



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:36 AM UTC

PDB ID : 5VL0 / pdb_00005vl0
Title : horse liver alcohol dehydrogenase complexed with NADH and N-benzyformamide
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Deposited on : 2017-04-24
Resolution : 1.20 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

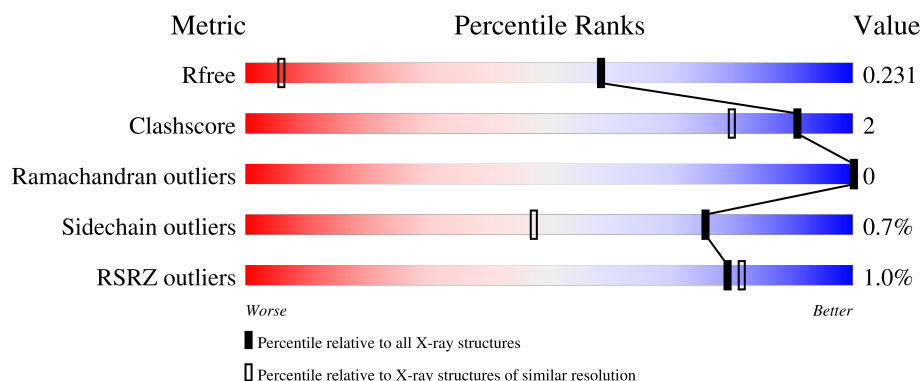
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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	374	2% 95% 5%
1	B	374	2% 97% •
1	C	374	2% 94% 5% •
1	D	374	2% 94% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12940 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

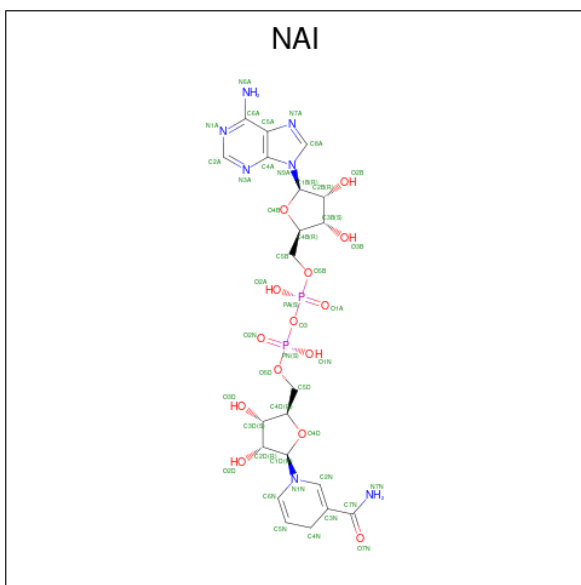
- Molecule 1 is a protein called Alcohol dehydrogenase E chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	9	0
			2821	1797	474	523	27			
1	B	374	Total	C	N	O	S	0	13	0
			2846	1810	480	532	24			
1	C	374	Total	C	N	O	S	0	14	0
			2845	1812	479	528	26			
1	D	374	Total	C	N	O	S	0	12	0
			2831	1801	475	529	26			

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

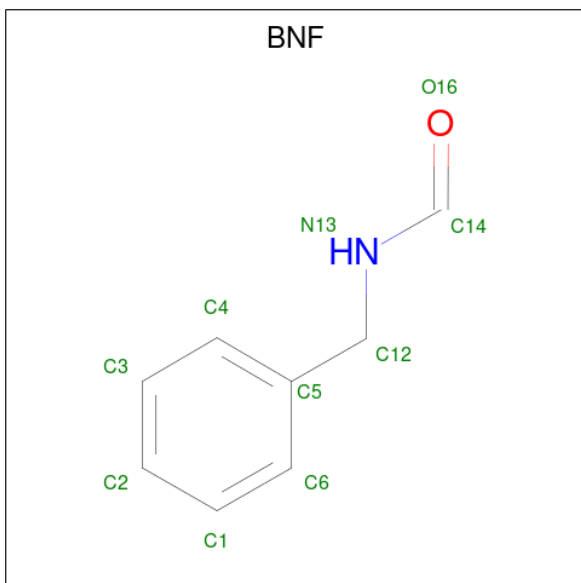
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



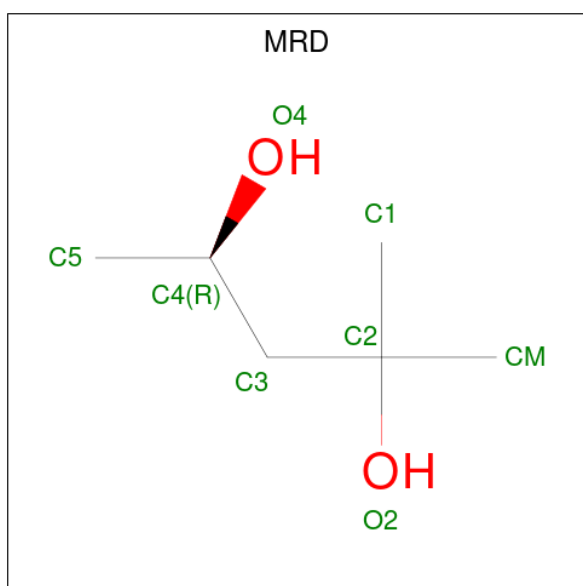
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is N-BENZYLFORMAMIDE (CCD ID: BNF) (formula: $\text{C}_8\text{H}_9\text{NO}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	8	1	1		
4	B	1	Total	C	N	O	0	0
			10	8	1	1		
4	C	1	Total	C	N	O	0	0
			10	8	1	1		
4	D	1	Total	C	N	O	0	0
			10	8	1	1		

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	324	Total	O	0	4
			326	326		
6	B	322	Total	O	0	3
			323	323		
6	C	367	Total	O	0	12
			371	371		
6	D	334	Total	O	0	8
			337	337		

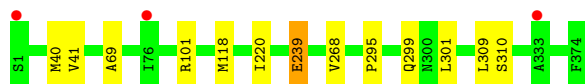
3 Residue-property plots [i](#)

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: Alcohol dehydrogenase E chain



- Molecule 1: Alcohol dehydrogenase E chain



- Molecule 1: Alcohol dehydrogenase E chain



- Molecule 1: Alcohol dehydrogenase E chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.16Å 180.29Å 86.92Å 90.00° 106.18° 90.00°	Depositor
Resolution (Å)	19.95 – 1.20 19.95 – 1.20	Depositor EDS
% Data completeness (in resolution range)	79.4 (19.95-1.20) 79.4 (19.95-1.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.158 , 0.199 (Not available) , 0.231	Depositor DCC
R_{free} test set	3775 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12940	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 67.13 % 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 5.4128e-06. 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: NAI, ZN, BNF, MRD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.25	2/2909 (0.1%)	1.13	5/3927 (0.1%)
1	B	1.19	1/2947 (0.0%)	1.09	1/3978 (0.0%)
1	C	1.25	7/2953 (0.2%)	1.12	2/3987 (0.1%)
1	D	1.21	3/2933 (0.1%)	1.13	4/3961 (0.1%)
All	All	1.23	13/11742 (0.1%)	1.12	12/15853 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	VAL	CA-C	9.86	1.61	1.52
1	C	241	VAL	N-CA	-7.21	1.37	1.46
1	C	315	LYS	CA-CB	-6.55	1.42	1.53
1	D	287	GLY	CA-C	6.15	1.58	1.52
1	D	292	VAL	CA-C	6.07	1.58	1.52
1	A	12	ALA	N-CA	-5.57	1.39	1.46
1	B	41	VAL	N-CA	-5.55	1.40	1.46
1	C	76	ILE	CA-C	-5.54	1.46	1.52
1	C	295	PRO	C-O	-5.37	1.18	1.24
1	C	328	VAL	CA-C	5.31	1.57	1.52
1	C	294	VAL	C-O	-5.19	1.17	1.24
1	D	315	LYS	CA-CB	-5.09	1.44	1.53
1	C	99	LYS	C-O	5.06	1.30	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	VAL	O-C-N	8.77	126.30	120.07
1	D	267	GLU	CB-CG-CD	6.45	123.56	112.60
1	A	229	PHE	N-CA-C	5.98	117.88	111.36
1	D	328	VAL	O-C-N	5.98	124.25	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	GLU	N-CA-C	5.76	118.34	111.71
1	D	284	GLU	N-CA-C	5.44	117.96	111.71
1	D	252	GLU	N-CA-C	5.43	116.88	111.07
1	A	294	VAL	CA-C-N	5.21	125.75	120.38
1	A	294	VAL	C-N-CA	5.21	125.75	120.38
1	C	267	GLU	CB-CG-CD	5.18	121.41	112.60
1	B	310	SER	N-CA-C	5.15	118.66	112.38
1	C	120	ARG	CA-CB-CG	5.11	124.33	114.10

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	2821	0	2904	9	0
1	B	2846	0	2920	9	0
1	C	2845	0	2928	11	0
1	D	2831	0	2902	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	44	0	27	1	0
3	B	44	0	27	0	0
3	C	44	0	27	0	0
3	D	44	0	27	0	0
4	A	10	0	9	1	0
4	B	10	0	9	0	0
4	C	10	0	9	2	0
4	D	10	0	9	0	0
5	B	8	0	14	2	0
5	C	8	0	14	0	0
6	A	326	0	0	2	0
6	B	323	0	0	1	0
6	C	371	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	337	0	0	3	0
All	All	12940	0	11826	40	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 2.

All (40) 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:241[B]:VAL:HG21	1:D:250:ILE:HD11	1.59	0.84
5:B:405:MRD:H5C3	5:B:405:MRD:H1C2	1.61	0.82
1:D:251:GLN:HA	1:D:281[B]:CYS:SG	2.24	0.77
1:D:241[B]:VAL:CG2	1:D:250:ILE:HD11	2.19	0.73
1:C:309[B]:LEU:HD11	1:D:295:PRO:HD3	1.73	0.70
1:A:286:TYR:OH	1:B:101[B]:ARG:NE	2.31	0.64
1:B:220:ILE:HG12	1:B:239[A]:GLU:HG3	1.83	0.61
1:A:17:GLU:OE1	6:A:501:HOH:O	2.16	0.59
1:A:209[B]:MET:HE1	1:A:341:ALA:O	2.04	0.57
1:C:101[A]:ARG:NH1	6:C:502:HOH:O	2.38	0.55
1:C:40[A]:MET:HE1	1:C:150:THR:HG22	1.90	0.54
1:D:40[A]:MET:HE1	1:D:150:THR:HG22	1.90	0.54
1:A:309[B]:LEU:HD11	1:B:295:PRO:HD3	1.89	0.53
1:D:212:LYS:NZ	6:D:506:HOH:O	2.42	0.53
1:C:309[B]:LEU:CD1	1:D:295:PRO:HD3	2.38	0.53
1:C:295:PRO:HD3	1:D:309[A]:LEU:HD11	1.91	0.51
1:A:360:ASP:OD1	6:A:502:HOH:O	2.20	0.50
6:C:667[B]:HOH:O	1:D:295:PRO:HB2	2.10	0.49
1:C:40[A]:MET:HE1	1:C:150:THR:CG2	2.42	0.49
4:C:404:BNF:H2	1:D:309[B]:LEU:HD23	1.95	0.48
1:C:116[B]:LEU:HD13	1:C:318[B]:ILE:HD12	1.94	0.48
5:B:405:MRD:H1C2	5:B:405:MRD:C5	2.40	0.48
1:A:295:PRO:HD3	1:B:309[B]:LEU:HD11	1.95	0.47
1:D:40[A]:MET:HE1	1:D:150:THR:CG2	2.45	0.46
1:B:40[B]:MET:HE2	1:B:69:ALA:HB1	1.97	0.46
1:B:299[B]:GLN:OE1	6:B:501:HOH:O	2.21	0.45
1:C:357[B]:GLU:HG3	6:C:723:HOH:O	2.16	0.45
1:A:309[B]:LEU:CD1	1:B:295:PRO:HD3	2.47	0.44
4:A:404:BNF:H2	1:B:309[A]:LEU:HD23	1.99	0.44
1:A:301:LEU:HD12	1:A:301:LEU:C	2.41	0.44
1:C:238:THR:C	1:C:239:GLU:HG3	2.43	0.44
1:C:40[A]:MET:HE2	1:C:40[A]:MET:HB2	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:GLN:HG2	6:D:752:HOH:O	2.18	0.42
1:B:301:LEU:C	1:B:301:LEU:HD12	2.45	0.42
4:C:404:BNF:H2	1:D:309[B]:LEU:CD2	2.50	0.42
1:C:350:LEU:O	1:C:372:LEU:HA	2.20	0.41
1:D:350:LEU:O	1:D:372:LEU:HA	2.20	0.41
1:D:120:ARG:HB2	6:D:651:HOH:O	2.21	0.41
1:A:174:CYS:SG	3:A:403:NAI:H5N	2.61	0.41
1:D:83:VAL:HG12	1:D:159:LYS:HB2	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	381/374 (102%)	370 (97%)	11 (3%)	0	100	100
1	B	385/374 (103%)	374 (97%)	11 (3%)	0	100	100
1	C	386/374 (103%)	375 (97%)	11 (3%)	0	100	100
1	D	384/374 (103%)	374 (97%)	10 (3%)	0	100	100
All	All	1536/1496 (103%)	1493 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	317/308 (103%)	313 (99%)	4 (1%)	61	25
1	B	320/308 (104%)	316 (99%)	4 (1%)	61	25
1	C	322/308 (104%)	320 (99%)	2 (1%)	78	52
1	D	320/308 (104%)	319 (100%)	1 (0%)	86	67
All	All	1279/1232 (104%)	1268 (99%)	11 (1%)	76	40

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	268	VAL
1	A	330[A]	LYS
1	A	330[B]	LYS
1	B	118	MET
1	B	239[A]	GLU
1	B	239[B]	GLU
1	B	268	VAL
1	C	239	GLU
1	C	268	VAL
1	D	268	VAL

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

Mol	Chain	Res	Type
1	A	300	ASN
1	B	138	HIS
1	B	300	ASN
1	C	300	ASN
1	D	124	GLN
1	D	138	HIS
1	D	300	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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
5	MRD	B	405	-	7,7,7	0.50	0	9,10,10	1.19	0
4	BNF	A	404	2	10,10,10	0.99	0	10,11,11	4.12	6 (60%)
4	BNF	C	404	2	10,10,10	1.04	0	10,11,11	4.04	4 (40%)
3	NAI	C	403	-	47,48,48	1.75	10 (21%)	64,73,73	1.90	15 (23%)
3	NAI	D	403	-	47,48,48	1.51	8 (17%)	64,73,73	1.67	11 (17%)
3	NAI	A	403	-	47,48,48	1.93	10 (21%)	64,73,73	1.66	9 (14%)
5	MRD	C	405[A]	-	7,7,7	0.46	0	9,10,10	0.86	0
3	NAI	B	403	-	47,48,48	1.59	8 (17%)	64,73,73	1.49	8 (12%)
4	BNF	B	404	2	10,10,10	0.83	0	10,11,11	3.58	4 (40%)
4	BNF	D	404	2	10,10,10	0.84	0	10,11,11	2.74	3 (30%)

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	MRD	B	405	-	-	3/5/5/5	-
4	BNF	A	404	2	-	0/4/4/4	0/1/1/1
4	BNF	C	404	2	-	0/4/4/4	0/1/1/1
3	NAI	C	403	-	-	3/29/72/72	0/5/5/5
3	NAI	D	403	-	-	2/29/72/72	0/5/5/5
3	NAI	A	403	-	-	2/29/72/72	0/5/5/5
5	MRD	C	405[A]	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAI	B	403	-	-	3/29/72/72	0/5/5/5
4	BNF	B	404	2	-	0/4/4/4	0/1/1/1
4	BNF	D	404	2	-	1/4/4/4	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	NAI	C2A-N1A	7.04	1.46	1.33
3	A	403	NAI	PN-O3	-6.16	1.52	1.59
3	D	403	NAI	C2A-N3A	5.54	1.43	1.33
3	A	403	NAI	C6A-N1A	-5.42	1.20	1.35
3	C	403	NAI	C6A-N1A	-5.06	1.21	1.35
3	C	403	NAI	C5A-C4A	-4.59	1.30	1.39
3	A	403	NAI	C4N-C5N	-4.22	1.38	1.49
3	C	403	NAI	C2A-N1A	4.13	1.41	1.33
3	A	403	NAI	PA-O3	3.79	1.63	1.59
3	A	403	NAI	C5A-N7A	-3.45	1.32	1.39
3	C	403	NAI	C4N-C3N	3.42	1.56	1.50
3	C	403	NAI	C8A-N9A	3.42	1.43	1.37
3	A	403	NAI	C2A-N1A	2.93	1.39	1.33
3	C	403	NAI	C1D-N1N	-2.90	1.38	1.46
3	B	403	NAI	C6A-N1A	-2.82	1.27	1.35
3	C	403	NAI	C6N-N1N	2.73	1.43	1.37
3	A	403	NAI	C4A-N3A	2.70	1.39	1.34
3	B	403	NAI	PA-O3	2.69	1.62	1.59
3	A	403	NAI	C2A-N3A	2.64	1.38	1.33
3	D	403	NAI	C1D-N1N	-2.50	1.39	1.46
3	C	403	NAI	C2A-N3A	2.49	1.38	1.33
3	D	403	NAI	O4B-C4B	-2.34	1.39	1.45
3	D	403	NAI	C6A-N1A	-2.28	1.29	1.35
3	B	403	NAI	C6N-N1N	2.26	1.42	1.37
3	C	403	NAI	O4D-C4D	-2.22	1.40	1.45
3	D	403	NAI	PN-O3	-2.20	1.57	1.59
3	D	403	NAI	C4A-N3A	2.17	1.38	1.34
3	B	403	NAI	C5A-N7A	-2.16	1.35	1.39
3	A	403	NAI	C6A-N6A	-2.14	1.28	1.34
3	B	403	NAI	C8A-N7A	2.13	1.35	1.31
3	B	403	NAI	C2A-N3A	2.08	1.37	1.33
3	D	403	NAI	PA-O3	2.04	1.61	1.59
3	A	403	NAI	C6N-N1N	2.04	1.42	1.37
3	B	403	NAI	C5D-C4D	2.02	1.57	1.51
3	D	403	NAI	C4N-C5N	-2.01	1.43	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	NAI	PA-O3	-2.00	1.57	1.59

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	404	BNF	O16-C14-N13	11.55	139.06	125.03
4	B	404	BNF	O16-C14-N13	9.83	136.96	125.03
4	A	404	BNF	O16-C14-N13	9.66	136.76	125.03
4	D	404	BNF	O16-C14-N13	7.73	134.41	125.03
3	C	403	NAI	N3A-C2A-N1A	-7.31	117.51	128.58
3	D	403	NAI	N3A-C2A-N1A	-7.16	117.74	128.58
3	A	403	NAI	N3A-C2A-N1A	-5.56	120.16	128.58
3	A	403	NAI	C2A-N1A-C6A	5.45	127.68	118.73
3	B	403	NAI	C6N-N1N-C2N	-5.39	113.55	119.32
3	B	403	NAI	N3A-C2A-N1A	-5.10	120.87	128.58
3	C	403	NAI	N9A-C8A-N7A	-4.98	106.87	113.94
3	D	403	NAI	C2A-N1A-C6A	4.60	126.29	118.73
4	A	404	BNF	C6-C5-C4	4.32	124.66	118.23
4	A	404	BNF	C2-C3-C4	-4.21	115.05	120.24
3	C	403	NAI	C6N-N1N-C2N	-4.12	114.91	119.32
3	B	403	NAI	C3N-C2N-N1N	4.08	129.19	123.20
3	A	403	NAI	C5A-N7A-C8A	3.95	109.66	103.45
4	A	404	BNF	C5-C12-N13	3.75	119.37	112.61
4	A	404	BNF	C1-C6-C5	-3.68	115.44	120.61
4	C	404	BNF	C5-C12-N13	3.54	118.99	112.61
3	D	403	NAI	C5A-N7A-C8A	3.51	108.97	103.45
3	C	403	NAI	C3N-C2N-N1N	3.45	128.28	123.20
3	A	403	NAI	C2D-C1D-N1N	3.42	121.72	113.31
4	B	404	BNF	C6-C5-C4	3.35	123.21	118.23
3	A	403	NAI	N9A-C8A-N7A	-3.34	109.20	113.94
3	D	403	NAI	N9A-C8A-N7A	-3.30	109.26	113.94
3	C	403	NAI	C5A-C4A-N3A	-3.22	122.28	126.72
3	C	403	NAI	C2A-N1A-C6A	3.03	123.70	118.73
3	A	403	NAI	C6N-N1N-C2N	-3.02	116.09	119.32
3	C	403	NAI	C5A-C6A-N6A	-2.94	116.00	123.29
3	A	403	NAI	C4A-C5A-N7A	-2.93	107.23	110.58
3	C	403	NAI	O4D-C1D-N1N	2.93	113.67	108.08
3	D	403	NAI	O4D-C1D-N1N	2.80	113.43	108.08
3	C	403	NAI	N6A-C6A-N1A	2.79	124.58	118.38
3	C	403	NAI	C4A-N9A-C1B	-2.71	120.30	126.63
4	B	404	BNF	C1-C6-C5	-2.69	116.83	120.61
3	C	403	NAI	C1B-N9A-C8A	2.60	132.86	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	BNF	C3-C2-C1	2.57	123.39	119.87
3	B	403	NAI	N9A-C8A-N7A	-2.57	110.29	113.94
4	B	404	BNF	C2-C3-C4	-2.56	117.08	120.24
3	C	403	NAI	C2A-N3A-C4A	2.51	117.96	111.83
3	B	403	NAI	C2A-N1A-C6A	2.46	122.78	118.73
3	D	403	NAI	O2D-C2D-C1D	2.44	118.50	110.10
3	C	403	NAI	C5A-C4A-N9A	2.39	108.42	105.81
3	D	403	NAI	O4B-C4B-C3B	2.38	109.87	105.15
4	D	404	BNF	C6-C5-C4	2.35	121.72	118.23
3	D	403	NAI	O1N-PN-O2N	2.35	123.36	112.44
3	B	403	NAI	O3-PA-O1A	-2.34	103.67	110.70
3	B	403	NAI	O2A-PA-O1A	2.33	123.27	112.44
3	B	403	NAI	C5A-N7A-C8A	2.24	106.97	103.45
3	D	403	NAI	C5A-C4A-N3A	-2.20	123.69	126.72
3	C	403	NAI	C2D-C1D-N1N	2.17	118.64	113.31
3	A	403	NAI	C5A-C4A-N3A	-2.15	123.75	126.72
4	C	404	BNF	C6-C5-C4	2.13	121.41	118.23
3	D	403	NAI	C2D-C1D-N1N	2.09	118.44	113.31
3	C	403	NAI	O1N-PN-O3	2.07	112.87	107.27
4	C	404	BNF	C2-C3-C4	-2.07	117.69	120.24
4	D	404	BNF	C2-C3-C4	-2.05	117.71	120.24
3	A	403	NAI	O4D-C1D-C2D	-2.04	102.25	106.62
3	D	403	NAI	C4A-C5A-N7A	-2.00	108.30	110.58

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	405	MRD	C2-C3-C4-O4
5	B	405	MRD	C2-C3-C4-C5
5	C	405[A]	MRD	C2-C3-C4-O4
3	B	403	NAI	C2D-C1D-N1N-C2N
3	A	403	NAI	C2D-C1D-N1N-C2N
3	C	403	NAI	C2D-C1D-N1N-C2N
3	D	403	NAI	C2D-C1D-N1N-C2N
3	B	403	NAI	O4D-C1D-N1N-C2N
3	C	403	NAI	O4D-C1D-N1N-C2N
3	D	403	NAI	O4D-C1D-N1N-C2N
3	A	403	NAI	O4D-C1D-N1N-C2N
4	D	404	BNF	O16-C14-N13-C12
5	C	405[A]	MRD	O2-C2-C3-C4
5	B	405	MRD	C1-C2-C3-C4

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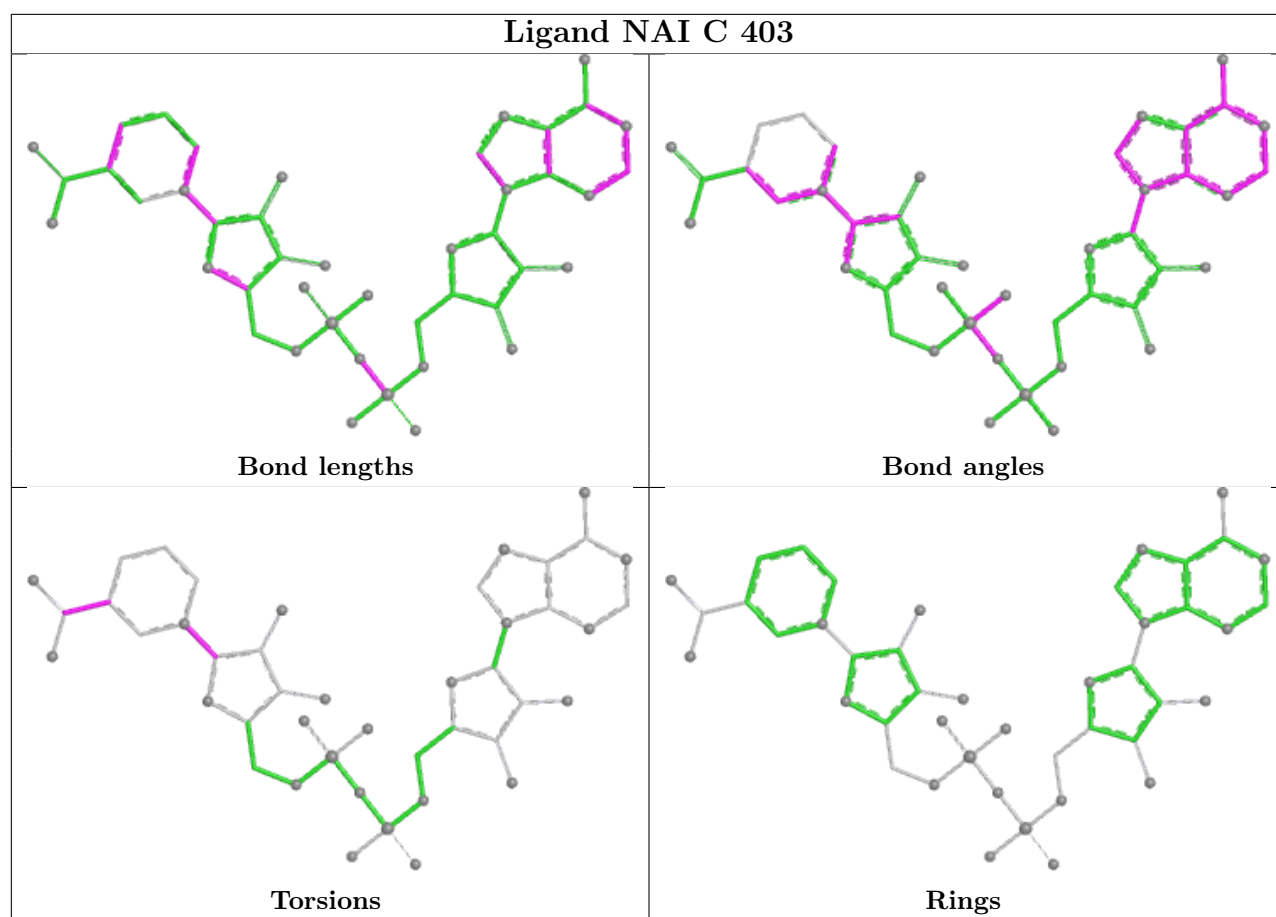
Mol	Chain	Res	Type	Atoms
3	B	403	NAI	O4B-C4B-C5B-O5B
3	C	403	NAI	C2N-C3N-C7N-O7N

There are no ring outliers.

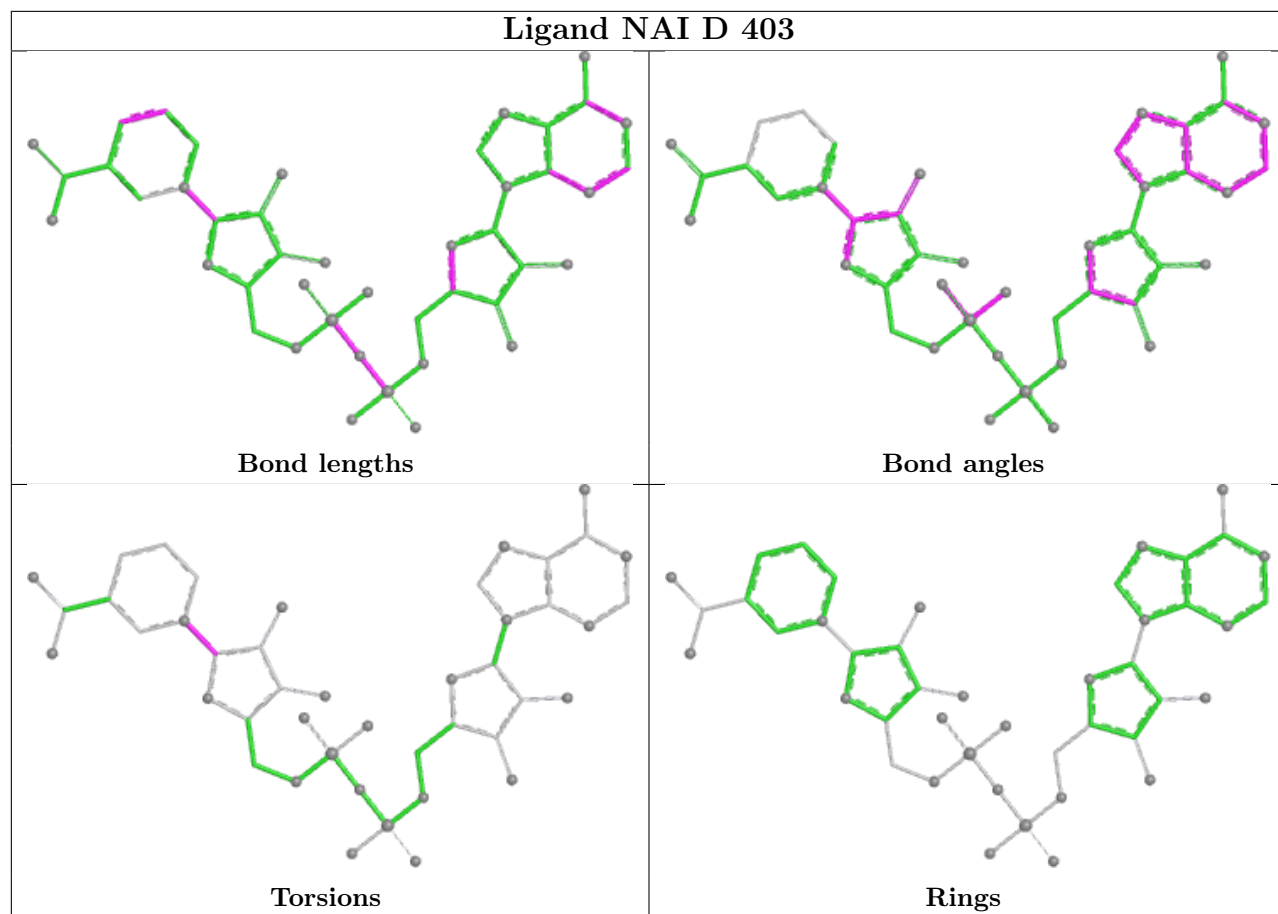
4 monomers are involved in 6 short contacts:

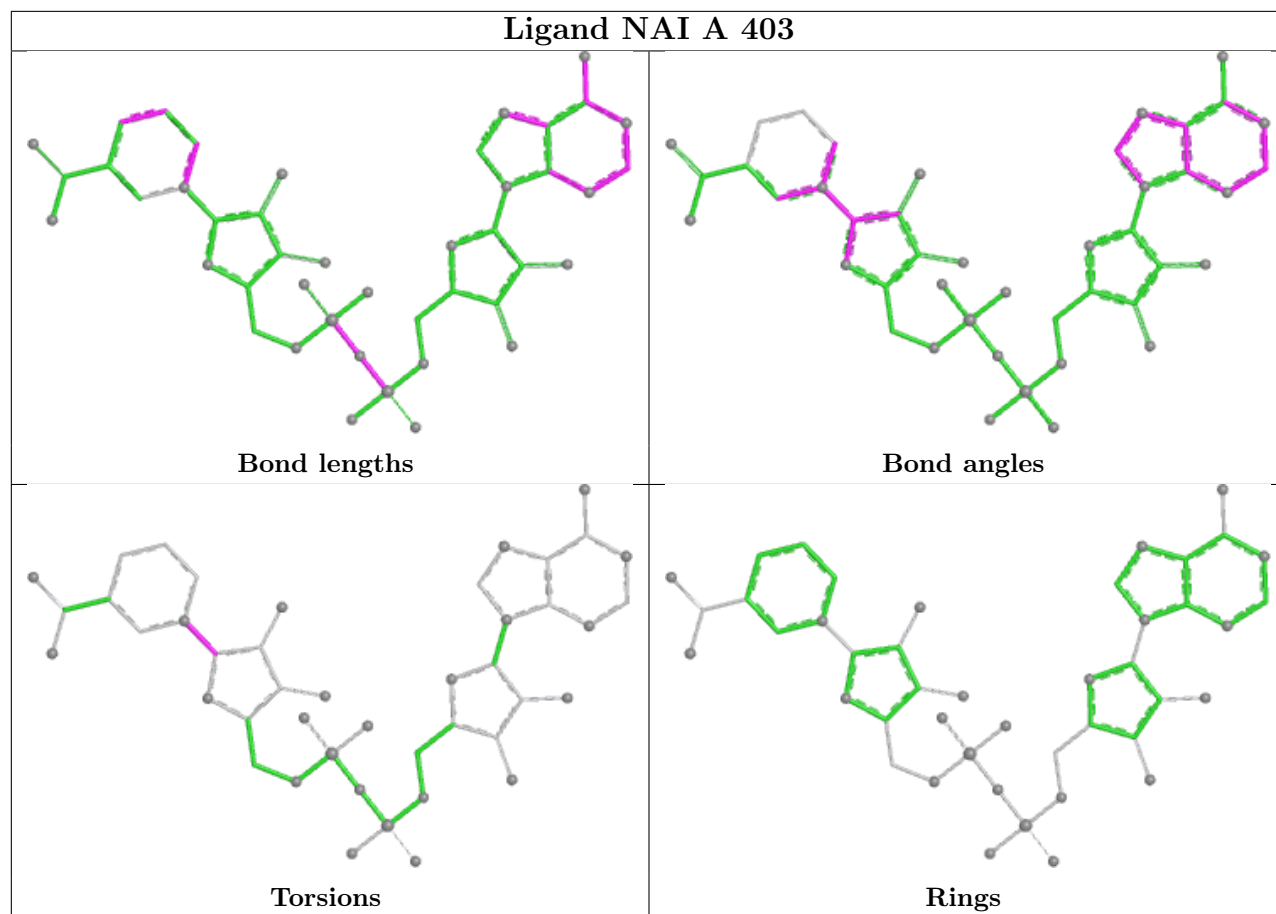
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	405	MRD	2	0
4	A	404	BNF	1	0
4	C	404	BNF	2	0
3	A	403	NAI	1	0

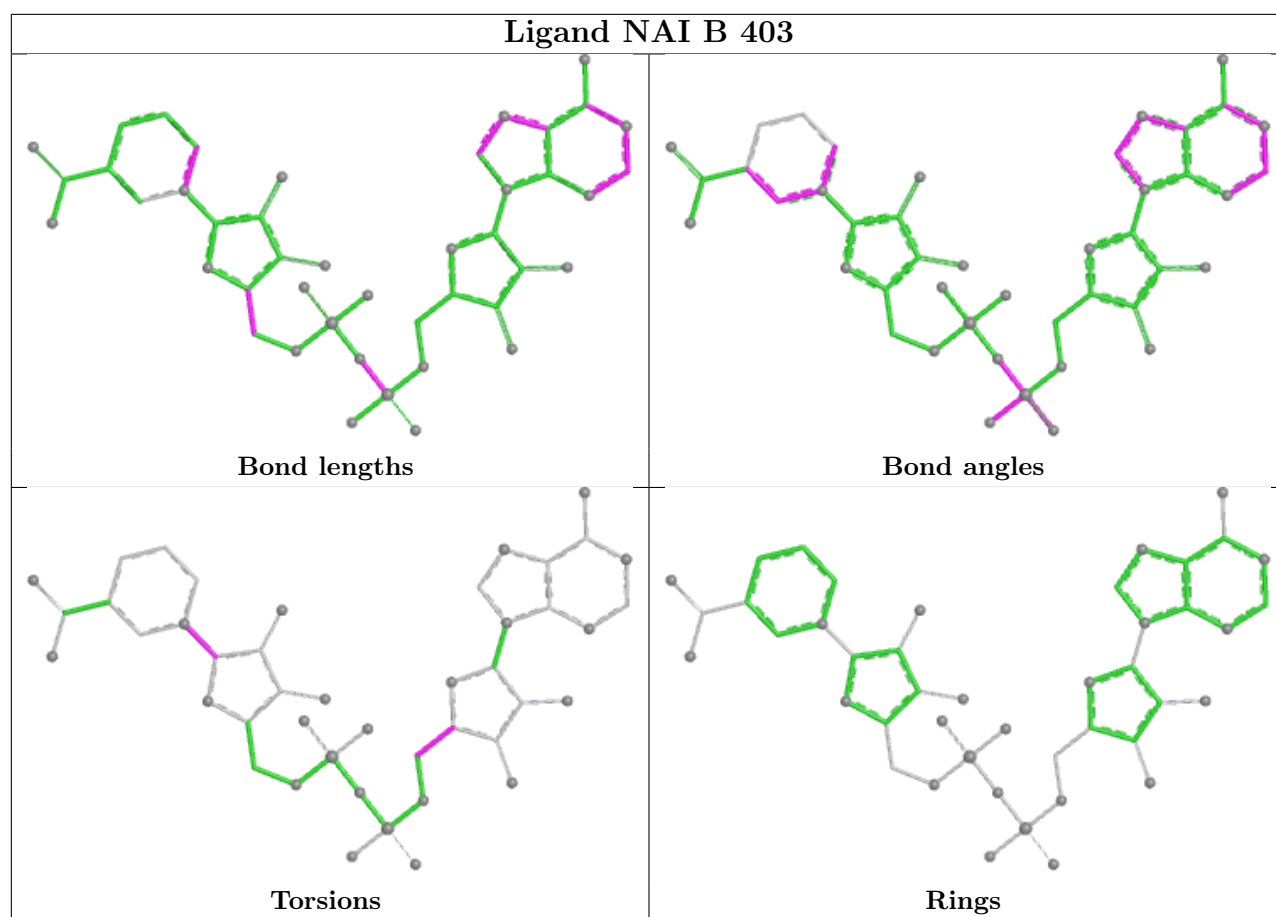
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand NAI D 403







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	374/374 (100%)	0.20	2 (0%) 87 89	10, 18, 29, 40	9 (2%)
1	B	374/374 (100%)	0.30	3 (0%) 82 86	10, 18, 30, 42	13 (3%)
1	C	374/374 (100%)	0.21	4 (1%) 78 79	8, 17, 27, 42	14 (3%)
1	D	374/374 (100%)	0.30	6 (1%) 70 71	10, 18, 30, 40	12 (3%)
All	All	1496/1496 (100%)	0.25	15 (1%) 79 82	8, 18, 29, 42	48 (3%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	255	THR	3.3
1	D	341	ALA	3.0
1	D	162	ALA	2.8
1	A	374	PHE	2.6
1	C	374	PHE	2.6
1	A	341	ALA	2.5
1	C	162	ALA	2.4
1	D	253	VAL	2.4
1	B	333	ALA	2.4
1	B	1	SER	2.2
1	C	163	ALA	2.2
1	D	33	ALA	2.2
1	D	180	TYR	2.1
1	C	333	ALA	2.1
1	B	76	ILE	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

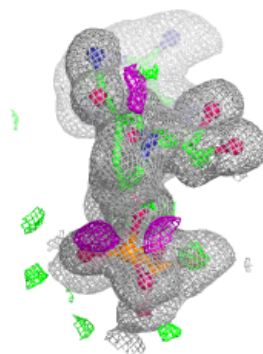
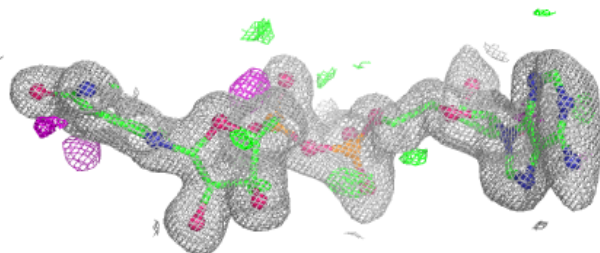
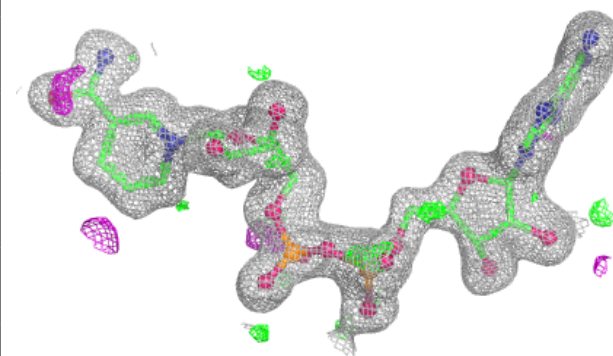
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MRD	C	405[A]	8/8	0.83	0.14	31,35,40,42	8
5	MRD	B	405	8/8	0.86	0.12	35,41,43,50	0
4	BNF	B	404	10/10	0.91	0.09	16,28,35,35	0
4	BNF	D	404	10/10	0.93	0.07	16,32,33,34	0
4	BNF	A	404	10/10	0.93	0.08	16,24,27,27	0
4	BNF	C	404	10/10	0.93	0.07	17,22,26,27	0
3	NAI	A	403	44/44	0.97	0.06	12,16,23,27	0
3	NAI	B	403	44/44	0.98	0.04	12,14,20,23	0
3	NAI	C	403	44/44	0.98	0.05	11,14,21,27	0
3	NAI	D	403	44/44	0.98	0.06	12,16,22,30	0
2	ZN	B	402	1/1	0.99	0.04	17,17,17,17	0
2	ZN	C	401	1/1	0.99	0.04	15,15,15,15	0
2	ZN	C	402	1/1	0.99	0.02	17,17,17,17	0
2	ZN	D	401	1/1	0.99	0.07	16,16,16,16	0
2	ZN	A	401	1/1	0.99	0.05	15,15,15,15	0
2	ZN	A	402	1/1	0.99	0.03	15,15,15,15	0
2	ZN	B	401	1/1	0.99	0.06	16,16,16,16	0
2	ZN	D	402	1/1	1.00	0.02	16,16,16,16	0

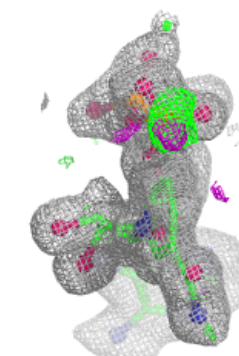
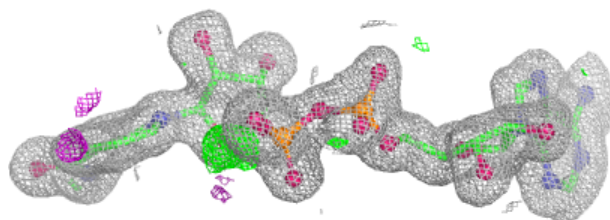
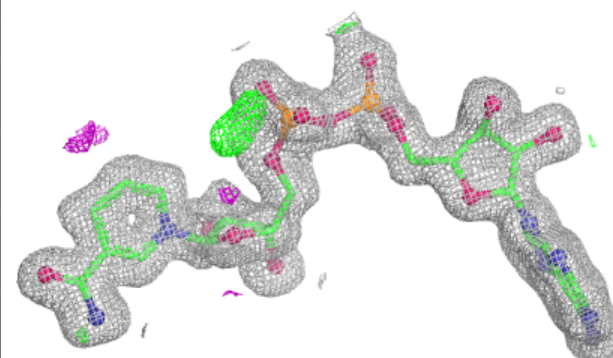
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI A 403:

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

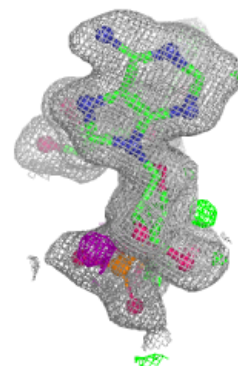
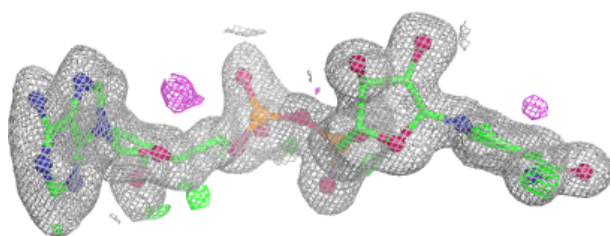
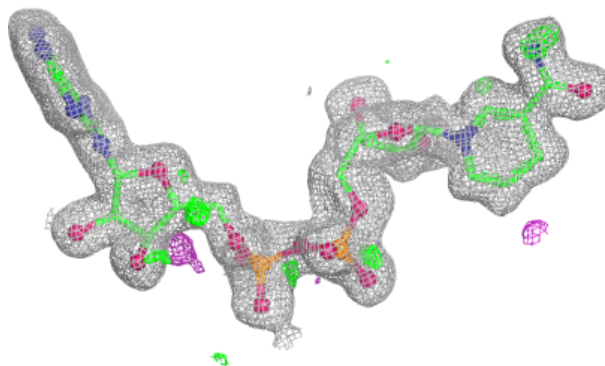
**Electron density around NAI B 403:**

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

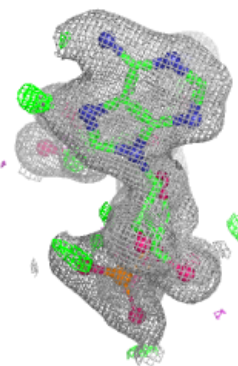
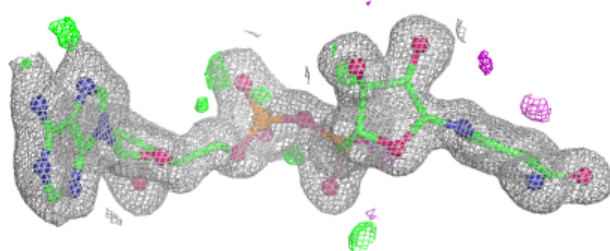
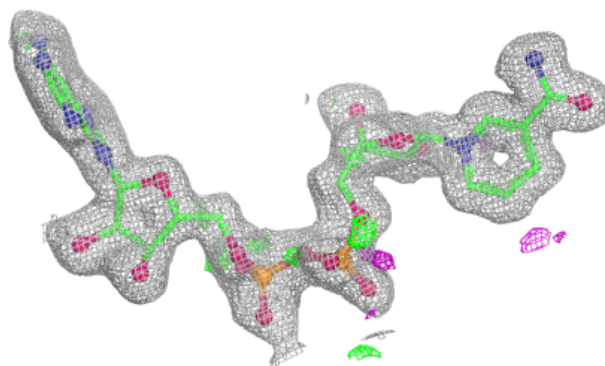


Electron density around NAI C 403:

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

**Electron density around NAI D 403:**

$2mF_o-DF_c$ (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.