



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:06 PM UTC

PDB ID : 4GX2 / pdb_00004gx2
Title : GsuK channel bound to NAD
Authors : Kong, C.; Zeng, W.; Ye, S.; Chen, L.; Sauer, D.B.; Lam, Y.; Derebe, M.G.; Jiang, Y.
Deposited on : 2012-09-03
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

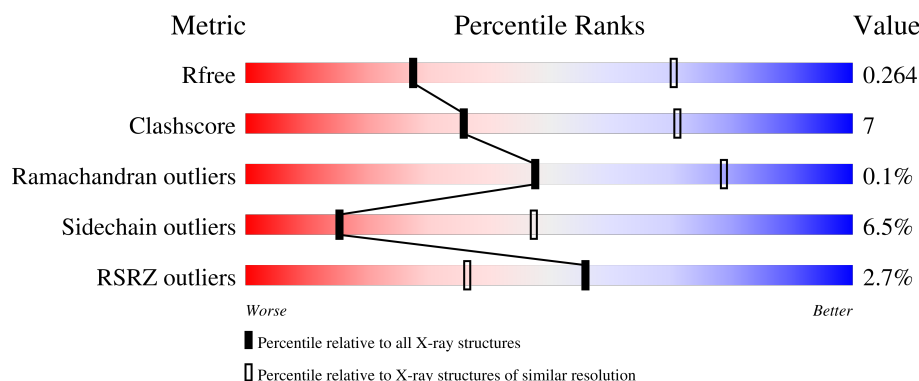
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	565	56% 9% . 34%
1	B	565	4% 73% 22% . .
1	C	565	3% 77% 18% . .
1	D	565	% 53% 12% . 33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14511 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 TrkA domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2922	1880	506	525	11			
1	B	548	Total	C	N	O	S	0	0	0
			4208	2693	729	771	15			
1	C	547	Total	C	N	O	S	0	0	0
			4197	2687	725	770	15			
1	D	376	Total	C	N	O	S	0	0	0
			2928	1883	507	527	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	expression tag	UNP Q74FS9
A	5	GLN	-	expression tag	UNP Q74FS9
A	6	ARG	-	expression tag	UNP Q74FS9
A	7	GLY	-	expression tag	UNP Q74FS9
A	8	SER	-	expression tag	UNP Q74FS9
A	52	ALA	GLU	engineered mutation	UNP Q74FS9
A	77	GLU	GLN	engineered mutation	UNP Q74FS9
A	97	ASP	LEU	engineered mutation	UNP Q74FS9
A	565	LEU	-	expression tag	UNP Q74FS9
A	566	VAL	-	expression tag	UNP Q74FS9
A	567	PRO	-	expression tag	UNP Q74FS9
A	568	ARG	-	expression tag	UNP Q74FS9
B	4	MET	-	expression tag	UNP Q74FS9
B	5	GLN	-	expression tag	UNP Q74FS9
B	6	ARG	-	expression tag	UNP Q74FS9
B	7	GLY	-	expression tag	UNP Q74FS9
B	8	SER	-	expression tag	UNP Q74FS9
B	52	ALA	GLU	engineered mutation	UNP Q74FS9
B	77	GLU	GLN	engineered mutation	UNP Q74FS9
B	97	ASP	LEU	engineered mutation	UNP Q74FS9
B	565	LEU	-	expression tag	UNP Q74FS9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	566	VAL	-	expression tag	UNP Q74FS9
B	567	PRO	-	expression tag	UNP Q74FS9
B	568	ARG	-	expression tag	UNP Q74FS9
C	4	MET	-	expression tag	UNP Q74FS9
C	5	GLN	-	expression tag	UNP Q74FS9
C	6	ARG	-	expression tag	UNP Q74FS9
C	7	GLY	-	expression tag	UNP Q74FS9
C	8	SER	-	expression tag	UNP Q74FS9
C	52	ALA	GLU	engineered mutation	UNP Q74FS9
C	77	GLU	GLN	engineered mutation	UNP Q74FS9
C	97	ASP	LEU	engineered mutation	UNP Q74FS9
C	565	LEU	-	expression tag	UNP Q74FS9
C	566	VAL	-	expression tag	UNP Q74FS9
C	567	PRO	-	expression tag	UNP Q74FS9
C	568	ARG	-	expression tag	UNP Q74FS9
D	4	MET	-	expression tag	UNP Q74FS9
D	5	GLN	-	expression tag	UNP Q74FS9
D	6	ARG	-	expression tag	UNP Q74FS9
D	7	GLY	-	expression tag	UNP Q74FS9
D	8	SER	-	expression tag	UNP Q74FS9
D	52	ALA	GLU	engineered mutation	UNP Q74FS9
D	77	GLU	GLN	engineered mutation	UNP Q74FS9
D	97	ASP	LEU	engineered mutation	UNP Q74FS9
D	565	LEU	-	expression tag	UNP Q74FS9
D	566	VAL	-	expression tag	UNP Q74FS9
D	567	PRO	-	expression tag	UNP Q74FS9
D	568	ARG	-	expression tag	UNP Q74FS9

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total K 5 5	0	0
2	B	1	Total K 1 1	0	0
2	C	5	Total K 5 5	0	0
2	D	1	Total K 1 1	0	0

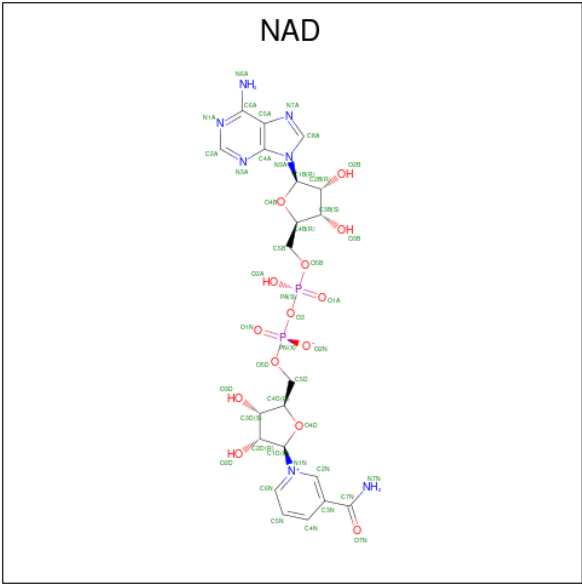
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	2	Total	Ca	0	0
			2	2		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



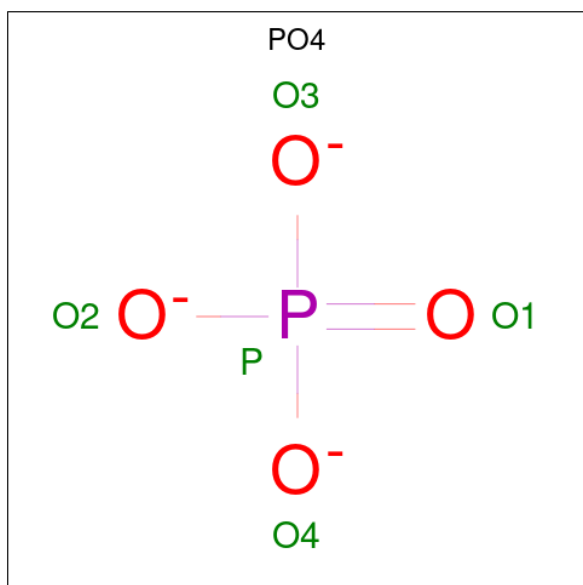
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
5	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



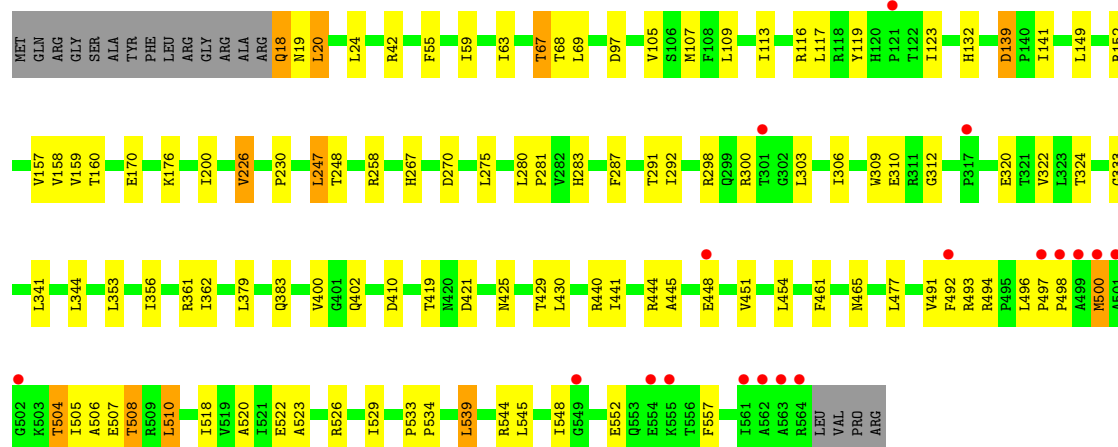
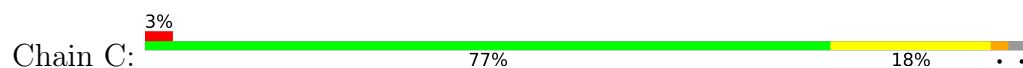
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P		
			5	4	1		
6	C	1	Total	O	P		
			5	4	1		

- Molecule 7 is water.

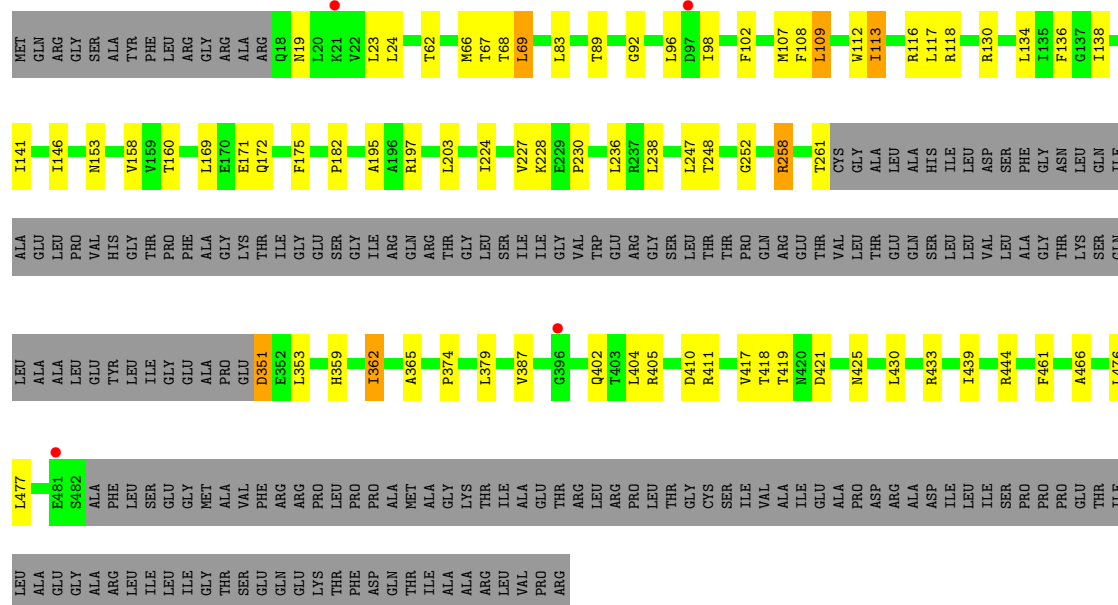
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total	O		
			17	17		
7	B	9	Total	O		
			9	9		
7	C	18	Total	O		
			18	18		
7	D	6	Total	O		
			6	6		



• Molecule 1: TrkA domain protein



• Molecule 1: TrkA domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	232.55Å 111.10Å 164.56Å 90.00° 134.78° 90.00°	Depositor
Resolution (Å)	41.14 – 3.20 41.14 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.5 (41.14-3.20) 94.1 (41.14-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.230 , 0.270 0.224 , 0.264	Depositor DCC
R_{free} test set	2384 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	88.7	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 83.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.206 for h+2*k,-h-l 0.023 for h,-k,-h-l 0.028 for -h-2*k,-k,l	Xtriage
F_o , F_c correlation	0.92	EDS
Total number of atoms	14511	wwPDB-VP
Average B, all atoms (Å ²)	117.0	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 37.45 % 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 4.2821e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, CA, PO4, ZN, K

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	0.30	0/2982	0.75	1/4060 (0.0%)
1	B	0.31	0/4291	0.75	3/5843 (0.1%)
1	C	0.32	0/4280	0.75	0/5829
1	D	0.31	0/2988	0.76	0/4068
All	All	0.31	0/14541	0.75	4/19800 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	GLU	CA-C-N	5.60	125.97	119.47
1	B	229	GLU	C-N-CA	5.60	125.97	119.47
1	A	109	LEU	N-CA-C	-5.31	107.17	113.97
1	B	345	ILE	N-CA-C	5.16	115.37	110.42

There are no chirality outliers.

There are no planarity outliers.

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	2922	0	2957	33	0
1	B	4208	0	4282	79	0
1	C	4197	0	4269	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2928	0	2962	43	0
2	A	5	0	0	0	0
2	B	1	0	0	0	0
2	C	5	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	44	0	26	6	0
5	B	44	0	26	4	0
5	C	44	0	26	6	0
5	D	44	0	26	6	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
7	A	17	0	0	0	0
7	B	9	0	0	0	0
7	C	18	0	0	0	0
7	D	6	0	0	0	0
All	All	14511	0	14574	211	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 (211) 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:C:69:LEU:HD23	1:D:68:THR:HA	1.59	0.84
1:A:247:LEU:H	5:A:608:NAD:H4N	1.45	0.82
1:C:226:VAL:HG12	5:C:610:NAD:H5N	1.62	0.80
1:A:69:LEU:HD22	1:B:70:GLY:HA3	1.62	0.80
1:A:69:LEU:CD2	1:B:70:GLY:HA3	2.13	0.79
1:C:419:THR:HG22	1:C:421:ASP:H	1.48	0.79
1:D:130:ARG:HG3	1:D:195:ALA:HB1	1.71	0.73
1:C:493:ARG:HD2	1:C:544:ARG:HD3	1.68	0.73
1:C:419:THR:HB	1:C:425:ASN:HD21	1.54	0.71
1:D:419:THR:HG22	1:D:421:ASP:H	1.56	0.68
1:A:247:LEU:N	5:A:608:NAD:H4N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:VAL:HG22	1:D:236:LEU:HD22	1.75	0.67
1:C:444:ARG:HE	1:C:465:ASN:HD21	1.44	0.66
1:B:523:ALA:HB3	1:B:526:ARG:HB2	1.79	0.65
1:A:157:VAL:HG22	1:A:176:LYS:HB3	1.79	0.64
1:D:247:LEU:H	5:D:603:NAD:H4N	1.63	0.64
1:A:119:TYR:HB2	1:B:118:ARG:HH22	1.62	0.63
1:C:248:THR:HB	1:C:362:ILE:HG12	1.81	0.63
1:A:419:THR:HG22	1:A:421:ASP:H	1.62	0.63
1:A:138:ILE:HG21	1:A:169:LEU:HD11	1.82	0.62
1:D:248:THR:HB	1:D:362:ILE:HG12	1.82	0.62
1:D:247:LEU:N	5:D:603:NAD:H4N	2.15	0.61
1:D:230:PRO:HD3	5:D:603:NAD:H72N	1.66	0.61
1:D:203:LEU:O	1:D:228:LYS:NZ	2.29	0.60
1:C:247:LEU:H	5:C:610:NAD:H4N	1.66	0.59
1:C:496:LEU:HD22	1:C:497:PRO:HD2	1.84	0.59
1:A:69:LEU:CD2	1:B:70:GLY:CA	2.80	0.59
1:C:504:THR:HG22	1:C:507:GLU:H	1.68	0.59
1:D:228:LYS:HD2	5:D:603:NAD:H1D	1.84	0.59
1:C:523:ALA:HB3	1:C:526:ARG:HB2	1.85	0.58
1:C:496:LEU:HD23	1:C:545:LEU:HD11	1.84	0.58
1:B:353:LEU:HB3	1:B:412:ALA:HA	1.86	0.58
1:B:496:LEU:HD23	1:B:545:LEU:HD11	1.84	0.58
1:D:113:ILE:HB	1:D:117:LEU:HD12	1.86	0.58
1:B:216:ARG:NH1	1:B:242:ASN:OD1	2.38	0.57
1:C:67:THR:O	1:C:68:THR:OG1	2.22	0.57
1:D:138:ILE:HG21	1:D:169:LEU:HD11	1.87	0.56
1:C:500:MET:HG3	1:C:508:THR:HG21	1.88	0.56
1:D:109:LEU:HA	1:D:112:TRP:HB3	1.86	0.56
1:B:493:ARG:HD3	1:B:544:ARG:HD2	1.86	0.56
1:C:505:ILE:HD13	1:C:518:ILE:HG21	1.87	0.56
1:B:270:ASP:HA	1:B:276:GLN:HG3	1.87	0.56
1:C:230:PRO:HD3	5:C:610:NAD:H72N	1.71	0.56
1:C:419:THR:HB	1:C:425:ASN:ND2	2.21	0.55
1:B:258:ARG:O	1:B:440:ARG:HD3	2.07	0.55
1:B:169:LEU:HB3	1:B:175:PHE:HE1	1.71	0.55
1:B:291:THR:HG22	1:B:322:VAL:HG22	1.89	0.55
1:B:496:LEU:HD22	1:B:497:PRO:HD2	1.88	0.55
1:B:356:ILE:HB	1:B:379:LEU:HD23	1.89	0.54
1:C:63:ILE:O	1:C:67:THR:HB	2.08	0.54
1:C:491:VAL:HG22	1:C:548:ILE:HG12	1.89	0.54
1:D:112:TRP:CE3	1:D:113:ILE:HG22	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:HA	1:A:111:PRO:HD2	1.91	0.53
1:B:353:LEU:HD12	1:B:411:ARG:HG2	1.90	0.53
1:C:258:ARG:HG2	1:C:461:PHE:CD1	2.45	0.52
1:B:520:ALA:HB3	1:B:546:ILE:HB	1.92	0.52
1:A:178:VAL:HG11	1:A:191:LEU:HD21	1.91	0.52
1:D:402:GLN:HB3	1:D:405:ARG:CZ	2.39	0.52
1:C:287:PHE:HE1	1:C:341:LEU:HD21	1.75	0.51
1:A:419:THR:HB	1:A:425:ASN:OD1	2.10	0.51
1:C:303:LEU:HD23	1:C:333:GLY:HA3	1.92	0.51
1:A:228:LYS:HD2	5:A:608:NAD:H1D	1.93	0.50
1:B:113:ILE:HG23	1:B:117:LEU:HD13	1.93	0.50
1:B:489:MET:HG2	1:B:550:THR:HA	1.93	0.50
1:A:105:VAL:HG23	1:A:109:LEU:HD23	1.93	0.50
1:B:419:THR:HG22	1:B:421:ASP:H	1.77	0.50
1:D:136:PHE:CD1	1:D:182:PRO:HB3	2.47	0.50
1:C:504:THR:HG23	1:C:506:ALA:H	1.77	0.50
1:B:146:ILE:HG21	1:B:175:PHE:HD2	1.77	0.49
1:D:197:ARG:NH1	1:D:477:LEU:O	2.37	0.49
1:B:188:LEU:HA	1:B:191:LEU:HD12	1.94	0.49
1:C:67:THR:HG21	1:D:89:THR:HG23	1.95	0.49
1:D:112:TRP:CD1	1:D:116:ARG:HD2	2.48	0.49
1:C:105:VAL:HG13	1:C:109:LEU:HD23	1.95	0.49
1:C:247:LEU:N	5:C:610:NAD:H4N	2.27	0.49
1:D:258:ARG:HG2	1:D:461:PHE:CD1	2.47	0.49
1:B:520:ALA:HB1	1:B:529:ILE:HD11	1.94	0.48
1:C:18:GLN:HB2	1:C:19:ASN:H	1.44	0.48
1:D:351:ASP:N	1:D:351:ASP:OD1	2.44	0.48
1:B:482:SER:HA	1:B:485:LEU:HB2	1.96	0.48
1:A:107:MET:HG2	1:A:108:PHE:HD2	1.78	0.48
1:B:67:THR:HG23	1:B:69:LEU:H	1.78	0.48
1:B:272:PHE:CE2	1:B:274:ASN:HB3	2.49	0.48
1:D:433:ARG:NH1	1:D:439:ILE:O	2.47	0.48
1:B:227:VAL:HG22	1:B:229:GLU:H	1.79	0.48
1:C:298:ARG:NH1	1:C:523:ALA:O	2.46	0.48
1:A:359:HIS:CD2	1:A:379:LEU:HD13	2.49	0.48
1:C:157:VAL:HG22	1:C:176:LYS:HB3	1.96	0.48
1:A:356:ILE:HB	1:A:379:LEU:HD23	1.95	0.47
1:D:109:LEU:O	1:D:113:ILE:HG23	2.14	0.47
1:C:258:ARG:O	1:C:440:ARG:HD3	2.14	0.47
1:B:141:ILE:HD13	1:B:466:ALA:HA	1.96	0.47
1:C:42:ARG:HD2	1:C:55:PHE:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:TYR:HE2	1:A:170:GLU:HG2	1.80	0.47
1:C:400:VAL:HG11	1:D:387:VAL:HA	1.97	0.47
1:C:492:PHE:HD1	1:C:494:ARG:HD3	1.78	0.47
1:C:510:LEU:HD11	1:C:557:PHE:HE1	1.79	0.47
1:D:113:ILE:O	1:D:117:LEU:HB2	2.14	0.47
1:B:143:ARG:NH2	1:B:172:GLN:HE22	2.13	0.47
1:C:496:LEU:HD21	1:C:539:LEU:HD23	1.96	0.46
1:A:23:LEU:HB2	1:A:107:MET:HE1	1.98	0.46
1:A:103:GLY:O	1:A:107:MET:HB3	2.15	0.46
1:D:228:LYS:O	5:D:603:NAD:N7N	2.34	0.46
1:A:228:LYS:C	5:A:608:NAD:H71N	2.23	0.46
1:A:480:LYS:H	1:A:480:LYS:HD3	1.78	0.46
1:B:362:ILE:HD12	1:B:444:ARG:NE	2.31	0.46
1:D:67:THR:HG23	1:D:69:LEU:H	1.80	0.46
1:D:402:GLN:HB2	1:D:405:ARG:HB2	1.96	0.46
1:C:119:TYR:CE2	1:C:170:GLU:HG3	2.51	0.46
1:B:124:GLU:HG2	1:B:125:LEU:H	1.80	0.46
1:B:146:ILE:HG21	1:B:175:PHE:CD2	2.50	0.46
1:B:281:PRO:HB2	1:B:283:HIS:CD2	2.51	0.46
1:C:105:VAL:O	1:C:109:LEU:HB3	2.15	0.46
1:D:19:ASN:HB3	1:D:107:MET:HE3	1.97	0.46
1:D:252:GLY:HA3	1:D:365:ALA:HB3	1.98	0.46
1:A:161:ASP:HB3	1:A:182:PRO:HD3	1.97	0.46
1:B:173:GLU:HA	1:B:174:GLY:HA3	1.63	0.46
1:C:303:LEU:HD12	1:C:341:LEU:HD12	1.98	0.45
1:B:292:ILE:HD11	1:B:308:VAL:HG21	1.98	0.45
1:A:92:GLY:O	1:A:96:LEU:HB2	2.16	0.45
1:B:271:SER:C	1:B:273:GLY:H	2.24	0.45
1:D:359:HIS:CD2	1:D:379:LEU:HD13	2.51	0.45
1:B:63:ILE:O	1:B:67:THR:HG22	2.17	0.45
1:B:269:LEU:HG	1:B:271:SER:H	1.82	0.45
1:D:418:THR:HG22	1:D:444:ARG:HH11	1.81	0.45
1:C:362:ILE:HD12	1:C:444:ARG:NE	2.32	0.45
1:B:500:MET:HE2	1:B:508:THR:HG23	1.99	0.45
1:B:19:ASN:HB3	1:B:107:MET:SD	2.57	0.45
1:C:19:ASN:HB3	1:C:107:MET:HG3	1.99	0.45
1:B:496:LEU:HA	1:B:497:PRO:HD2	1.90	0.44
1:B:504:THR:HG22	1:B:507:GLU:H	1.82	0.44
1:C:200:ILE:HD11	1:C:477:LEU:HD11	2.00	0.44
1:C:429:THR:HG23	1:C:441:ILE:HG21	1.98	0.44
1:D:419:THR:HB	1:D:425:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:H	5:B:605:NAD:H4N	1.82	0.44
1:D:146:ILE:HG21	1:D:175:PHE:HD2	1.83	0.44
1:D:418:THR:HG23	1:D:444:ARG:HD3	1.99	0.44
1:B:352:GLU:O	1:B:376:PRO:HG2	2.17	0.44
1:B:111:PRO:HB3	1:B:115:ARG:CZ	2.47	0.44
1:B:149:LEU:HB2	1:B:156:PHE:HE1	1.82	0.44
1:D:247:LEU:HB2	5:D:603:NAD:C5N	2.48	0.44
1:B:200:ILE:HD13	1:B:224:ILE:HB	1.98	0.43
1:C:291:THR:HG22	1:C:322:VAL:HG22	2.00	0.43
1:C:448:GLU:HA	1:C:451:VAL:HG23	1.99	0.43
1:B:429:THR:HG23	1:B:441:ILE:HG21	2.00	0.43
1:C:300:ARG:HH21	1:C:344:LEU:HD22	1.83	0.43
1:B:287:PHE:HD2	1:B:295:SER:HB2	1.83	0.43
1:B:149:LEU:HB2	1:B:156:PHE:CE1	2.53	0.43
1:B:448:GLU:HA	1:B:451:VAL:HG23	2.01	0.43
1:B:492:PHE:HD1	1:B:494:ARG:HD3	1.83	0.43
1:A:224:ILE:HD13	1:A:476:LEU:HB3	1.99	0.43
1:B:119:TYR:HE2	1:B:170:GLU:HG3	1.84	0.43
1:C:522:GLU:HB2	1:C:544:ARG:HB3	2.00	0.43
1:B:494:ARG:HG2	1:B:557:PHE:CE2	2.54	0.43
1:B:521:ILE:HG13	1:B:533:PRO:HG2	2.01	0.43
1:A:360:GLY:HA3	5:A:608:NAD:PA	2.58	0.43
1:A:69:LEU:HD21	1:B:70:GLY:CA	2.47	0.43
1:B:476:LEU:O	1:B:480:LYS:HG2	2.19	0.43
1:C:309:TRP:CZ2	1:C:312:GLY:HA2	2.54	0.43
1:B:494:ARG:NH2	1:B:554:GLU:OE2	2.52	0.43
1:A:247:LEU:HB2	5:A:608:NAD:C5N	2.49	0.42
1:C:267:HIS:CE1	1:C:270:ASP:HB2	2.54	0.42
1:C:281:PRO:HB2	1:C:283:HIS:ND1	2.34	0.42
1:D:62:THR:HG22	1:D:66:MET:HE2	2.01	0.42
1:B:226:VAL:HG12	5:B:605:NAD:H5N	2.01	0.42
1:C:117:LEU:HD23	1:C:117:LEU:HA	1.85	0.42
1:A:136:PHE:CD1	1:A:182:PRO:HB3	2.54	0.42
1:B:272:PHE:HB2	1:B:490:ALA:HB1	2.00	0.42
1:A:110:ALA:HB3	1:A:111:PRO:HD3	2.02	0.42
1:C:298:ARG:HG3	1:C:303:LEU:O	2.20	0.42
1:B:162:ASN:HB3	1:B:165:GLN:HB3	2.00	0.42
1:C:275:LEU:HD23	1:C:491:VAL:HG12	2.02	0.42
1:C:356:ILE:HB	1:C:379:LEU:HD23	2.00	0.42
1:C:444:ARG:HE	1:C:465:ASN:ND2	2.11	0.42
1:A:474:GLY:O	1:A:478:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:THR:HG21	1:B:557:PHE:HD1	1.84	0.42
1:C:520:ALA:HB1	1:C:529:ILE:HD11	2.01	0.42
1:B:257:ILE:HG22	1:B:369:PHE:CZ	2.54	0.42
1:B:550:THR:C	1:B:552:GLU:H	2.28	0.42
1:A:67:THR:HG23	1:A:69:LEU:H	1.85	0.42
1:B:275:LEU:HD23	1:B:491:VAL:HG13	2.02	0.42
1:B:360:GLY:HA3	5:B:605:NAD:PA	2.60	0.42
1:C:445:ALA:HB2	1:C:454:LEU:HD12	2.02	0.41
1:B:309:TRP:CZ2	1:B:312:GLY:HA2	2.54	0.41
1:B:335:LYS:HE3	1:B:335:LYS:HB2	1.95	0.41
1:B:496:LEU:HD21	1:B:539:LEU:HD23	2.01	0.41
1:D:98:ILE:O	1:D:102:PHE:HB3	2.21	0.41
1:B:359:HIS:CD2	1:B:379:LEU:HD13	2.55	0.41
1:C:139:ASP:OD1	1:C:141:ILE:HG12	2.21	0.41
1:B:248:THR:HG23	5:B:605:NAD:C2N	2.51	0.41
1:C:280:LEU:HA	1:C:281:PRO:HD2	1.94	0.41
1:C:230:PRO:HD3	5:C:610:NAD:N7N	2.36	0.41
1:D:224:ILE:HD13	1:D:476:LEU:HB3	2.02	0.41
1:C:533:PRO:HA	1:C:534:PRO:HD2	1.90	0.41
1:B:181:SER:HA	1:B:182:PRO:HD3	1.90	0.41
1:B:307:GLY:HA2	1:B:317:PRO:HD3	2.01	0.41
1:D:117:LEU:HD23	1:D:117:LEU:HA	1.65	0.41
1:D:141:ILE:HD13	1:D:466:ALA:HA	2.02	0.41
1:B:110:ALA:HB3	1:B:111:PRO:HD3	2.03	0.40
1:B:258:ARG:HG2	1:B:461:PHE:CG	2.56	0.40
1:C:20:LEU:HD22	1:C:20:LEU:H	1.86	0.40
1:B:136:PHE:CD1	1:B:182:PRO:HB3	2.56	0.40
1:D:23:LEU:HB2	1:D:107:MET:HE1	2.03	0.40
1:D:92:GLY:O	1:D:96:LEU:HB2	2.20	0.40
1:A:440:ARG:HA	1:A:460:ASP:OD2	2.21	0.40
1:C:419:THR:HG23	5:C:610:NAD:C8A	2.51	0.40
1:C:497:PRO:HA	1:C:498:PRO:HD3	1.90	0.40
1:B:188:LEU:HD23	1:B:191:LEU:HD12	2.04	0.40
1:B:345:ILE:N	1:B:346:GLY:HA2	2.36	0.40
1:B:426:ILE:O	1:B:430:LEU:HB2	2.22	0.40
1:C:55:PHE:O	1:C:59:ILE:HG12	2.22	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	371/565 (66%)	348 (94%)	23 (6%)	0	100	100
1	B	546/565 (97%)	517 (95%)	28 (5%)	1 (0%)	43	73
1	C	545/565 (96%)	525 (96%)	20 (4%)	0	100	100
1	D	372/565 (66%)	358 (96%)	13 (4%)	1 (0%)	36	68
All	All	1834/2260 (81%)	1748 (95%)	84 (5%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	374	PRO
1	B	524	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	313/463 (68%)	293 (94%)	20 (6%)	16	48
1	B	449/463 (97%)	428 (95%)	21 (5%)	23	57
1	C	448/463 (97%)	414 (92%)	34 (8%)	12	42
1	D	314/463 (68%)	290 (92%)	24 (8%)	12	42
All	All	1524/1852 (82%)	1425 (94%)	99 (6%)	15	47

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	24	LEU
1	A	30	LEU
1	A	69	LEU
1	A	83	LEU
1	A	90	VAL
1	A	117	LEU
1	A	123	ILE
1	A	132	HIS
1	A	143	ARG
1	A	160	THR
1	A	172	GLN
1	A	197	ARG
1	A	220	GLN
1	A	238	LEU
1	A	243	GLN
1	A	353	LEU
1	A	403	THR
1	A	411	ARG
1	A	440	ARG
1	B	69	LEU
1	B	83	LEU
1	B	105	VAL
1	B	134	LEU
1	B	143	ARG
1	B	145	LEU
1	B	158	VAL
1	B	160	THR
1	B	167	LEU
1	B	172	GLN
1	B	226	VAL
1	B	274	ASN
1	B	347	GLU
1	B	353	LEU
1	B	371	ASP
1	B	372	ARG
1	B	418	THR
1	B	430	LEU
1	B	480	LYS
1	B	504	THR
1	B	556	THR
1	C	18	GLN
1	C	20	LEU

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Mol	Chain	Res	Type
1	C	24	LEU
1	C	67	THR
1	C	97	ASP
1	C	113	ILE
1	C	116	ARG
1	C	123	ILE
1	C	132	HIS
1	C	139	ASP
1	C	149	LEU
1	C	152	ARG
1	C	158	VAL
1	C	159	VAL
1	C	160	THR
1	C	226	VAL
1	C	247	LEU
1	C	292	ILE
1	C	306	ILE
1	C	310	GLU
1	C	320	GLU
1	C	324	THR
1	C	353	LEU
1	C	361	ARG
1	C	383	GLN
1	C	402	GLN
1	C	410	ASP
1	C	430	LEU
1	C	500	MET
1	C	504	THR
1	C	508	THR
1	C	510	LEU
1	C	539	LEU
1	C	552	GLU
1	D	24	LEU
1	D	69	LEU
1	D	83	LEU
1	D	108	PHE
1	D	109	LEU
1	D	113	ILE
1	D	118	ARG
1	D	134	LEU
1	D	153	ASN
1	D	158	VAL

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Mol	Chain	Res	Type
1	D	160	THR
1	D	171	GLU
1	D	172	GLN
1	D	238	LEU
1	D	258	ARG
1	D	261	THR
1	D	351	ASP
1	D	353	LEU
1	D	362	ILE
1	D	404	LEU
1	D	410	ASP
1	D	411	ARG
1	D	417	VAL
1	D	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	402	GLN
1	A	453	GLN
1	B	47	HIS
1	B	172	GLN
1	B	283	HIS
1	B	402	GLN
1	C	165	GLN
1	C	276	GLN
1	C	425	ASN
1	C	434	HIS
1	C	436	HIS
1	C	465	ASN
1	C	475	ASN
1	D	406	GLN
1	D	479	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 20 are monoatomic - leaving 6 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	$\# Z > 2$
6	PO4	B	604	-	4,4,4	0.94	0	6,6,6	0.43	0
6	PO4	C	609	-	4,4,4	0.95	0	6,6,6	0.51	0
5	NAD	C	610	-	46,48,48	1.67	8 (17%)	64,73,73	1.83	14 (21%)
5	NAD	A	608	-	46,48,48	1.68	8 (17%)	64,73,73	1.87	15 (23%)
5	NAD	B	605	-	46,48,48	1.67	9 (19%)	64,73,73	1.77	15 (23%)
5	NAD	D	603	-	46,48,48	1.68	8 (17%)	64,73,73	1.90	14 (21%)

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
5	NAD	A	608	-	-	14/30/62/62	0/5/5/5
5	NAD	B	605	-	-	13/30/62/62	0/5/5/5
5	NAD	D	603	-	-	13/30/62/62	0/5/5/5
5	NAD	C	610	-	-	18/30/62/62	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	610	NAD	C7N-N7N	5.61	1.43	1.33
5	B	605	NAD	C7N-N7N	5.60	1.43	1.33
5	D	603	NAD	C7N-N7N	5.51	1.43	1.33
5	A	608	NAD	C7N-N7N	5.50	1.43	1.33
5	B	605	NAD	C2D-C3D	-4.04	1.42	1.53
5	A	608	NAD	C2D-C3D	-4.04	1.42	1.53
5	C	610	NAD	C2D-C3D	-4.02	1.42	1.53
5	D	603	NAD	C2D-C3D	-4.02	1.42	1.53
5	D	603	NAD	C6A-N6A	3.49	1.43	1.34
5	C	610	NAD	C6A-N6A	3.47	1.43	1.34
5	B	605	NAD	C6A-N6A	3.45	1.43	1.34
5	A	608	NAD	C6A-N6A	3.43	1.43	1.34
5	C	610	NAD	C2B-C3B	-3.30	1.44	1.53
5	A	608	NAD	C2B-C3B	-3.29	1.44	1.53
5	B	605	NAD	C2B-C3B	-3.29	1.44	1.53
5	D	603	NAD	C2B-C3B	-3.25	1.44	1.53
5	D	603	NAD	O4D-C4D	-2.82	1.38	1.45
5	A	608	NAD	O4D-C4D	-2.76	1.38	1.45
5	C	610	NAD	O4D-C4D	-2.72	1.39	1.45
5	B	605	NAD	O4D-C4D	-2.63	1.39	1.45
5	D	603	NAD	O5D-C5D	-2.17	1.36	1.44
5	A	608	NAD	O5D-C5D	-2.14	1.36	1.44
5	C	610	NAD	C5A-N7A	-2.11	1.35	1.39
5	C	610	NAD	O5D-C5D	-2.10	1.36	1.44
5	B	605	NAD	C5A-N7A	-2.09	1.35	1.39
5	D	603	NAD	C8A-N7A	2.08	1.35	1.31
5	A	608	NAD	C5A-N7A	-2.08	1.35	1.39
5	B	605	NAD	O5D-C5D	-2.08	1.36	1.44
5	A	608	NAD	C8A-N7A	2.06	1.35	1.31
5	B	605	NAD	C8A-N7A	2.06	1.35	1.31
5	C	610	NAD	C8A-N7A	2.03	1.35	1.31
5	B	605	NAD	C3D-C4D	-2.01	1.47	1.53
5	D	603	NAD	C5A-N7A	-2.01	1.35	1.39

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	603	NAD	C4D-O4D-C1D	-5.66	104.74	109.92
5	C	610	NAD	N3A-C2A-N1A	-5.09	120.87	128.58
5	D	603	NAD	N3A-C2A-N1A	-5.05	120.94	128.58
5	B	605	NAD	N3A-C2A-N1A	-5.04	120.95	128.58
5	A	608	NAD	C4D-O4D-C1D	-5.01	105.33	109.92
5	A	608	NAD	N3A-C2A-N1A	-4.98	121.05	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	610	NAD	C5A-C4A-N3A	-4.91	119.95	126.72
5	D	603	NAD	C5A-C4A-N3A	-4.87	120.01	126.72
5	C	610	NAD	C4D-O4D-C1D	-4.84	105.49	109.92
5	A	608	NAD	C5A-C4A-N3A	-4.83	120.06	126.72
5	B	605	NAD	C5A-C4A-N3A	-4.81	120.10	126.72
5	A	608	NAD	N9A-C8A-N7A	-4.02	108.23	113.94
5	B	605	NAD	N9A-C8A-N7A	-3.98	108.28	113.94
5	D	603	NAD	N9A-C8A-N7A	-3.98	108.29	113.94
5	C	610	NAD	N9A-C8A-N7A	-3.84	108.49	113.94
5	B	605	NAD	C4D-O4D-C1D	-3.73	106.51	109.92
5	C	610	NAD	O4B-C1B-N9A	3.64	115.08	108.09
5	C	610	NAD	C2A-N3A-C4A	3.57	120.55	111.83
5	D	603	NAD	C2A-N3A-C4A	3.54	120.47	111.83
5	B	605	NAD	C2A-N3A-C4A	3.52	120.42	111.83
5	A	608	NAD	C2A-N3A-C4A	3.48	120.33	111.83
5	D	603	NAD	C3N-C7N-N7N	3.45	121.99	117.74
5	D	603	NAD	O4B-C1B-N9A	3.40	114.62	108.09
5	A	608	NAD	O4B-C1B-N9A	3.38	114.58	108.09
5	A	608	NAD	C5A-N7A-C8A	3.34	108.70	103.45
5	B	605	NAD	C5A-N7A-C8A	3.32	108.67	103.45
5	D	603	NAD	C5A-N7A-C8A	3.30	108.64	103.45
5	B	605	NAD	O4B-C1B-N9A	3.27	114.38	108.09
5	C	610	NAD	C5A-N7A-C8A	3.26	108.57	103.45
5	C	610	NAD	N3A-C4A-N9A	3.25	132.70	127.17
5	D	603	NAD	N3A-C4A-N9A	3.24	132.69	127.17
5	A	608	NAD	C3N-C7N-N7N	3.22	121.70	117.74
5	A	608	NAD	N3A-C4A-N9A	3.21	132.62	127.17
5	B	605	NAD	N3A-C4A-N9A	3.18	132.57	127.17
5	A	608	NAD	C4A-C5A-N7A	-3.11	107.03	110.58
5	B	605	NAD	C4A-C5A-N7A	-3.11	107.03	110.58
5	C	610	NAD	C4A-C5A-N7A	-3.08	107.06	110.58
5	D	603	NAD	C4A-C5A-N7A	-3.06	107.08	110.58
5	C	610	NAD	O5B-C5B-C4B	2.90	118.88	108.99
5	A	608	NAD	C4A-N9A-C8A	2.84	108.72	105.74
5	D	603	NAD	C3B-C2B-C1B	2.83	106.81	101.46
5	D	603	NAD	C4A-N9A-C8A	2.81	108.69	105.74
5	B	605	NAD	C4A-N9A-C8A	2.80	108.68	105.74
5	D	603	NAD	O7N-C7N-N7N	-2.77	118.61	122.62
5	C	610	NAD	C3B-C2B-C1B	2.75	106.66	101.46
5	C	610	NAD	C4A-N9A-C8A	2.66	108.53	105.74
5	A	608	NAD	C3B-C2B-C1B	2.66	106.49	101.46
5	A	608	NAD	O7N-C7N-N7N	-2.55	118.93	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	605	NAD	O7N-C7N-N7N	-2.44	119.08	122.62
5	B	605	NAD	O5B-C5B-C4B	2.44	117.31	108.99
5	B	605	NAD	C3B-C2B-C1B	2.32	105.85	101.46
5	C	610	NAD	O7N-C7N-N7N	-2.30	119.30	122.62
5	C	610	NAD	C2B-C3B-C4B	2.27	107.00	102.61
5	B	605	NAD	C2B-C3B-C4B	2.23	106.91	102.61
5	A	608	NAD	C2B-C3B-C4B	2.21	106.88	102.61
5	B	605	NAD	C3N-C7N-N7N	2.17	120.41	117.74
5	D	603	NAD	C2B-C3B-C4B	2.10	106.67	102.61
5	A	608	NAD	O5B-C5B-C4B	2.09	116.13	108.99

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	608	NAD	C5B-O5B-PA-O2A
5	A	608	NAD	C5B-O5B-PA-O3
5	A	608	NAD	C5D-O5D-PN-O3
5	A	608	NAD	C5D-O5D-PN-O2N
5	A	608	NAD	O4D-C4D-C5D-O5D
5	A	608	NAD	C2D-C1D-N1N-C6N
5	B	605	NAD	C5D-O5D-PN-O3
5	B	605	NAD	C5D-O5D-PN-O1N
5	B	605	NAD	C5D-O5D-PN-O2N
5	B	605	NAD	O4D-C1D-N1N-C2N
5	B	605	NAD	O4D-C1D-N1N-C6N
5	B	605	NAD	C2D-C1D-N1N-C2N
5	B	605	NAD	C2D-C1D-N1N-C6N
5	C	610	NAD	C5B-O5B-PA-O1A
5	C	610	NAD	C5B-O5B-PA-O3
5	C	610	NAD	C5D-O5D-PN-O3
5	C	610	NAD	C5D-O5D-PN-O1N
5	C	610	NAD	C5D-O5D-PN-O2N
5	C	610	NAD	O4D-C1D-N1N-C2N
5	C	610	NAD	O4D-C1D-N1N-C6N
5	C	610	NAD	C2D-C1D-N1N-C2N
5	C	610	NAD	C2D-C1D-N1N-C6N
5	D	603	NAD	C5B-O5B-PA-O2A
5	D	603	NAD	C5B-O5B-PA-O3
5	D	603	NAD	C5D-O5D-PN-O3
5	D	603	NAD	C5D-O5D-PN-O2N
5	D	603	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
5	D	603	NAD	C2D-C1D-N1N-C6N
5	A	608	NAD	C2N-C3N-C7N-N7N
5	A	608	NAD	O4B-C4B-C5B-O5B
5	C	610	NAD	O4D-C4D-C5D-O5D
5	C	610	NAD	C3D-C4D-C5D-O5D
5	D	603	NAD	O4B-C4B-C5B-O5B
5	A	608	NAD	C2N-C3N-C7N-O7N
5	A	608	NAD	C4N-C3N-C7N-N7N
5	A	608	NAD	C3D-C4D-C5D-O5D
5	B	605	NAD	O4B-C4B-C5B-O5B
5	B	605	NAD	O4D-C4D-C5D-O5D
5	D	603	NAD	O4D-C4D-C5D-O5D
5	D	603	NAD	C3D-C4D-C5D-O5D
5	A	608	NAD	C4N-C3N-C7N-O7N
5	B	605	NAD	C3B-C4B-C5B-O5B
5	D	603	NAD	C3B-C4B-C5B-O5B
5	A	608	NAD	C3B-C4B-C5B-O5B
5	C	610	NAD	O4B-C4B-C5B-O5B
5	C	610	NAD	C4N-C3N-C7N-O7N
5	C	610	NAD	C2N-C3N-C7N-O7N
5	B	605	NAD	C3D-C4D-C5D-O5D
5	C	610	NAD	C4B-C5B-O5B-PA
5	A	608	NAD	C2D-C1D-N1N-C2N
5	D	603	NAD	C2D-C1D-N1N-C2N
5	B	605	NAD	C4D-C5D-O5D-PN
5	D	603	NAD	O4D-C1D-N1N-C2N
5	C	610	NAD	C4N-C3N-C7N-N7N
5	B	605	NAD	C4B-C5B-O5B-PA
5	C	610	NAD	C4D-C5D-O5D-PN
5	D	603	NAD	C4B-C5B-O5B-PA
5	C	610	NAD	C3B-C4B-C5B-O5B

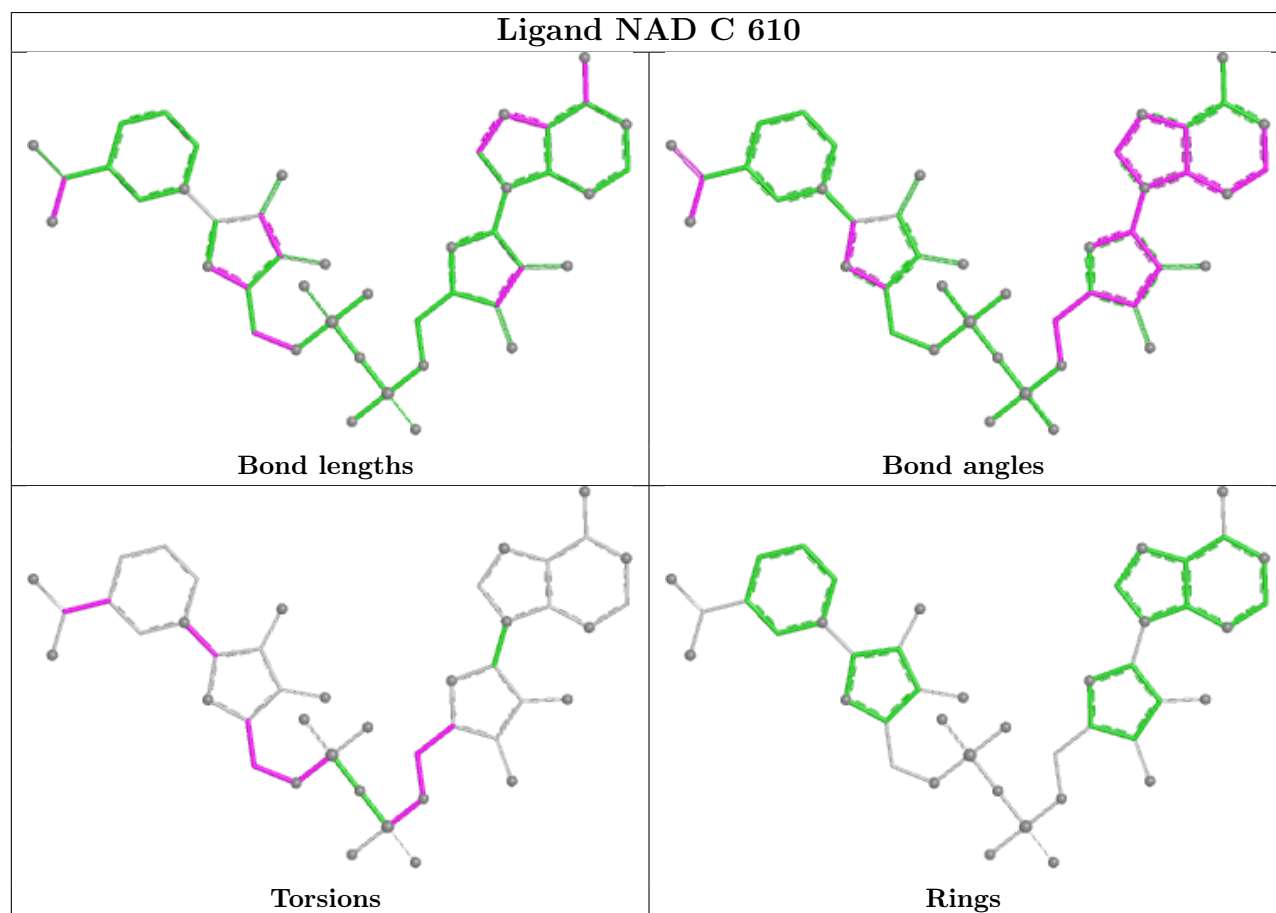
There are no ring outliers.

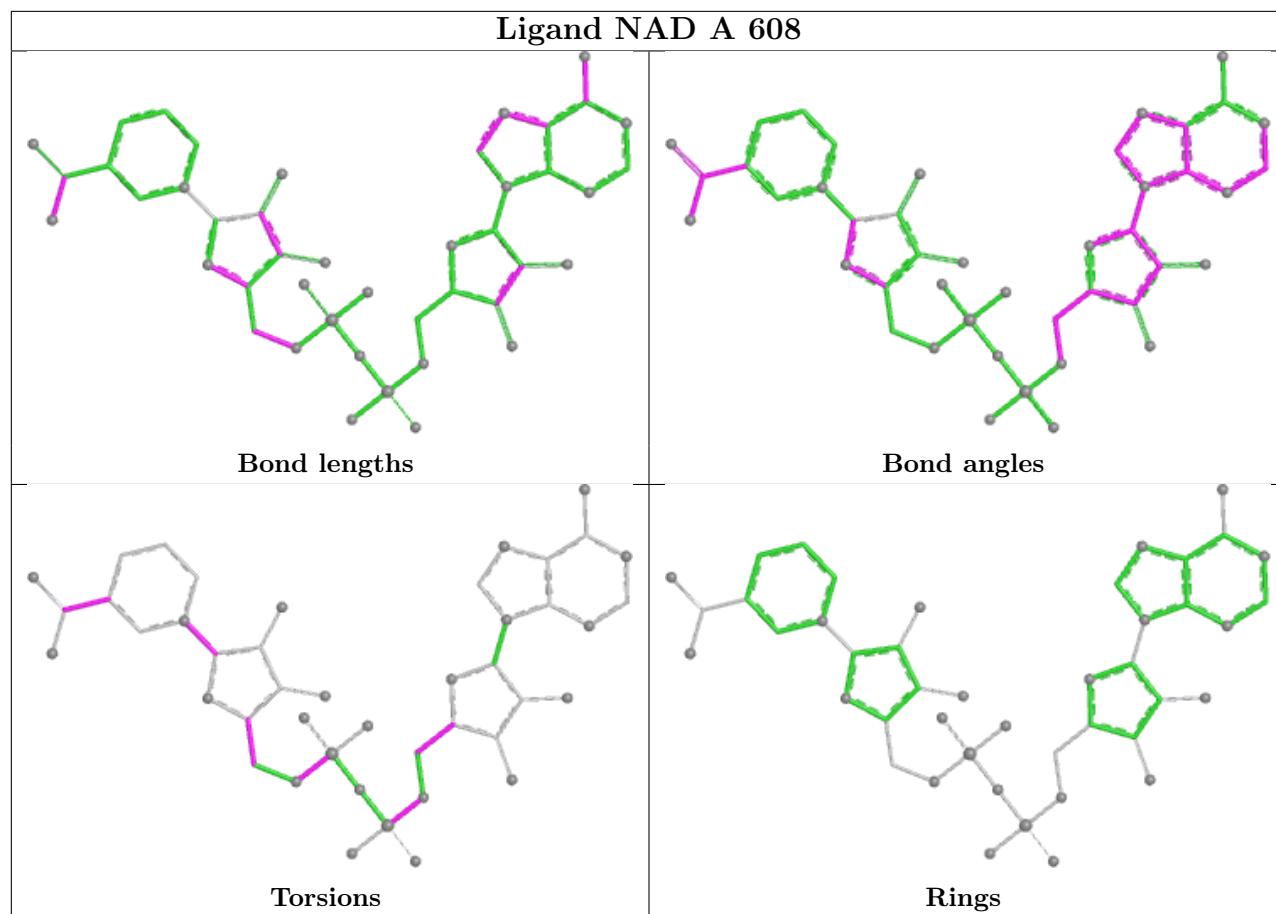
4 monomers are involved in 22 short contacts:

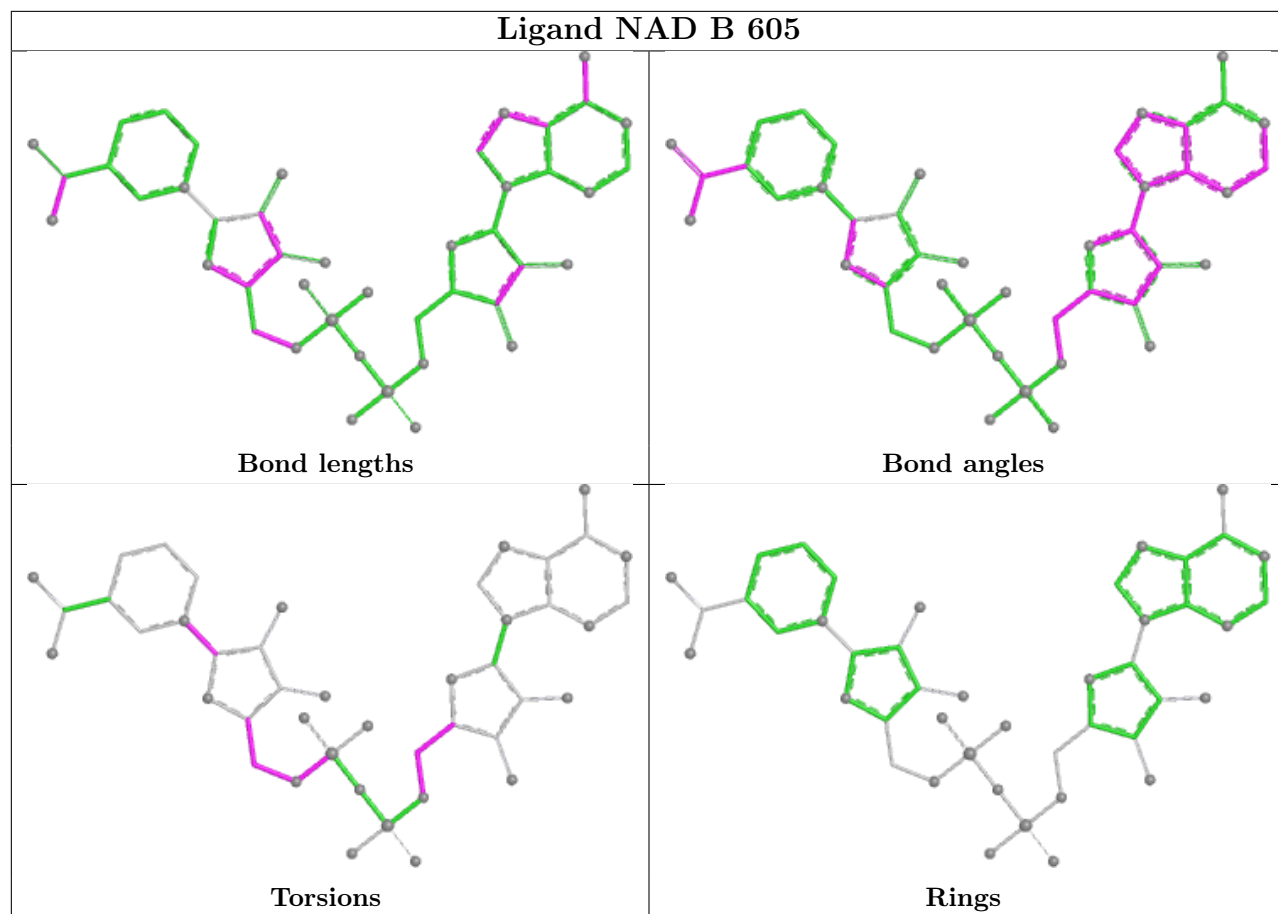
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	610	NAD	6	0
5	A	608	NAD	6	0
5	B	605	NAD	4	0
5	D	603	NAD	6	0

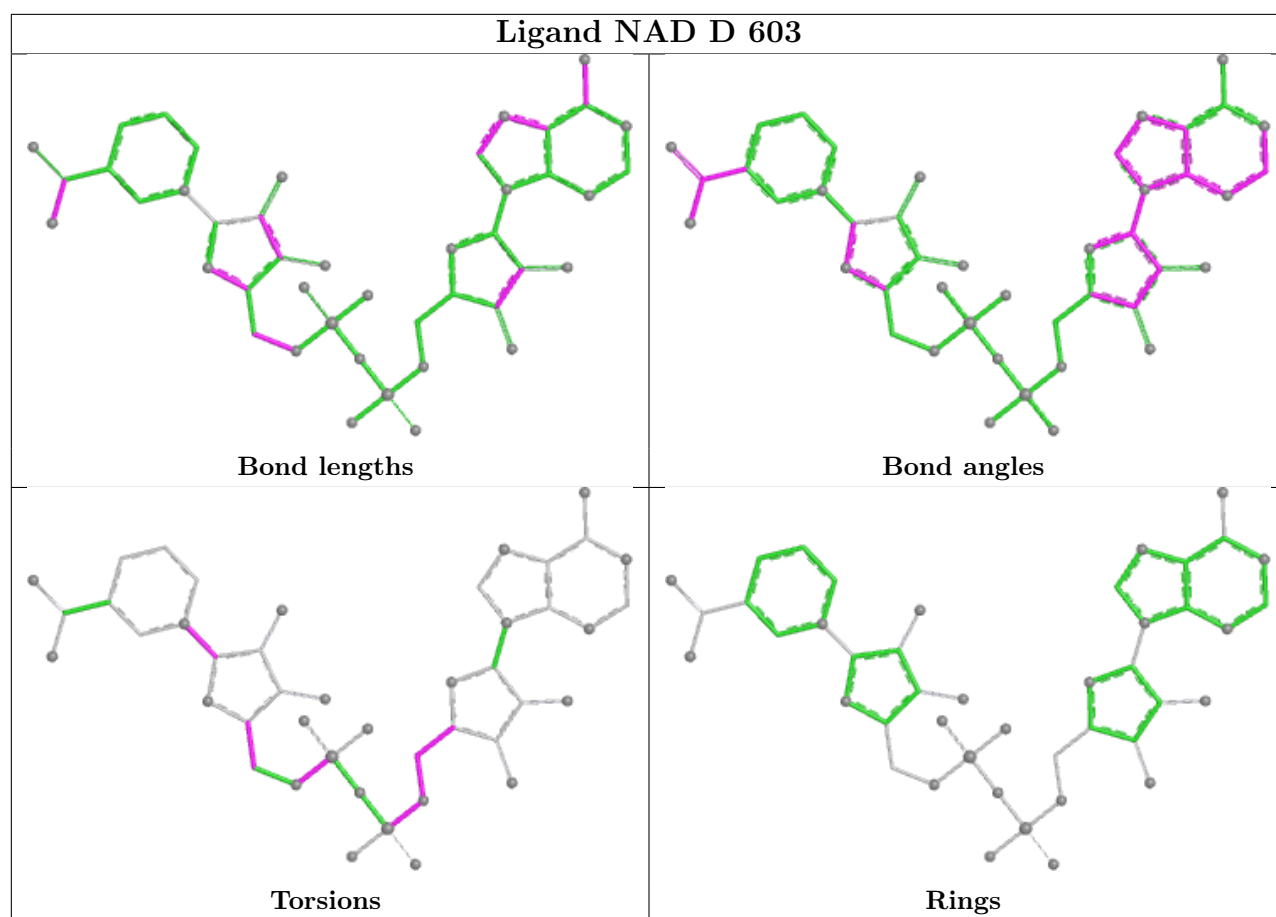
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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	375/565 (66%)	-0.68	2 (0%) 87 76	64, 90, 166, 214	0
1	B	548/565 (96%)	-0.17	25 (4%) 37 23	67, 115, 249, 357	0
1	C	547/565 (96%)	-0.21	18 (3%) 49 30	66, 111, 192, 261	0
1	D	376/565 (66%)	-0.64	4 (1%) 78 61	60, 89, 168, 234	0
All	All	1846/2260 (81%)	-0.38	49 (2%) 56 36	60, 100, 212, 357	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	562	ALA	5.5
1	C	561	ILE	5.0
1	B	561	ILE	5.0
1	B	507	GLU	4.8
1	B	483	ALA	4.0
1	C	498	PRO	3.9
1	C	563	ALA	3.5
1	C	492	PHE	3.3
1	C	499	ALA	3.2
1	B	497	PRO	3.0
1	B	438	HIS	3.0
1	C	564	ARG	2.9
1	B	557	PHE	2.9
1	B	550	THR	2.8
1	D	481	GLU	2.8
1	B	530	LEU	2.8
1	B	492	PHE	2.7
1	B	525	ASP	2.7
1	D	97	ASP	2.6
1	B	506	ALA	2.6
1	B	542	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	448	GLU	2.5
1	B	543	ALA	2.5
1	B	560	THR	2.5
1	C	301	THR	2.4
1	D	396	GLY	2.4
1	B	371	ASP	2.4
1	B	558	ASP	2.4
1	C	502	GLY	2.4
1	B	448	GLU	2.4
1	B	528	ASP	2.3
1	C	448	GLU	2.3
1	A	403	THR	2.3
1	D	21	LYS	2.3
1	B	531	ILE	2.3
1	B	499	ALA	2.3
1	B	523	ALA	2.2
1	C	121	PRO	2.2
1	B	545	LEU	2.2
1	C	317	PRO	2.2
1	C	555	LYS	2.2
1	C	501	ALA	2.2
1	C	554	GLU	2.2
1	C	500	MET	2.1
1	B	540	ALA	2.1
1	B	562	ALA	2.1
1	B	97	ASP	2.1
1	C	497	PRO	2.1
1	C	549	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

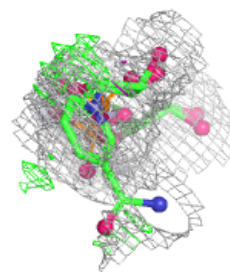
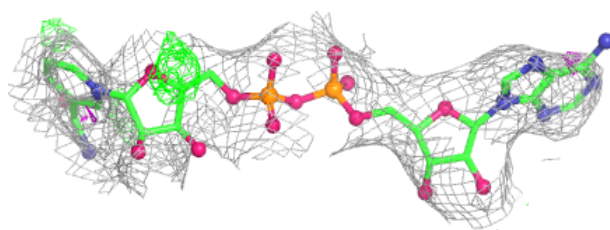
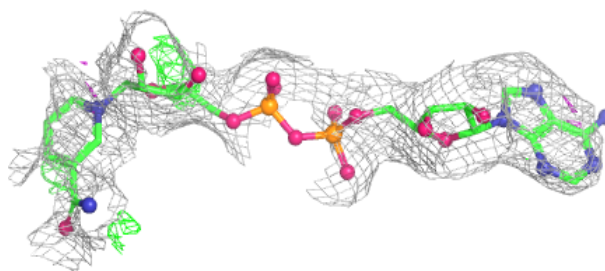
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	K	B	601	1/1	0.92	0.18	222,222,222,222	1
2	K	C	605	1/1	0.96	0.16	207,207,207,207	1
5	NAD	B	605	44/44	0.96	0.10	57,151,214,216	0
5	NAD	C	610	44/44	0.96	0.10	78,179,210,212	0
5	NAD	D	603	44/44	0.96	0.14	83,197,221,223	0
4	CA	B	603	1/1	0.98	0.08	89,89,89,89	0
4	CA	C	607	1/1	0.98	0.05	87,87,87,87	0
5	NAD	A	608	44/44	0.98	0.10	67,221,245,282	0
2	K	A	604	1/1	0.98	0.09	109,109,109,109	1
2	K	A	605	1/1	0.98	0.18	136,136,136,136	1
2	K	D	601	1/1	0.98	0.05	136,136,136,136	1
6	PO4	B	604	5/5	0.98	0.07	131,134,136,137	0
2	K	C	601	1/1	0.99	0.02	73,73,73,73	1
2	K	C	602	1/1	0.99	0.02	64,64,64,64	1
2	K	C	604	1/1	0.99	0.09	100,100,100,100	1
2	K	A	602	1/1	0.99	0.02	87,87,87,87	1
2	K	A	601	1/1	0.99	0.04	88,88,88,88	1
3	ZN	D	602	1/1	0.99	0.03	81,81,81,81	0
4	CA	A	607	1/1	0.99	0.05	89,89,89,89	0
6	PO4	C	609	5/5	0.99	0.08	139,139,142,142	0
3	ZN	C	606	1/1	1.00	0.05	87,87,87,87	0
2	K	C	603	1/1	1.00	0.03	68,68,68,68	1
2	K	A	603	1/1	1.00	0.01	71,71,71,71	1
3	ZN	A	606	1/1	1.00	0.04	91,91,91,91	0
3	ZN	B	602	1/1	1.00	0.04	92,92,92,92	0
4	CA	C	608	1/1	1.00	0.03	90,90,90,90	0

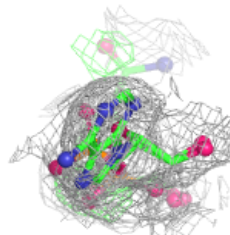
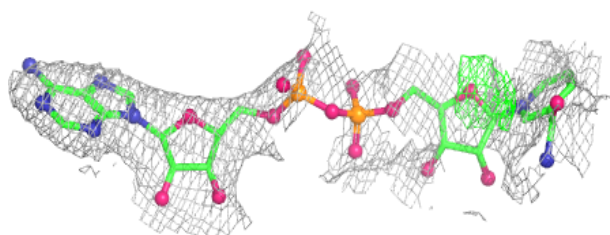
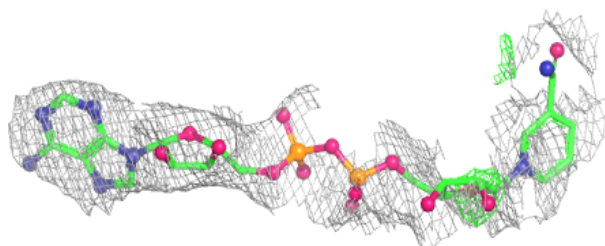
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 605:

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

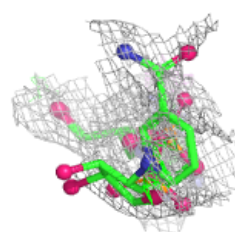
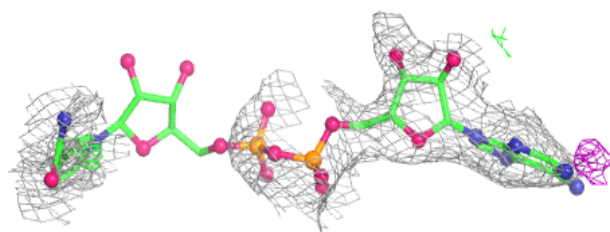
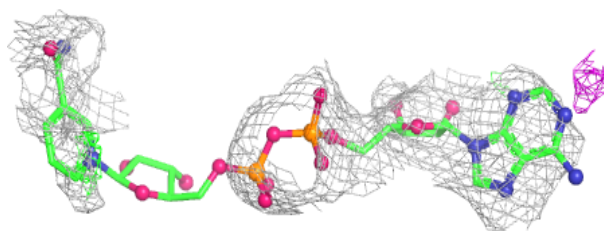
**Electron density around NAD C 610:**

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

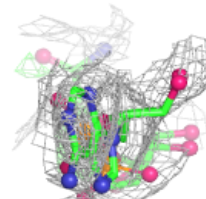
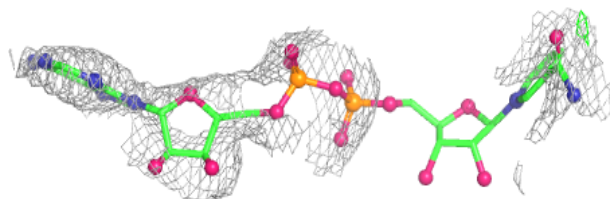
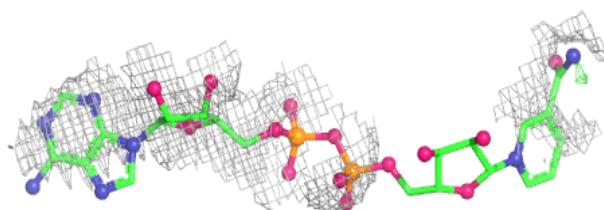


Electron density around NAD D 603:

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

**Electron density around 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.