



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:28 am BST

PDB ID : 2GRU
Title : Crystal structure of 2-deoxy-scylo-inosose synthase complexed with carbaglu
cose-6-phosphate, NAD⁺ and Co²⁺
Authors : Nango, E.; Kumasaka, T.
Deposited on : 2006-04-25
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

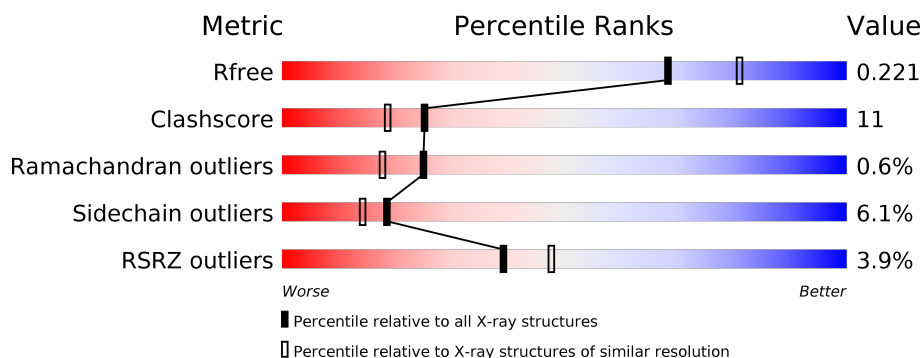
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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	368	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	368	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	608	-	-	X	-
5	NAD	B	604	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6183 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.

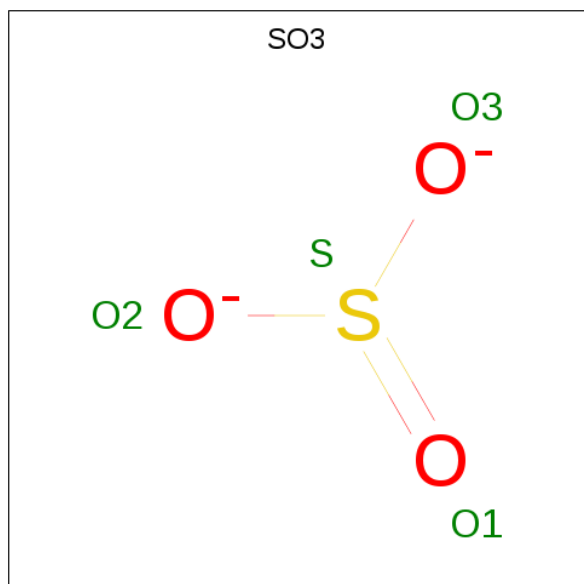
- Molecule 1 is a protein called 2-deoxy-scylo-inosose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	8	0
			2889	1848	488	537	16			
1	B	360	Total	C	N	O	S	0	10	0
			2828	1808	475	529	16			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 3 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



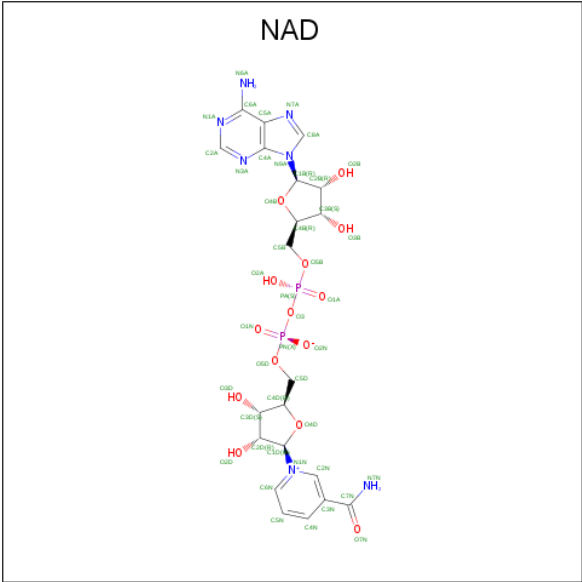
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			4	3	1		
3	B	1	Total	O	S	0	0
			4	3	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



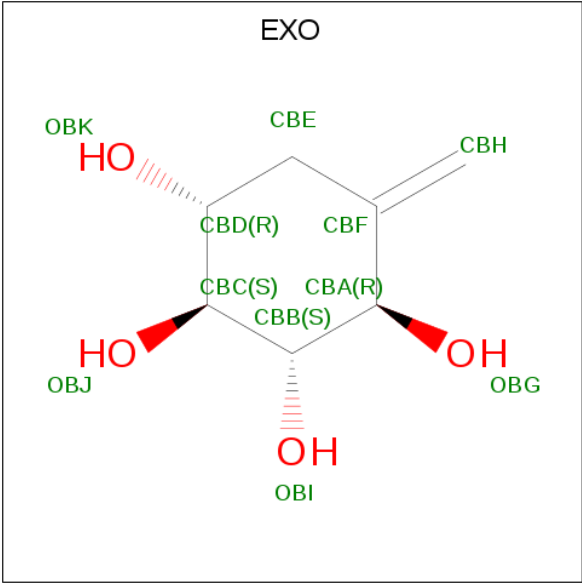
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



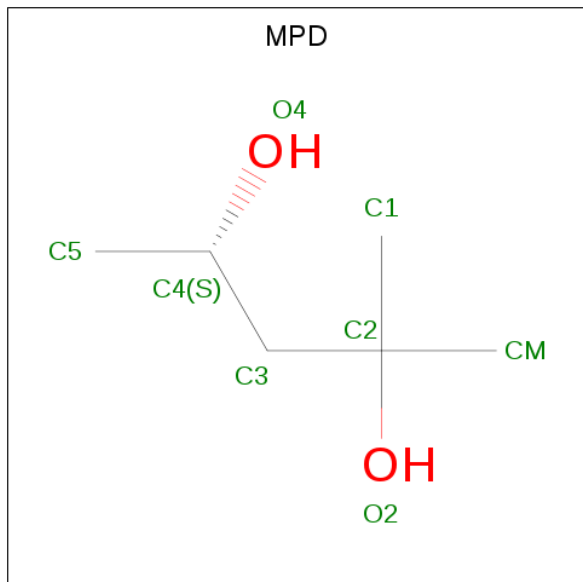
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
5	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 6 is (1R,2S,3S,4R)-5-METHYLENECYCLOHEXANE-1,2,3,4-TETRAOL (three-letter code: EXO) (formula: C₇H₁₂O₄).



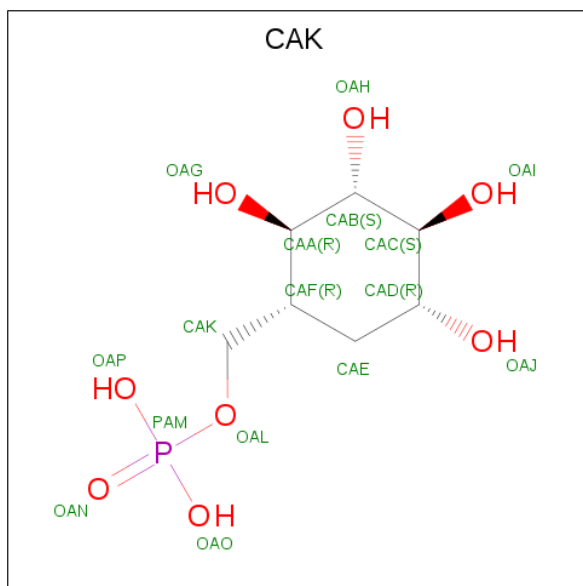
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	7	4		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is [(1R,2R,3S,4S,5R)-2,3,4,5-TETRAHYDROXYCYCLOHEXYL]METHYL DIHYDROGEN PHOSPHATE (three-letter code: CAK) (formula: $C_7H_{15}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O	P	0	0
			16	7	8	1		

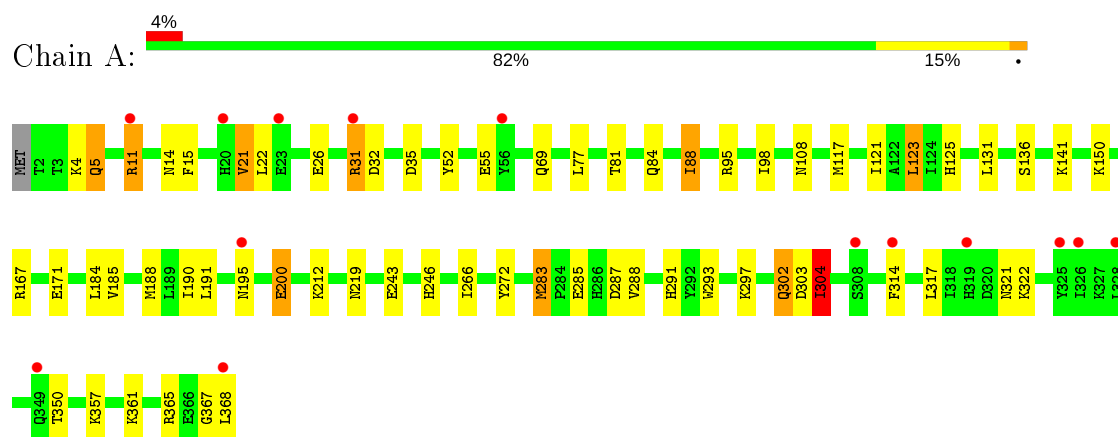
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	158	Total	O	0	0
			158	158		
9	B	162	Total	O	0	0
			162	162		

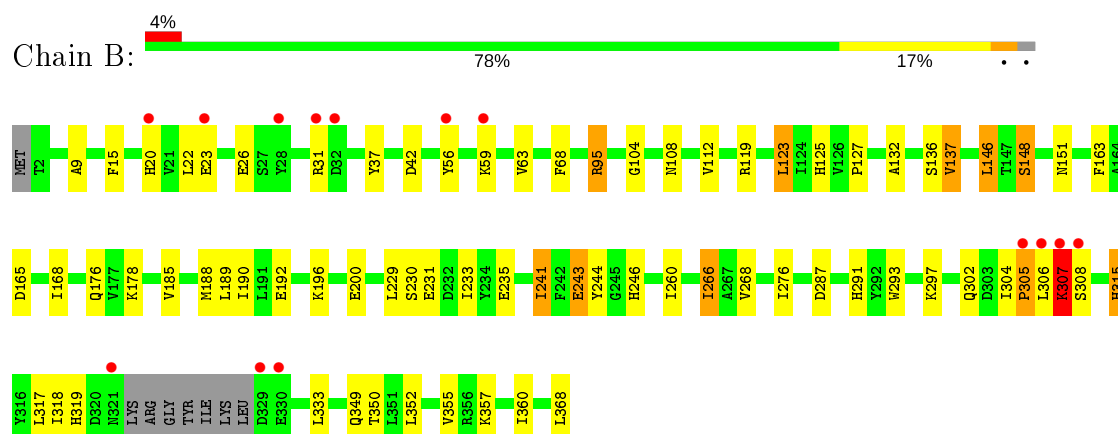
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: 2-deoxy-scylo-inosose synthase



• Molecule 1: 2-deoxy-scylo-inosose synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.57Å 70.11Å 81.57Å 90.00° 117.61° 90.00°	Depositor
Resolution (Å)	40.72 – 2.15 40.72 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.72-2.15) 99.2 (40.72-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.174 , 0.223 0.173 , 0.221	Depositor DCC
R_{free} test set	2171 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6183	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5105e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MPD, CO, NAD, EXO, PO4, CAK, SO3

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	0.91	0/2981	0.87	6/4030 (0.1%)
1	B	0.92	2/2924 (0.1%)	0.84	1/3953 (0.0%)
All	All	0.92	2/5905 (0.0%)	0.85	7/7983 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	VAL	CB-CG1	5.34	1.64	1.52
1	B	266	ILE	CB-CG2	5.02	1.68	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	123	LEU	CB-CG-CD2	6.76	122.50	111.00
1	B	123	LEU	CB-CG-CD2	5.82	120.89	111.00
1	A	35	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	283	MET	CG-SD-CE	-5.50	91.39	100.20
1	A	21	VAL	CB-CA-C	-5.37	101.20	111.40
1	A	317	LEU	CA-CB-CG	5.23	127.34	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2889	0	2886	56	0
1	B	2828	0	2806	66	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	5	0	0	2	0
5	A	44	0	25	5	0
5	B	44	0	25	10	0
6	A	11	0	10	2	0
7	A	8	0	14	3	0
7	B	8	0	14	1	0
8	B	16	0	11	0	0
9	A	158	0	0	4	0
9	B	162	0	0	8	0
All	All	6183	0	5791	125	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 11.

All (125) 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:31:ARG:HH11	1:A:31:ARG:HG2	1.07	1.12
1:B:350:THR:HG22	1:B:352:LEU:H	1.32	0.94
1:A:31:ARG:HG2	1:A:31:ARG:NH1	1.82	0.87
1:A:283:MET:HE1	1:A:288:VAL:HG22	1.61	0.81
1:A:4:LYS:HE3	1:A:219:ASN:HD21	1.47	0.79
1:A:88:ILE:HD13	1:B:146:LEU:HD23	1.67	0.77
1:A:283:MET:CE	1:A:288:VAL:N	2.48	0.77
5:A:603:NAD:H6N	9:A:728:HOH:O	1.85	0.74
1:B:355:VAL:CG1	1:B:360:ILE:HD11	2.16	0.74
1:B:108:ASN:HD21	5:B:604:NAD:C2N	2.01	0.73
4:A:608:PO4:O3	6:A:607:EXO:HBH2	1.89	0.72
1:A:98:ILE:CD1	1:A:121:ILE:HD11	2.19	0.72
1:B:315:HIS:NE2	9:B:721:HOH:O	2.20	0.71
1:B:151:ASN:ND2	5:B:604:NAD:N7N	2.38	0.71
1:A:200:GLU:H	1:A:200:GLU:CD	1.94	0.71
1:B:355:VAL:HG11	1:B:360:ILE:HD11	1.72	0.71
1:A:88:ILE:HD13	1:B:146:LEU:CD2	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:608:PO4:O3	6:A:607:EXO:CBH	2.40	0.69
1:A:283:MET:HE1	1:A:288:VAL:CG2	2.23	0.68
1:A:185:VAL:HG22	1:A:188[B]:MET:CE	2.24	0.68
1:B:260:ILE:CG2	1:B:305:PRO:HD2	2.24	0.67
1:B:125:HIS:HE1	9:B:710:HOH:O	1.77	0.66
5:B:604:NAD:N7N	9:B:693:HOH:O	2.27	0.65
1:A:283:MET:HE3	1:A:287:ASP:C	2.17	0.65
1:A:283:MET:HE3	1:A:288:VAL:N	2.14	0.62
1:A:31:ARG:HH11	1:A:31:ARG:CG	1.97	0.62
1:A:287:ASP:O	1:A:291:HIS:HD2	1.82	0.62
1:A:136:SER:HB2	5:A:603:NAD:C4N	2.29	0.62
1:A:171:GLU:OE1	7:A:611:MPD:H51	2.00	0.62
1:B:95:ARG:NH2	9:B:768:HOH:O	2.28	0.60
1:A:88:ILE:HG21	1:B:148:SER:CB	2.31	0.60
1:A:32:ASP:O	1:A:95:ARG:NH1	2.35	0.60
1:B:246:HIS:CE1	1:B:266:ILE:HG12	2.36	0.60
1:A:185:VAL:HA	1:A:188[B]:MET:HE2	1.82	0.59
1:A:4:LYS:HE3	1:A:219:ASN:ND2	2.14	0.59
1:A:302:GLN:HE21	1:A:302:GLN:N	2.01	0.58
1:B:185:VAL:HG22	1:B:188[B]:MET:CE	2.33	0.58
1:B:230:SER:O	1:B:233[B]:ILE:HD11	2.04	0.58
1:B:260:ILE:CG2	1:B:305:PRO:CD	2.81	0.58
1:B:20:HIS:HB3	1:B:23:GLU:CD	2.24	0.58
1:B:355:VAL:HG11	1:B:360:ILE:CD1	2.33	0.57
1:A:283:MET:CE	1:A:288:VAL:CA	2.83	0.57
1:A:314[B]:PHE:HZ	1:A:357:LYS:HD3	1.69	0.56
1:A:125:HIS:HE1	9:A:715:HOH:O	1.89	0.55
1:B:276:ILE:HD13	1:B:360:ILE:HD12	1.87	0.55
1:B:355:VAL:CG1	1:B:360:ILE:CD1	2.84	0.55
1:A:365:ARG:HD3	9:A:742:HOH:O	2.05	0.55
1:B:244:TYR:OH	1:B:291:HIS:HE1	1.90	0.55
1:B:26:GLU:OE2	1:B:59:LYS:HB3	2.06	0.55
1:B:178:LYS:NZ	1:B:302:GLN:HE21	2.05	0.54
1:A:246:HIS:CE1	1:A:266:ILE:HG12	2.42	0.54
1:A:293:TRP:CZ2	1:A:297:LYS:NZ	2.73	0.54
1:A:98:ILE:HD13	1:A:121:ILE:HD11	1.89	0.54
1:B:305:PRO:C	1:B:307:LYS:H	2.10	0.53
1:B:176:GLN:NE2	9:B:725:HOH:O	2.41	0.53
1:B:287:ASP:O	1:B:291:HIS:HD2	1.91	0.53
1:B:306:LEU:C	1:B:308:SER:H	2.13	0.53
1:B:188[A]:MET:HG2	1:B:196[A]:LYS:HE2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:PRO:HB2	1:B:307:LYS:HE2	1.91	0.52
1:A:136:SER:HB2	5:A:603:NAD:C3N	2.40	0.52
1:B:243:GLU:HG3	1:B:246:HIS:HB2	1.92	0.52
1:B:136:SER:HB3	5:B:604:NAD:H5N	1.92	0.52
1:A:69:GLN:NE2	9:A:706:HOH:O	2.33	0.51
1:B:22:LEU:HB2	9:B:746:HOH:O	2.09	0.51
1:A:5[A]:GLN:HG3	1:A:14:ASN:OD1	2.11	0.51
1:A:185:VAL:HA	1:A:188[B]:MET:CE	2.40	0.51
1:A:272:TYR:OH	1:A:367:GLY:HA2	2.11	0.51
7:B:610:MPD:H53	7:B:610:MPD:H11	1.92	0.51
1:B:317:LEU:HD21	1:B:360:ILE:HG21	1.91	0.51
1:A:184:LEU:HD23	1:A:188[B]:MET:HE2	1.93	0.51
1:A:88:ILE:HG21	1:B:148:SER:HB2	1.93	0.51
1:A:283:MET:CE	1:A:288:VAL:HA	2.41	0.50
1:A:283:MET:CE	1:A:288:VAL:CG2	2.90	0.49
1:B:23:GLU:HG2	1:B:56:TYR:CZ	2.46	0.49
1:A:304:ILE:O	1:A:304:ILE:CG2	2.61	0.49
1:B:136:SER:HB3	5:B:604:NAD:C5N	2.43	0.49
1:B:151:ASN:HD21	5:B:604:NAD:H71N	1.61	0.49
1:B:104:GLY:O	9:B:767:HOH:O	2.20	0.48
1:A:302:GLN:HE21	1:A:302:GLN:H	1.61	0.48
1:B:20:HIS:HB3	1:B:23:GLU:OE2	2.14	0.48
1:A:283:MET:HE2	1:A:288:VAL:N	2.26	0.48
1:B:244:TYR:OH	1:B:291:HIS:CE1	2.67	0.48
1:B:127:PRO:HD2	1:B:163:PHE:O	2.14	0.48
1:A:141:LYS:HD2	1:B:119:ARG:CZ	2.44	0.47
1:A:88:ILE:HD12	1:A:117:MET:HE3	1.96	0.47
1:B:108:ASN:HD21	5:B:604:NAD:H2N	1.78	0.47
1:B:9:ALA:N	1:B:233[B]:ILE:HD11	2.29	0.47
1:A:190:ILE:HG13	1:A:191:LEU:HG	1.97	0.47
1:B:132:ALA:O	1:B:137:VAL:HB	2.14	0.47
1:A:131:LEU:HD23	5:A:603:NAD:O2N	2.15	0.47
1:A:185:VAL:HG22	1:A:188[B]:MET:HE3	1.97	0.47
1:A:52:TYR:CD1	7:A:611:MPD:H11	2.50	0.46
1:B:260:ILE:HG21	1:B:305:PRO:HD2	1.98	0.46
1:A:283:MET:HE1	1:A:288:VAL:HA	1.99	0.45
1:B:268:VAL:HG13	1:B:368:LEU:HD21	1.98	0.45
1:B:243:GLU:O	1:B:246:HIS:HB2	2.17	0.45
1:A:22:LEU:HA	1:A:22:LEU:HD23	1.86	0.44
5:B:604:NAD:C2N	5:B:604:NAD:O2D	2.65	0.44
1:A:26:GLU:OE1	1:A:31:ARG:NH2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:611:MPD:O2	7:A:611:MPD:H53	2.17	0.44
1:B:190:ILE:HB	1:B:241:ILE:CD1	2.48	0.44
1:B:231:GLU:HG3	9:B:732:HOH:O	2.18	0.44
1:B:200:GLU:HG2	1:B:293:TRP:CH2	2.54	0.43
1:B:9:ALA:H	1:B:233[B]:ILE:HD11	1.83	0.43
1:B:318:ILE:HG13	1:B:319:HIS:HD2	1.83	0.43
1:B:355:VAL:HG12	1:B:360:ILE:HD11	1.99	0.43
1:A:283:MET:HE1	1:A:288:VAL:CA	2.48	0.43
1:B:231:GLU:O	1:B:233[B]:ILE:HD12	2.19	0.42
1:B:108:ASN:ND2	5:B:604:NAD:C2N	2.77	0.42
1:B:260:ILE:HG22	1:B:305:PRO:HD3	2.00	0.42
1:B:333:LEU:HG	1:B:357:LYS:HG2	2.00	0.42
5:B:604:NAD:H2N	5:B:604:NAD:H71N	1.62	0.42
1:A:314[A]:PHE:CE1	1:A:361:LYS:HA	2.55	0.41
1:B:185:VAL:HG22	1:B:188[B]:MET:HE2	2.00	0.41
1:B:260:ILE:HG21	1:B:260:ILE:HD13	1.86	0.41
1:A:81:THR:HA	1:A:84:GLN:HE21	1.85	0.41
1:B:229:LEU:HD22	1:B:235:GLU:HG2	2.02	0.41
1:A:243:GLU:O	1:A:246:HIS:HB2	2.21	0.40
1:B:37:TYR:HB2	1:B:63:VAL:HG22	2.03	0.40
1:B:355:VAL:HG12	1:B:360:ILE:CD1	2.51	0.40
1:B:360:ILE:HD13	1:B:360:ILE:N	2.36	0.40
1:B:42:ASP:HB3	1:B:68:PHE:CZ	2.57	0.40
1:B:165:ASP:HB3	1:B:168:ILE:HD12	2.03	0.40
1:A:108:ASN:OD1	5:A:603:NAD:H1D	2.21	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	372/368 (101%)	359 (96%)	11 (3%)	2 (0%)	29 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	363/368 (99%)	348 (96%)	13 (4%)	2 (1%)	25	18
All	All	735/736 (100%)	707 (96%)	24 (3%)	4 (0%)	25	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	ASP
1	B	305	PRO
1	B	307	LYS
1	A	304	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	314/308 (102%)	291 (93%)	23 (7%)	14	9
1	B	309/308 (100%)	293 (95%)	16 (5%)	23	19
All	All	623/616 (101%)	584 (94%)	39 (6%)	18	13

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5[A]	GLN
1	A	5[B]	GLN
1	A	11[A]	ARG
1	A	11[B]	ARG
1	A	15	PHE
1	A	21	VAL
1	A	31	ARG
1	A	55	GLU
1	A	77	LEU
1	A	88	ILE
1	A	123	LEU
1	A	150	LYS

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Mol	Chain	Res	Type
1	A	167	ARG
1	A	195	ASN
1	A	200	GLU
1	A	212	LYS
1	A	285	GLU
1	A	302	GLN
1	A	304	ILE
1	A	321	ASN
1	A	322	LYS
1	A	350	THR
1	A	368	LEU
1	B	15	PHE
1	B	31	ARG
1	B	95	ARG
1	B	123	LEU
1	B	137	VAL
1	B	146	LEU
1	B	148	SER
1	B	189	LEU
1	B	192	GLU
1	B	241	ILE
1	B	243	GLU
1	B	297	LYS
1	B	304	ILE
1	B	307	LYS
1	B	315	HIS
1	B	349	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	84	GLN
1	A	125	HIS
1	A	219	ASN
1	A	250	HIS
1	A	291	HIS
1	A	302	GLN
1	A	319	HIS
1	B	69	GLN
1	B	84	GLN
1	B	108	ASN

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Mol	Chain	Res	Type
1	B	125	HIS
1	B	176	GLN
1	B	291	HIS
1	B	302	GLN
1	B	348	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\# Z > 2$
7	MPD	A	611	-	7,7,7	0.27	0	9,10,10	0.39	0
8	CAK	B	609	2	16,16,16	1.15	1 (6%)	21,24,24	1.33	1 (4%)
5	NAD	B	604	-	42,48,48	1.98	12 (28%)	50,73,73	2.00	10 (20%)
4	PO4	A	608	-	4,4,4	0.97	0	6,6,6	0.82	0
3	SO3	B	606	-	1,3,3	0.95	0	0,3,3	0.00	-
5	NAD	A	603	-	42,48,48	2.40	14 (33%)	50,73,73	2.05	18 (36%)
6	EXO	A	607	2	11,11,11	1.46	1 (9%)	13,16,16	1.99	3 (23%)
3	SO3	A	605	-	1,3,3	0.46	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MPD	B	610	-	7,7,7	0.47	0	9,10,10	0.81	0

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
7	MPD	A	611	-	-	4/5/5/5	-
5	NAD	B	604	-	1/1/11/11	3/26/62/62	0/5/5/5
8	CAK	B	609	2	-	0/6/26/26	0/1/1/1
5	NAD	A	603	-	-	1/26/62/62	0/5/5/5
6	EXO	A	607	2	-	-	0/1/1/1
7	MPD	B	610	-	-	1/5/5/5	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	603	NAD	C2N-N1N	7.67	1.44	1.35
5	A	603	NAD	O7N-C7N	7.19	1.37	1.24
5	B	604	NAD	O7N-C7N	6.08	1.35	1.24
5	B	604	NAD	O4B-C1B	4.97	1.48	1.41
5	B	604	NAD	C2N-N1N	4.90	1.40	1.35
5	A	603	NAD	O4B-C1B	4.46	1.47	1.41
5	A	603	NAD	O3B-C3B	3.92	1.52	1.43
6	A	607	EXO	CBD-CBC	3.52	1.57	1.52
5	A	603	NAD	C6N-N1N	3.26	1.43	1.35
5	A	603	NAD	C2B-C3B	-3.18	1.44	1.53
5	A	603	NAD	O4D-C1D	2.92	1.45	1.41
5	B	604	NAD	O4B-C4B	2.85	1.51	1.45
5	B	604	NAD	C2B-C3B	-2.81	1.45	1.53
5	A	603	NAD	O2B-C2B	-2.68	1.36	1.43
5	B	604	NAD	C5D-C4D	2.60	1.59	1.51
5	A	603	NAD	PN-O5D	2.55	1.69	1.59
5	B	604	NAD	C6N-N1N	2.52	1.41	1.35
5	B	604	NAD	O4D-C1D	2.51	1.44	1.41
5	A	603	NAD	PA-O5B	2.37	1.68	1.59
5	A	603	NAD	PN-O2N	-2.33	1.44	1.55
5	A	603	NAD	C3N-C7N	2.30	1.54	1.50
5	B	604	NAD	O2B-C2B	-2.25	1.37	1.43
5	A	603	NAD	C2B-C1B	-2.21	1.50	1.53
8	B	609	CAK	CAD-CAC	2.20	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	604	NAD	C2D-C1D	-2.19	1.50	1.53
5	A	603	NAD	O2D-C2D	2.15	1.48	1.43
5	B	604	NAD	PN-O2N	-2.13	1.45	1.55
5	B	604	NAD	C2B-C1B	-2.12	1.50	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	604	NAD	O4B-C1B-C2B	-6.35	97.64	106.93
5	B	604	NAD	N3A-C2A-N1A	-4.84	121.11	128.68
5	A	603	NAD	O7N-C7N-N7N	4.58	129.08	122.58
5	B	604	NAD	O2B-C2B-C3B	4.41	126.08	111.82
5	A	603	NAD	O4D-C1D-C2D	-4.33	100.60	106.93
5	A	603	NAD	N3A-C2A-N1A	-4.33	121.92	128.68
5	A	603	NAD	O4B-C1B-C2B	-4.08	100.96	106.93
5	B	604	NAD	C3N-C7N-N7N	-4.00	112.95	117.75
8	B	609	CAK	OAP-PAM-OAL	-3.94	96.25	106.73
6	A	607	EXO	OBJ-CBC-CBD	3.91	117.48	109.99
5	B	604	NAD	C1B-N9A-C4A	-3.80	119.96	126.64
5	B	604	NAD	O3B-C3B-C4B	3.49	121.15	111.05
6	A	607	EXO	OBK-CBD-CBC	3.37	116.89	110.14
5	A	603	NAD	C6N-N1N-C2N	-3.36	118.91	121.97
5	A	603	NAD	O3B-C3B-C4B	3.16	120.17	111.05
5	A	603	NAD	C1B-N9A-C4A	-3.15	121.10	126.64
5	B	604	NAD	C3B-C2B-C1B	3.13	105.69	100.98
5	B	604	NAD	O2B-C2B-C1B	3.12	122.38	110.85
5	A	603	NAD	O7N-C7N-C3N	-2.96	116.09	119.63
5	A	603	NAD	C4A-C5A-N7A	-2.92	106.35	109.40
6	A	607	EXO	CBA-CBF-CBH	-2.88	118.81	122.25
5	B	604	NAD	C6N-N1N-C2N	-2.74	119.47	121.97
5	A	603	NAD	O3B-C3B-C2B	2.73	120.64	111.82
5	A	603	NAD	C5A-C6A-N6A	2.49	124.13	120.35
5	A	603	NAD	O4B-C4B-C3B	-2.48	100.22	105.11
5	A	603	NAD	C3N-C7N-N7N	-2.45	114.81	117.75
5	B	604	NAD	O7N-C7N-C3N	2.36	122.46	119.63
5	A	603	NAD	C5D-C4D-C3D	2.36	124.03	115.18
5	A	603	NAD	O4D-C4D-C5D	-2.34	101.66	109.37
5	A	603	NAD	C2N-C3N-C4N	2.19	120.74	118.26
5	A	603	NAD	C2B-C3B-C4B	2.09	106.70	102.64
5	A	603	NAD	O2D-C2D-C3D	2.01	118.31	111.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	604	NAD	C2B

All (9) torsion outliers are listed below:

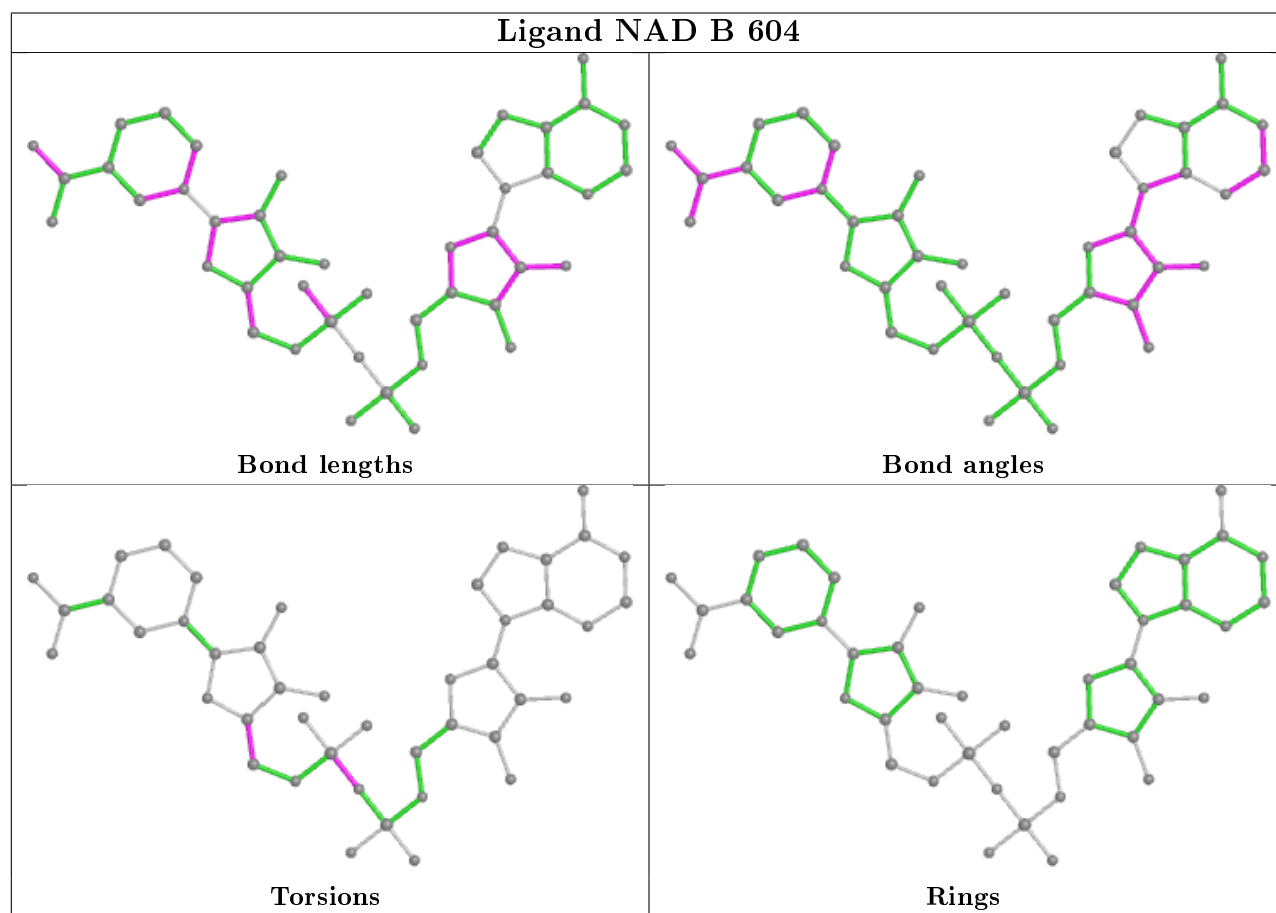
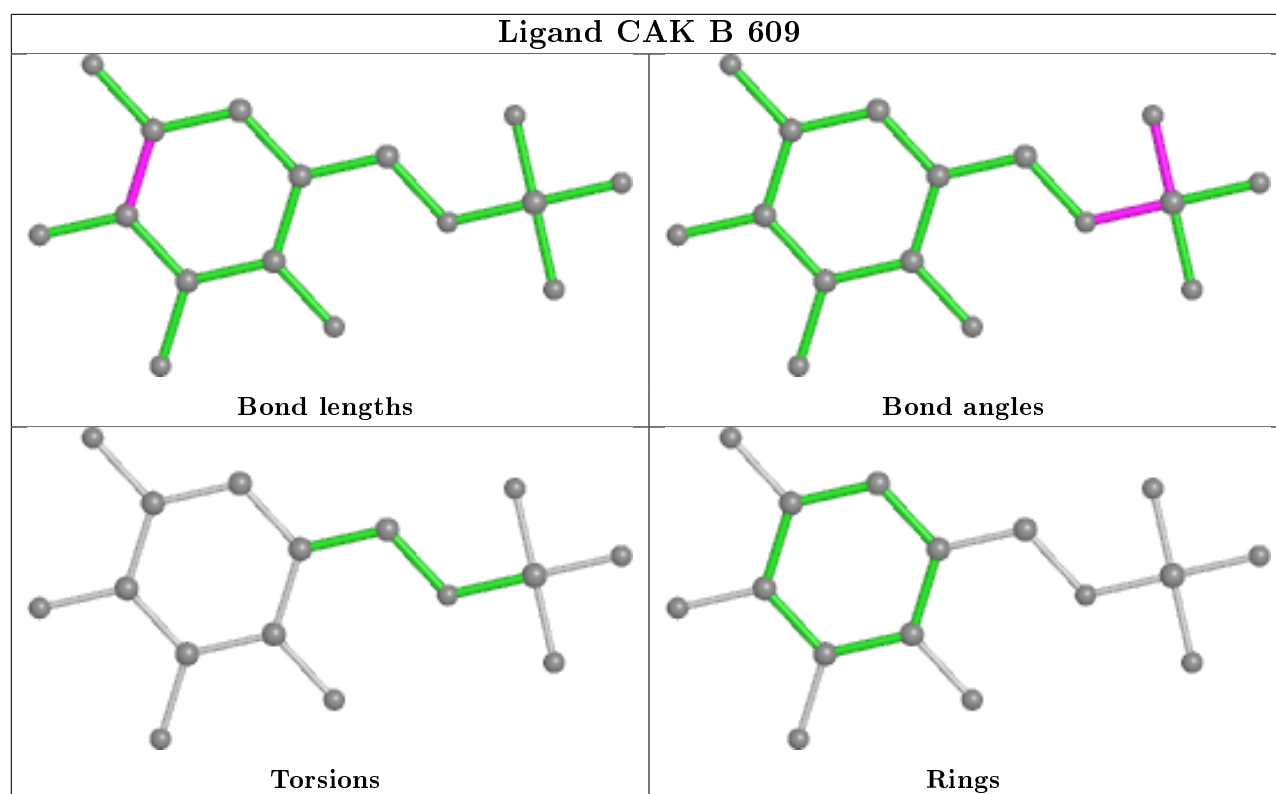
Mol	Chain	Res	Type	Atoms
5	B	604	NAD	PA-O3-PN-O5D
5	B	604	NAD	C3D-C4D-C5D-O5D
5	B	604	NAD	O4D-C4D-C5D-O5D
7	A	611	MPD	O2-C2-C3-C4
5	A	603	NAD	PA-O3-PN-O5D
7	B	610	MPD	C2-C3-C4-C5
7	A	611	MPD	C1-C2-C3-C4
7	A	611	MPD	CM-C2-C3-C4
7	A	611	MPD	C2-C3-C4-C5

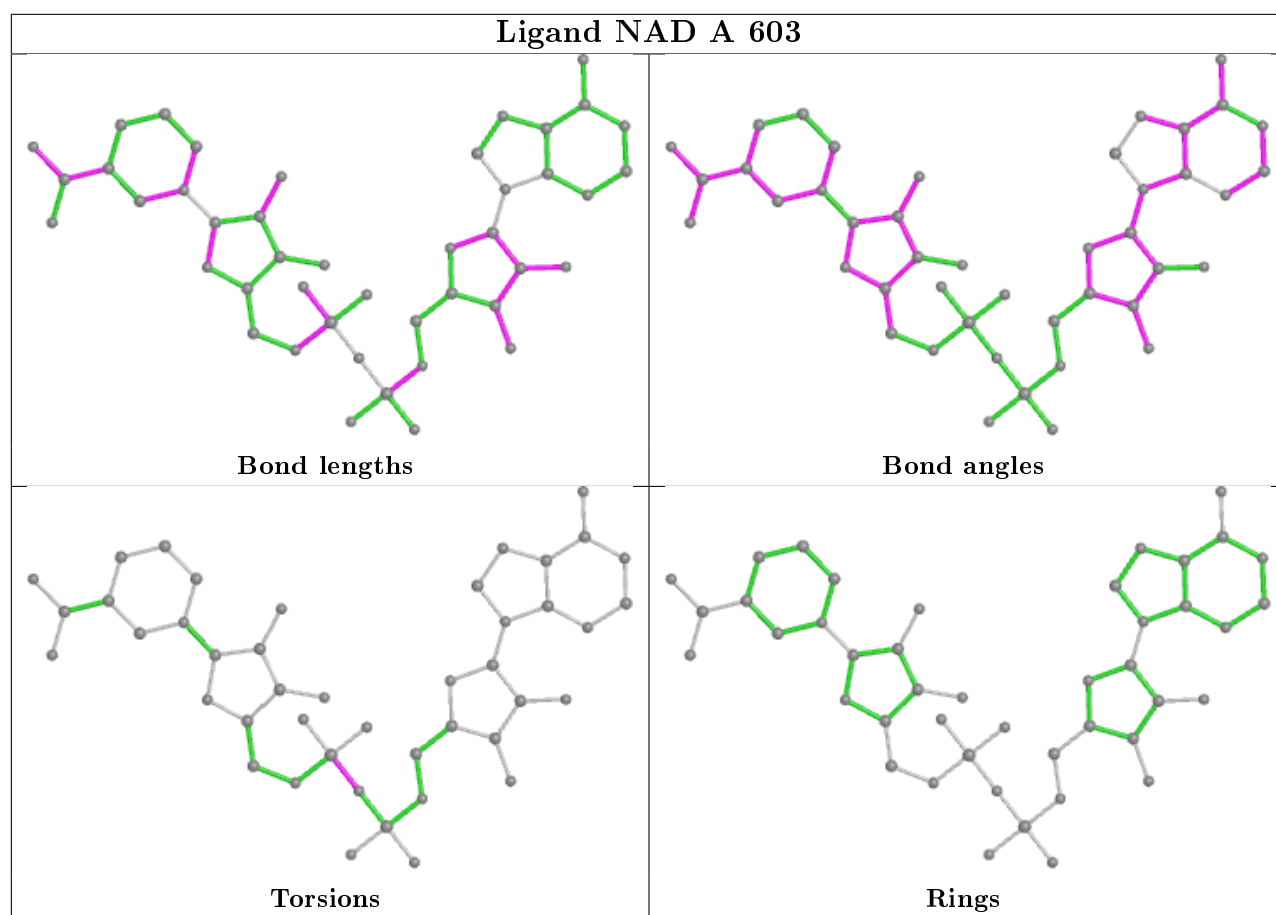
There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	611	MPD	3	0
5	B	604	NAD	10	0
4	A	608	PO4	2	0
5	A	603	NAD	5	0
6	A	607	EXO	2	0
7	B	610	MPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	367/368 (99%)	-0.23	14 (3%)	40 49	11, 20, 47, 70	0
1	B	360/368 (97%)	-0.21	14 (3%)	39 48	10, 23, 45, 62	0
All	All	727/736 (98%)	-0.22	28 (3%)	39 48	10, 21, 46, 70	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	LEU	7.7
1	B	305	PRO	4.1
1	B	32[A]	ASP	3.9
1	B	31	ARG	3.8
1	A	31	ARG	3.8
1	A	195	ASN	3.7
1	B	56	TYR	3.5
1	A	325	TYR	3.2
1	B	307	LYS	3.0
1	B	308	SER	2.9
1	B	329	ASP	2.9
1	B	59	LYS	2.8
1	B	321[A]	ASN	2.7
1	A	314[A]	PHE	2.6
1	A	326	ILE	2.6
1	B	28	TYR	2.5
1	A	368	LEU	2.5
1	A	328	LEU	2.4
1	B	330	GLU	2.4
1	A	20	HIS	2.4
1	B	23	GLU	2.3
1	A	23	GLU	2.3
1	B	20	HIS	2.2
1	A	56	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	319	HIS	2.1
1	A	349	GLN	2.1
1	A	308	SER	2.1
1	A	11[A]	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

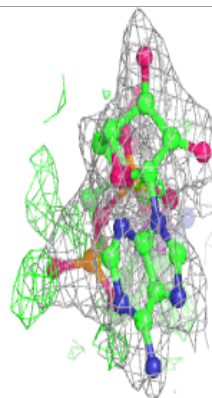
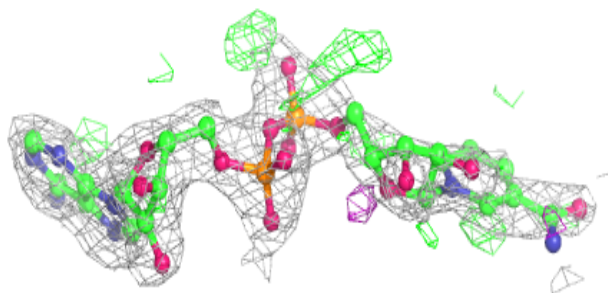
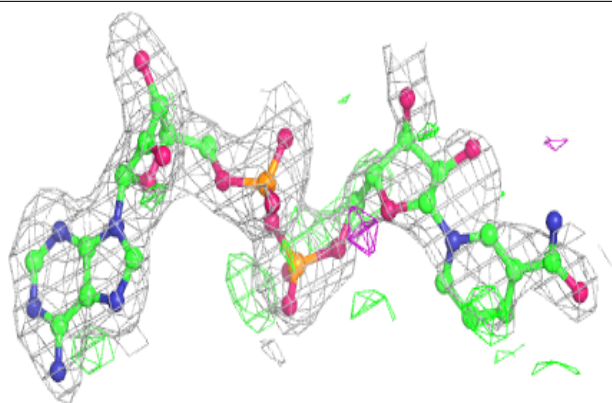
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MPD	B	610	8/8	0.82	0.25	39,41,42,43	8
7	MPD	A	611	8/8	0.87	0.18	27,30,33,36	8
6	EXO	A	607	11/11	0.89	0.18	20,30,35,38	0
5	NAD	B	604	44/44	0.93	0.20	15,25,39,40	44
5	NAD	A	603	44/44	0.95	0.12	23,31,39,40	0
8	CAK	B	609	16/16	0.95	0.13	19,32,38,38	0
4	PO4	A	608	5/5	0.95	0.17	37,38,39,41	5
3	SO3	A	605	4/4	0.97	0.09	10,11,12,21	4
3	SO3	B	606	4/4	0.98	0.06	9,14,16,24	4
2	CO	B	602	1/1	1.00	0.09	14,14,14,14	0
2	CO	A	601	1/1	1.00	0.10	14,14,14,14	0

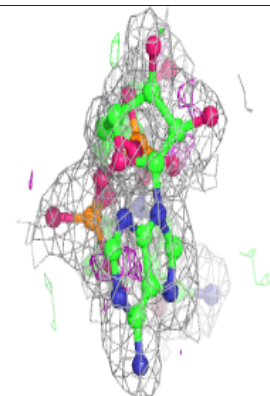
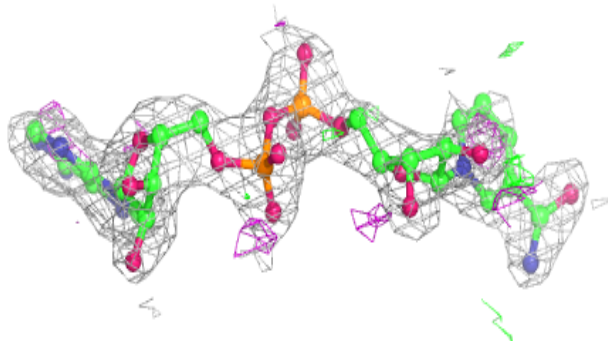
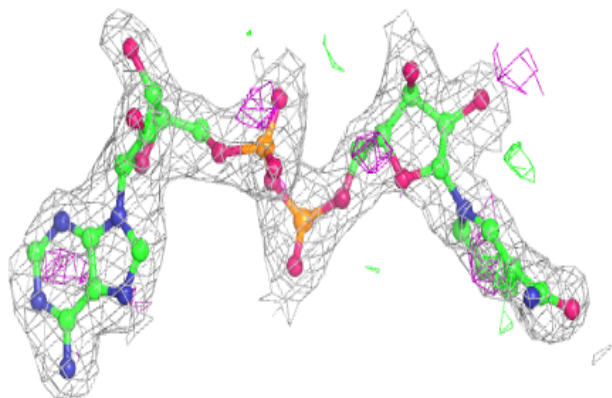
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 604:

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

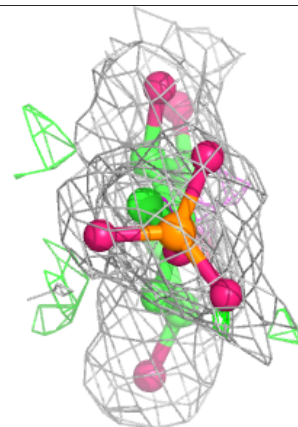
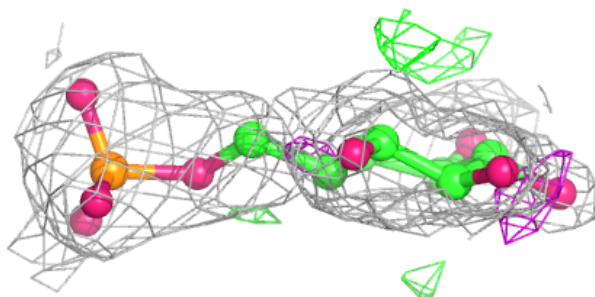
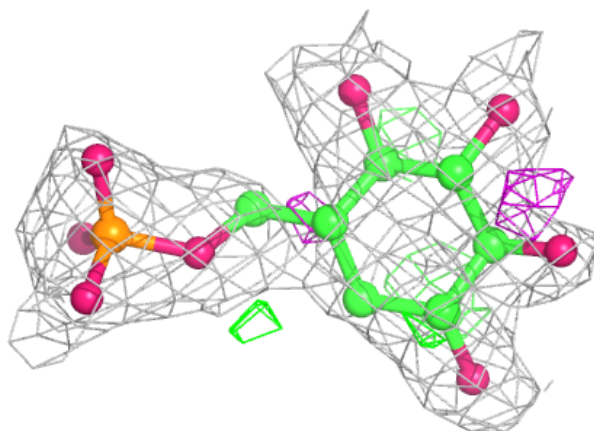
**Electron density around NAD A 603:**

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



Electron density around CAK B 609:

$2mF_o-DF_c$ (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.