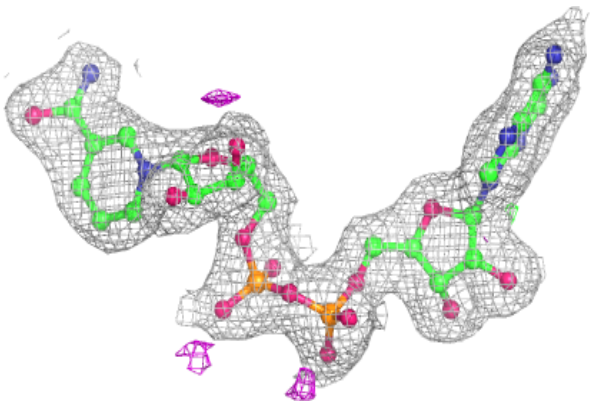


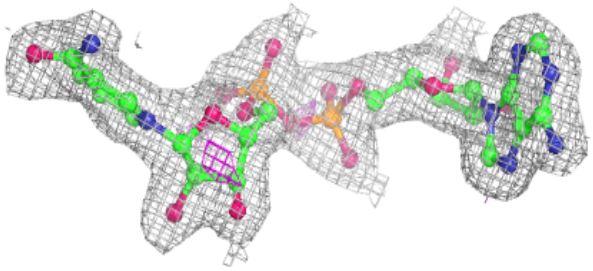


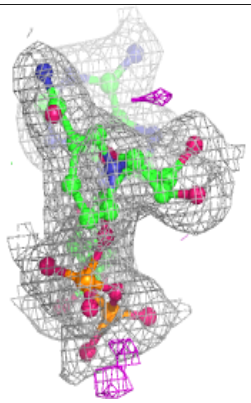


Electron density around NAD C 608:

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

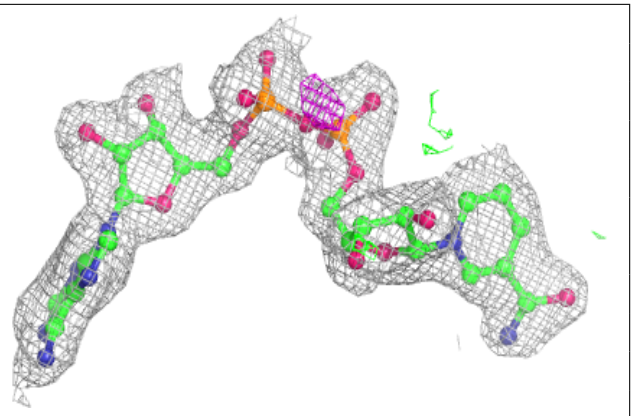


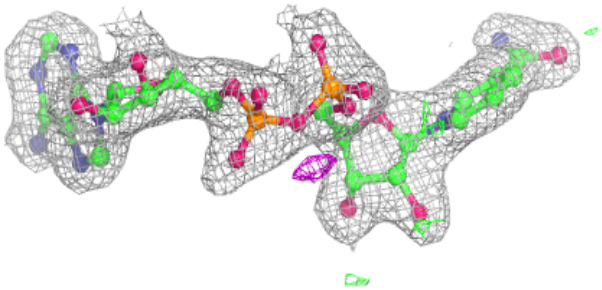


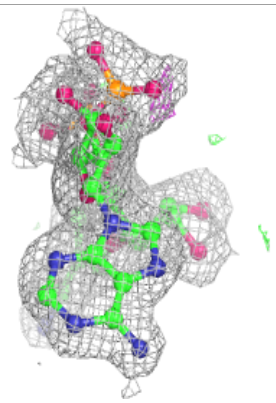


Electron density around NAD B 608:

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

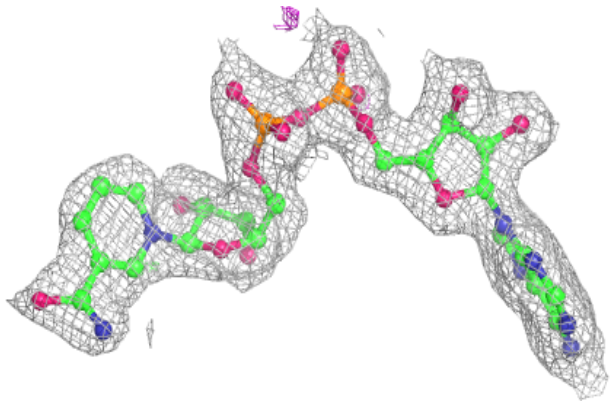


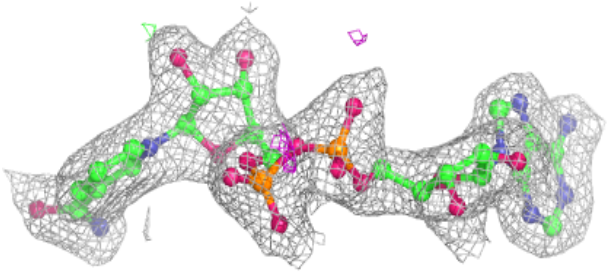


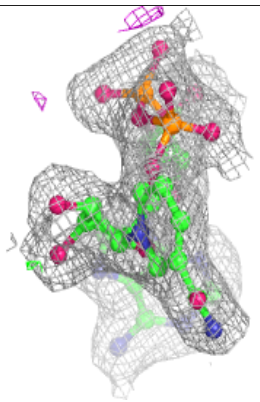


Electron density around NAD A 608:

$2mF_o$-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.