



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 12:57 pm BST

PDB ID : 2VHW
Title : Crystal structure of holo L-alanine dehydrogenase from Mycobacterium tuberculosis in the open and closed conformation
Authors : Agren, D.; Schneider, G.
Deposited on : 2007-11-26
Resolution : 2.00 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

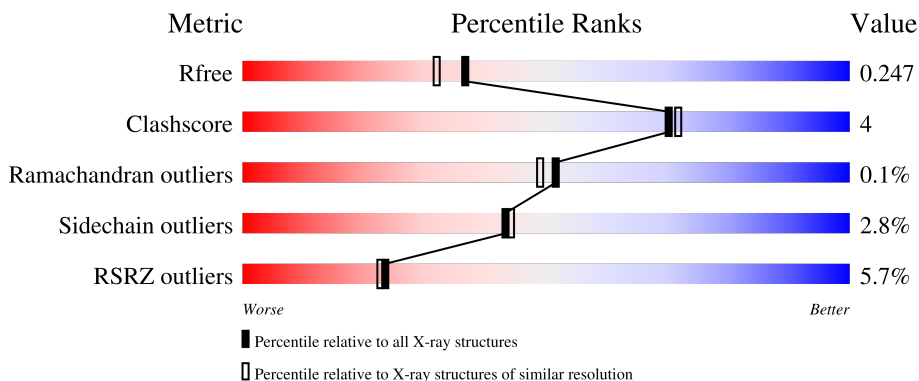
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



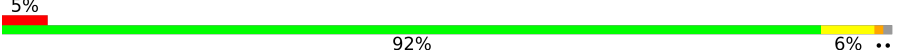
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	377	 4% 88% 9% ..
1	B	377	 2% 91% 7% ..
1	C	377	 9% 87% 10% ..
1	D	377	 % 90% 7% ..
1	E	377	 12% 92% 6% ..

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Mol	Chain	Length	Quality of chain
1	F	377	 5% 92% 6% **

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18159 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 ALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	371	2719	1710	479	517	13	0	0	0
1	B	370	2730	1717	479	521	13	0	3	0
1	C	371	2719	1710	479	517	13	0	0	0
1	D	370	2714	1707	478	516	13	0	0	0
1	E	373	2747	1727	488	519	13	0	1	0
1	F	373	2752	1730	488	521	13	0	2	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

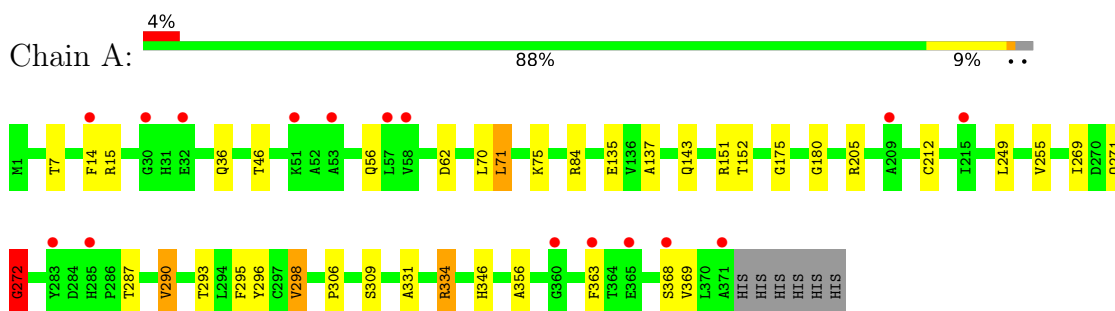
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).

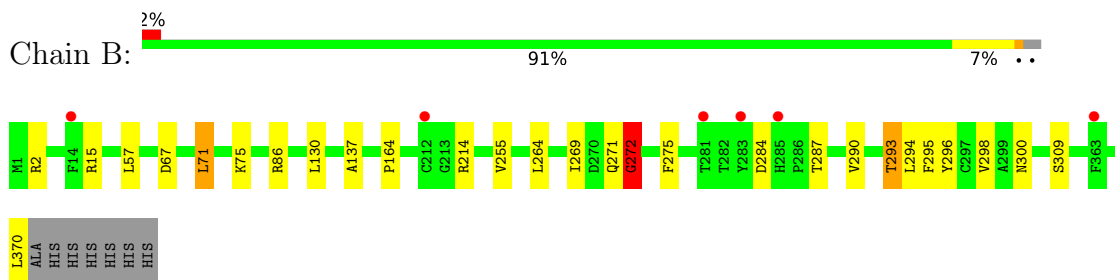
3 Residue-property plots

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.

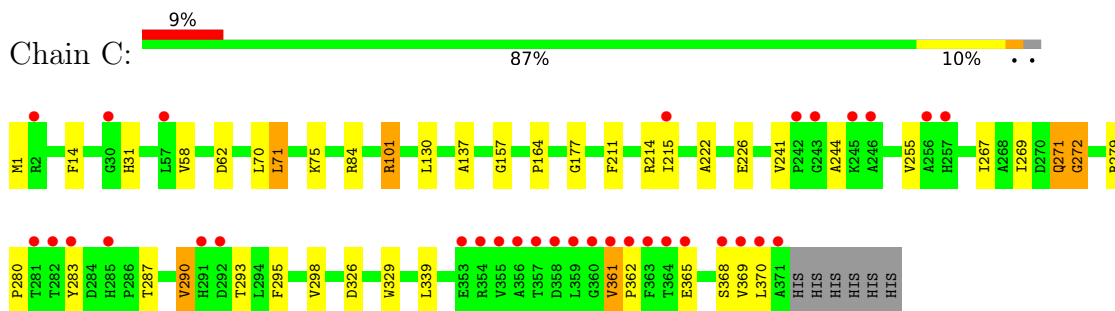
- Molecule 1: ALANINE DEHYDROGENASE



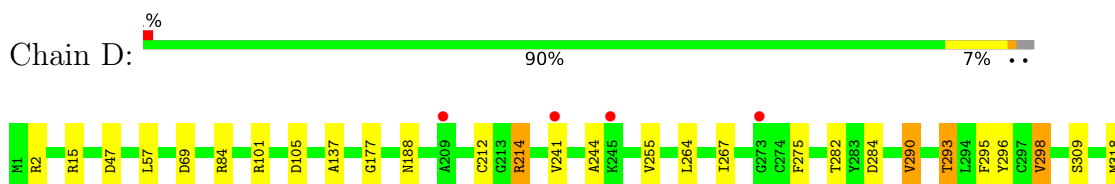
- Molecule 1: ALANINE DEHYDROGENASE

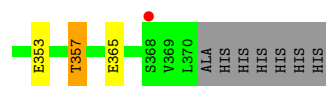


- Molecule 1: ALANINE DEHYDROGENASE

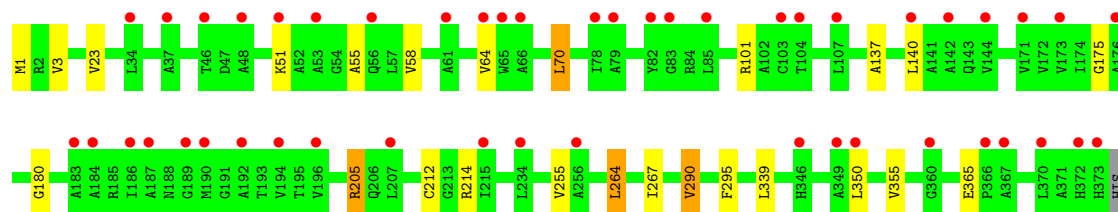
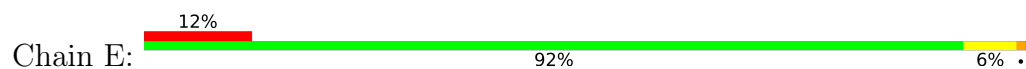


- Molecule 1: ALANINE DEHYDROGENASE

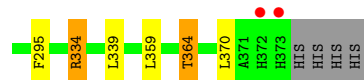
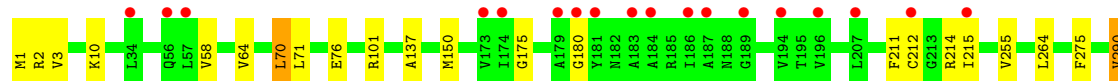
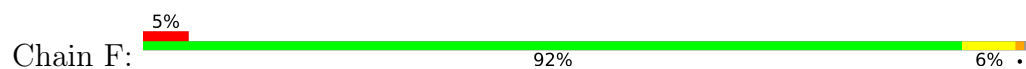




- Molecule 1: ALANINE DEHYDROGENASE



- Molecule 1: ALANINE DEHYDROGENASE



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	177.03Å 172.01Å 98.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 49.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-2.00) 94.6 (49.56-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.212 0.219 , 0.247	Depositor DCC
R_{free} test set	9699 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.257	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18159	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, MG

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	0.56	1/2769 (0.0%)	0.72	3/3773 (0.1%)
1	B	0.60	0/2789	0.76	4/3800 (0.1%)
1	C	0.53	0/2769	0.66	2/3773 (0.1%)
1	D	0.58	0/2764	0.67	1/3766 (0.0%)
1	E	0.52	0/2802	0.67	3/3817 (0.1%)
1	F	0.56	0/2810	0.68	1/3828 (0.0%)
All	All	0.56	1/16703 (0.0%)	0.69	14/22757 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	THR	CB-OG1	-5.76	1.31	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	GLY	N-CA-C	-10.27	87.42	113.10
1	B	272	GLY	N-CA-C	-8.68	91.39	113.10
1	E	205	ARG	NE-CZ-NH2	-8.31	116.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	272	GLY	N-CA-C	-7.83	93.51	113.10
1	E	205	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	E	264	LEU	CA-CB-CG	7.35	132.21	115.30
1	F	334	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	71	LEU	CA-CB-CG	-6.25	100.92	115.30
1	D	214	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	294	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	71	LEU	CA-CB-CG	-5.41	102.86	115.30
1	C	71	LEU	CA-CB-CG	-5.31	103.09	115.30
1	A	46	THR	OG1-CB-CG2	5.11	121.76	110.00
1	B	86	ARG	NE-CZ-NH1	-5.06	117.77	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	GLN	Peptide
1	B	271	GLN	Peptide
1	C	271	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2719	0	2732	21	0
1	B	2730	0	2743	14	0
1	C	2719	0	2732	32	0
1	D	2714	0	2727	23	0
1	E	2747	0	2759	19	0
1	F	2752	0	2763	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	44	0	27	1	0
3	B	44	0	27	1	0
3	C	44	0	27	3	0
3	D	44	0	27	3	0
3	E	44	0	27	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	44	0	27	1	0
4	A	219	0	0	0	0
4	B	310	0	0	1	0
4	C	211	0	0	1	0
4	D	297	0	0	3	0
4	E	195	0	0	3	0
4	F	280	0	0	3	0
All	All	18159	0	16618	120	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 4.

All (120) 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:101:ARG:HG3	1:C:101:ARG:HH21	1.18	1.04
1:C:241:VAL:HG23	1:C:244:ALA:HB3	1.57	0.87
1:C:101:ARG:HH21	1:C:101:ARG:CG	1.87	0.86
1:D:282:THR:HG22	1:D:284:ASP:H	1.43	0.83
1:B:255:VAL:HG11	1:B:290:VAL:HG22	1.63	0.78
1:C:329:TRP:HH2	1:C:369:VAL:HG12	1.49	0.76
1:D:214:ARG:NH2	1:F:212:CYS:O	2.20	0.72
1:C:101:ARG:HG3	1:C:101:ARG:NH2	1.96	0.71
1:D:241:VAL:HG23	1:D:244:ALA:HB3	1.72	0.70
1:C:329:TRP:HH2	1:C:369:VAL:CG1	2.05	0.70
1:C:361:VAL:HG22	1:C:362:PRO:HD2	1.72	0.70
1:D:318:MET:HG3	4:D:2126:HOH:O	1.92	0.69
1:D:353:GLU:O	1:D:357:THR:HG23	1.92	0.69
1:E:205:ARG:NH2	4:E:2104:HOH:O	2.26	0.68
1:F:334:ARG:HD2	1:F:370:LEU:O	1.95	0.67
1:E:350:LEU:HD21	1:E:355:VAL:HG12	1.78	0.66
1:C:75:LYS:NZ	4:C:2051:HOH:O	2.28	0.65
1:A:290:VAL:HG13	1:A:295:PHE:CD1	2.32	0.65
1:D:2:ARG:NH1	4:D:2002:HOH:O	2.29	0.64
1:B:296:TYR:CE2	1:B:298:VAL:HG13	2.32	0.64
1:C:214:ARG:HG3	1:E:214:ARG:HG3	1.81	0.63
1:E:255:VAL:HG11	1:E:290:VAL:HG22	1.79	0.62
1:C:31:HIS:HE1	1:C:326:ASP:OD1	1.85	0.60
1:D:290:VAL:HG13	1:D:295:PHE:CD1	2.37	0.59
1:A:255:VAL:HG11	1:A:290:VAL:HG22	1.84	0.59
1:C:241:VAL:CG2	1:C:244:ALA:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:GLU:HG3	4:D:2290:HOH:O	2.02	0.59
1:B:269:ILE:O	1:B:272:GLY:HA2	2.02	0.59
1:A:62:ASP:OD1	1:A:84:ARG:HD3	2.03	0.58
1:A:135:GLU:OE1	1:E:205:ARG:HD3	2.03	0.58
1:C:255:VAL:HG11	1:C:290:VAL:HG22	1.85	0.57
1:A:137:ALA:HB2	3:A:1373:NAI:H4N	1.86	0.57
1:F:255:VAL:HG11	1:F:290:VAL:HG22	1.85	0.56
1:C:101:ARG:CG	1:C:101:ARG:NH2	2.56	0.56
1:C:1:MET:N	1:C:31:HIS:HD2	2.04	0.56
1:E:214:ARG:NH2	4:E:2116:HOH:O	2.23	0.56
1:F:101[B]:ARG:NH2	1:F:359:LEU:O	2.37	0.56
1:B:214:ARG:NH2	4:B:2199:HOH:O	2.29	0.55
1:D:188:ASN:OD1	1:D:214:ARG:HD2	2.07	0.55
1:E:365:GLU:HG3	4:E:2192:HOH:O	2.07	0.55
1:C:269:ILE:O	1:C:272:GLY:HA2	2.06	0.55
1:D:264:LEU:HD13	1:D:293:THR:CG2	2.37	0.55
1:C:329:TRP:CH2	1:C:369:VAL:HG12	2.38	0.54
1:D:101:ARG:NH2	1:D:105:ASP:OD2	2.41	0.53
1:E:290:VAL:HG13	1:E:295:PHE:CD1	2.43	0.53
1:C:290:VAL:HG13	1:C:295:PHE:CD1	2.44	0.53
1:C:267:ILE:O	3:C:1372:NAI:H2N	2.09	0.52
1:F:137:ALA:HB2	3:F:1374:NAI:H4N	1.91	0.52
1:D:255:VAL:HG11	1:D:290:VAL:HG22	1.92	0.52
1:D:267:ILE:O	3:D:1371:NAI:H2N	2.10	0.52
1:F:290:VAL:HG13	1:F:295:PHE:CD1	2.45	0.51
1:B:137:ALA:HB2	3:B:1372:NAI:H4N	1.93	0.51
1:E:137:ALA:HB2	3:E:1374:NAI:H4N	1.93	0.51
1:F:10:LYS:HE3	1:F:76:GLU:OE2	2.10	0.51
1:D:264:LEU:HD13	1:D:293:THR:HG23	1.93	0.50
1:F:211:PHE:CD1	1:F:215:ILE:HD12	2.46	0.50
1:B:15:ARG:HD3	1:B:309:SER:HB3	1.94	0.50
1:A:306:PRO:HD2	1:C:157:GLY:HA3	1.94	0.49
1:F:214:ARG:NH2	4:F:2159:HOH:O	2.40	0.49
1:F:58:VAL:CG2	1:F:64:VAL:HG23	2.42	0.49
1:B:75:LYS:NZ	1:B:300:ASN:OD1	2.46	0.48
1:A:287:THR:HA	1:A:295:PHE:O	2.14	0.48
1:A:152:THR:HG21	1:C:283:TYR:CD2	2.48	0.48
1:A:346:HIS:CD2	1:A:369:VAL:HG21	2.48	0.48
1:B:2:ARG:HD3	1:B:67:ASP:O	2.14	0.48
1:A:7:THR:H	1:A:36:GLN:NE2	2.11	0.48
1:A:151:ARG:HD3	1:C:14:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:VAL:HG21	1:E:64:VAL:HG23	1.96	0.47
1:F:58:VAL:HG21	1:F:64:VAL:HG23	1.95	0.47
1:F:364:THR:CG2	4:F:2252:HOH:O	2.62	0.47
1:A:296:TYR:CE2	1:A:298:VAL:HG13	2.49	0.47
1:B:290:VAL:HG13	1:B:295:PHE:CD1	2.49	0.47
1:B:264:LEU:HB3	1:B:275:PHE:CE1	2.50	0.47
1:D:264:LEU:CD1	1:D:293:THR:HG23	2.45	0.47
1:F:364:THR:HG22	4:F:2252:HOH:O	2.14	0.46
1:B:287:THR:HA	1:B:295:PHE:O	2.14	0.46
1:D:15:ARG:HD3	1:D:309:SER:HB3	1.98	0.46
1:D:296:TYR:CE2	1:D:298:VAL:HG13	2.51	0.46
1:E:1:MET:SD	1:E:70:LEU:HB2	2.56	0.45
1:D:188:ASN:OD1	1:D:214:ARG:CD	2.64	0.45
1:E:58:VAL:CG2	1:E:64:VAL:HG23	2.47	0.45
1:C:279:ARG:HB2	1:C:280:PRO:HD2	1.98	0.45
1:A:175:GLY:O	1:A:180:GLY:HA3	2.17	0.44
1:A:331:ALA:HA	1:A:334:ARG:HD2	1.98	0.44
1:B:290:VAL:O	1:B:293:THR:HB	2.18	0.44
1:C:211:PHE:CD1	1:C:215:ILE:HD12	2.52	0.44
1:C:164:PRO:HG2	1:E:205:ARG:HG2	1.98	0.44
1:C:365:GLU:O	1:C:368:SER:HB2	2.18	0.44
1:D:177:GLY:HA3	3:D:1371:NAI:O5B	2.18	0.44
1:F:58:VAL:HG21	1:F:64:VAL:CG2	2.48	0.44
1:D:2:ARG:HD3	1:D:69:ASP:OD2	2.18	0.44
1:F:58:VAL:CG2	1:F:64:VAL:CG2	2.96	0.43
1:B:255:VAL:HG11	1:B:290:VAL:CG2	2.43	0.43
1:C:62:ASP:OD1	1:C:84:ARG:HD3	2.19	0.43
1:C:287:THR:HA	1:C:295:PHE:O	2.18	0.43
1:E:175:GLY:O	1:E:180:GLY:HA3	2.18	0.43
1:D:137:ALA:HB2	3:D:1371:NAI:H4N	2.01	0.42
1:A:205:ARG:HG2	1:B:164:PRO:HG2	2.01	0.42
1:A:269:ILE:O	1:A:272:GLY:HA2	2.19	0.42
1:E:23:VAL:HG11	1:E:55:ALA:HB2	2.00	0.42
1:A:75:LYS:HA	1:A:75:LYS:HD2	1.87	0.42
1:A:346:HIS:HD2	1:A:369:VAL:HG21	1.83	0.42
1:A:14:PHE:HB2	1:A:306:PRO:HG3	2.02	0.42
1:A:15:ARG:HD3	1:A:309:SER:HB3	2.02	0.42
1:D:47:ASP:HB3	1:D:57:LEU:HD13	2.02	0.42
1:D:264:LEU:HB3	1:D:275:PHE:CE1	2.54	0.42
1:C:177:GLY:HA3	3:C:1372:NAI:O5B	2.19	0.41
1:C:329:TRP:CH2	1:C:369:VAL:CG1	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101[A]:ARG:HE	1:E:101[A]:ARG:HB2	1.54	0.41
1:F:264:LEU:HB3	1:F:275:PHE:CE1	2.55	0.41
1:C:222:ALA:O	1:C:226:GLU:HG3	2.20	0.41
1:E:51:LYS:HB2	1:E:51:LYS:HE3	1.80	0.41
1:A:356:ALA:CB	1:A:363:PHE:HB2	2.50	0.41
1:C:137:ALA:HB2	3:C:1372:NAI:H4N	2.01	0.41
1:F:175:GLY:O	1:F:180:GLY:HA3	2.21	0.41
1:E:267:ILE:O	3:E:1374:NAI:H2N	2.20	0.41
1:F:1:MET:SD	1:F:70:LEU:HB2	2.61	0.41
1:F:2:ARG:HE	1:F:2:ARG:HB2	1.69	0.41
1:C:1:MET:H3	1:C:31:HIS:HD2	1.68	0.41
1:E:140:LEU:HD22	1:F:150:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	369/377 (98%)	362 (98%)	6 (2%)	1 (0%)	41	37
1	B	371/377 (98%)	364 (98%)	6 (2%)	1 (0%)	41	37
1	C	369/377 (98%)	361 (98%)	8 (2%)	0	100	100
1	D	368/377 (98%)	364 (99%)	4 (1%)	0	100	100
1	E	372/377 (99%)	366 (98%)	6 (2%)	0	100	100
1	F	373/377 (99%)	368 (99%)	5 (1%)	0	100	100
All	All	2222/2262 (98%)	2185 (98%)	35 (2%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	GLY

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Mol	Chain	Res	Type
1	B	272	GLY

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	276/282 (98%)	265 (96%)	11 (4%)	31 29
1	B	279/282 (99%)	273 (98%)	6 (2%)	52 55
1	C	276/282 (98%)	264 (96%)	12 (4%)	29 26
1	D	276/282 (98%)	270 (98%)	6 (2%)	52 55
1	E	279/282 (99%)	273 (98%)	6 (2%)	52 55
1	F	280/282 (99%)	274 (98%)	6 (2%)	53 57
All	All	1666/1692 (98%)	1619 (97%)	47 (3%)	43 44

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	70	LEU
1	A	71	LEU
1	A	143	GLN
1	A	212	CYS
1	A	249	LEU
1	A	290	VAL
1	A	293	THR
1	A	298	VAL
1	A	334	ARG
1	A	368	SER
1	B	57	LEU
1	B	71	LEU
1	B	130	LEU
1	B	284	ASP
1	B	293	THR
1	B	370	LEU

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Mol	Chain	Res	Type
1	C	58	VAL
1	C	70	LEU
1	C	71	LEU
1	C	101	ARG
1	C	130	LEU
1	C	271	GLN
1	C	290	VAL
1	C	293	THR
1	C	298	VAL
1	C	339	LEU
1	C	361	VAL
1	C	370	LEU
1	D	84	ARG
1	D	212	CYS
1	D	290	VAL
1	D	293	THR
1	D	298	VAL
1	D	357	THR
1	E	3	VAL
1	E	70	LEU
1	E	212	CYS
1	E	264	LEU
1	E	290	VAL
1	E	339	LEU
1	F	3	VAL
1	F	70	LEU
1	F	71	LEU
1	F	290	VAL
1	F	339	LEU
1	F	364	THR

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

Mol	Chain	Res	Type
1	A	36	GLN
1	B	12	ASN
1	B	87	HIS
1	B	271	GLN
1	C	31	HIS
1	C	121	GLN
1	C	148	HIS
1	D	96	HIS

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Mol	Chain	Res	Type
1	D	148	HIS
1	E	56	GLN
1	E	148	HIS
1	F	11	ASN
1	F	12	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 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$
3	NAI	E	1374	-	42,48,48	1.38	5 (11%)	47,73,73	1.38	5 (10%)
3	NAI	C	1372	-	42,48,48	1.37	4 (9%)	47,73,73	1.36	5 (10%)
3	NAI	B	1372	-	42,48,48	1.38	5 (11%)	47,73,73	1.43	7 (14%)
3	NAI	A	1373	-	42,48,48	1.39	4 (9%)	47,73,73	1.31	6 (12%)
3	NAI	F	1374	-	42,48,48	1.36	5 (11%)	47,73,73	1.47	8 (17%)
3	NAI	D	1371	-	42,48,48	1.42	4 (9%)	47,73,73	1.57	6 (12%)

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
3	NAI	E	1374	-	-	5/25/72/72	0/5/5/5
3	NAI	C	1372	-	-	6/25/72/72	0/5/5/5
3	NAI	B	1372	-	-	5/25/72/72	0/5/5/5
3	NAI	A	1373	-	-	5/25/72/72	0/5/5/5
3	NAI	F	1374	-	-	6/25/72/72	0/5/5/5
3	NAI	D	1371	-	-	6/25/72/72	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1373	NAI	C4N-C3N	-5.52	1.39	1.49
3	B	1372	NAI	C4N-C3N	-5.33	1.39	1.49
3	C	1372	NAI	C4N-C3N	-4.98	1.40	1.49
3	D	1371	NAI	C4N-C3N	-4.94	1.40	1.49
3	E	1374	NAI	C4N-C3N	-4.83	1.40	1.49
3	F	1374	NAI	C4N-C3N	-4.39	1.41	1.49
3	C	1372	NAI	C6N-C5N	3.98	1.40	1.33
3	D	1371	NAI	C6N-C5N	3.98	1.40	1.33
3	E	1374	NAI	C6N-C5N	3.85	1.40	1.33
3	A	1373	NAI	C4N-C5N	-3.79	1.39	1.48
3	F	1374	NAI	C6N-C5N	3.59	1.39	1.33
3	B	1372	NAI	C4N-C5N	-3.34	1.40	1.48
3	E	1374	NAI	C4N-C5N	-3.24	1.40	1.48
3	D	1371	NAI	C4N-C5N	-3.23	1.40	1.48
3	A	1373	NAI	C6N-C5N	3.15	1.39	1.33
3	B	1372	NAI	C6N-C5N	2.97	1.38	1.33
3	C	1372	NAI	C4N-C5N	-2.92	1.41	1.48
3	F	1374	NAI	C4N-C5N	-2.81	1.41	1.48
3	D	1371	NAI	C5A-C4A	2.68	1.48	1.40
3	E	1374	NAI	C5A-C4A	2.64	1.47	1.40
3	F	1374	NAI	C5A-C4A	2.63	1.47	1.40
3	C	1372	NAI	C5A-C4A	2.58	1.47	1.40
3	F	1374	NAI	C2A-N3A	2.47	1.36	1.32
3	B	1372	NAI	C5A-C4A	2.41	1.47	1.40
3	E	1374	NAI	C2A-N3A	2.40	1.36	1.32
3	B	1372	NAI	C2A-N3A	2.19	1.35	1.32
3	A	1373	NAI	C5A-C4A	2.05	1.46	1.40

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1371	NAI	O4D-C1D-N1N	5.34	118.50	108.06
3	E	1374	NAI	O4D-C1D-N1N	4.80	117.45	108.06
3	F	1374	NAI	O4D-C1D-N1N	4.46	116.78	108.06
3	C	1372	NAI	O4D-C1D-N1N	4.14	116.15	108.06
3	A	1373	NAI	N3A-C2A-N1A	-3.93	122.53	128.68
3	E	1374	NAI	N3A-C2A-N1A	-3.74	122.83	128.68
3	C	1372	NAI	C1D-N1N-C2N	-3.64	115.05	121.11
3	D	1371	NAI	N3A-C2A-N1A	-3.63	123.00	128.68
3	D	1371	NAI	C1D-N1N-C2N	-3.48	115.32	121.11
3	B	1372	NAI	N3A-C2A-N1A	-3.28	123.56	128.68
3	F	1374	NAI	C1D-N1N-C2N	-3.18	115.82	121.11
3	A	1373	NAI	C4A-C5A-N7A	-3.18	106.09	109.40
3	C	1372	NAI	N3A-C2A-N1A	-3.16	123.74	128.68
3	F	1374	NAI	N3A-C2A-N1A	-3.14	123.77	128.68
3	B	1372	NAI	O4D-C1D-N1N	3.13	114.18	108.06
3	B	1372	NAI	PN-O3-PA	-3.07	122.30	132.83
3	B	1372	NAI	C4A-C5A-N7A	-3.02	106.25	109.40
3	D	1371	NAI	C4A-C5A-N7A	-2.96	106.31	109.40
3	A	1373	NAI	C1D-N1N-C2N	-2.78	116.49	121.11
3	C	1372	NAI	C4A-C5A-N7A	-2.75	106.53	109.40
3	D	1371	NAI	C3N-C7N-N7N	2.74	122.53	117.67
3	E	1374	NAI	O4D-C1D-C2D	-2.66	100.84	106.64
3	A	1373	NAI	O4D-C1D-N1N	2.65	113.24	108.06
3	B	1372	NAI	O4B-C1B-C2B	-2.64	103.06	106.93
3	B	1372	NAI	C1D-N1N-C2N	-2.56	116.85	121.11
3	F	1374	NAI	N6A-C6A-N1A	2.36	123.46	118.57
3	C	1372	NAI	PN-O3-PA	-2.32	124.88	132.83
3	B	1372	NAI	O4D-C1D-C2D	-2.30	101.64	106.64
3	F	1374	NAI	PN-O3-PA	-2.23	125.17	132.83
3	A	1373	NAI	O4B-C1B-C2B	-2.21	103.70	106.93
3	D	1371	NAI	PN-O3-PA	-2.20	125.27	132.83
3	E	1374	NAI	C4A-C5A-N7A	-2.18	107.13	109.40
3	F	1374	NAI	C2A-N1A-C6A	2.18	122.48	118.75
3	A	1373	NAI	O4D-C1D-C2D	-2.17	101.92	106.64
3	E	1374	NAI	C1B-N9A-C4A	-2.15	122.86	126.64
3	F	1374	NAI	O4B-C1B-C2B	-2.15	103.78	106.93
3	F	1374	NAI	O4D-C1D-C2D	-2.04	102.19	106.64

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1371	NAI	C2D-C1D-N1N-C2N
3	D	1371	NAI	C2D-C1D-N1N-C6N
3	D	1371	NAI	O4D-C1D-N1N-C6N
3	A	1373	NAI	C2D-C1D-N1N-C2N
3	C	1372	NAI	C2D-C1D-N1N-C2N
3	C	1372	NAI	O4D-C1D-N1N-C2N
3	D	1371	NAI	O4D-C1D-N1N-C2N
3	C	1372	NAI	O4D-C1D-N1N-C6N
3	B	1372	NAI	C2D-C1D-N1N-C2N
3	A	1373	NAI	O4D-C1D-N1N-C2N
3	B	1372	NAI	O4D-C1D-N1N-C2N
3	F	1374	NAI	O4D-C1D-N1N-C2N
3	F	1374	NAI	C2D-C1D-N1N-C2N
3	E	1374	NAI	O4D-C1D-N1N-C2N
3	E	1374	NAI	C2D-C1D-N1N-C2N
3	F	1374	NAI	O4D-C1D-N1N-C6N
3	A	1373	NAI	C2D-C1D-N1N-C6N
3	B	1372	NAI	C2D-C1D-N1N-C6N
3	C	1372	NAI	C2D-C1D-N1N-C6N
3	F	1374	NAI	C2D-C1D-N1N-C6N
3	D	1371	NAI	O4B-C4B-C5B-O5B
3	E	1374	NAI	C2D-C1D-N1N-C6N
3	A	1373	NAI	O4D-C1D-N1N-C6N
3	B	1372	NAI	O4D-C1D-N1N-C6N
3	E	1374	NAI	O4D-C1D-N1N-C6N
3	B	1372	NAI	O4B-C4B-C5B-O5B
3	C	1372	NAI	O4B-C4B-C5B-O5B
3	E	1374	NAI	O4B-C4B-C5B-O5B
3	F	1374	NAI	O4B-C4B-C5B-O5B
3	C	1372	NAI	PN-O3-PA-O2A
3	D	1371	NAI	PN-O3-PA-O1A
3	F	1374	NAI	PN-O3-PA-O2A
3	A	1373	NAI	O4B-C4B-C5B-O5B

There are no ring outliers.

6 monomers are involved in 11 short contacts:

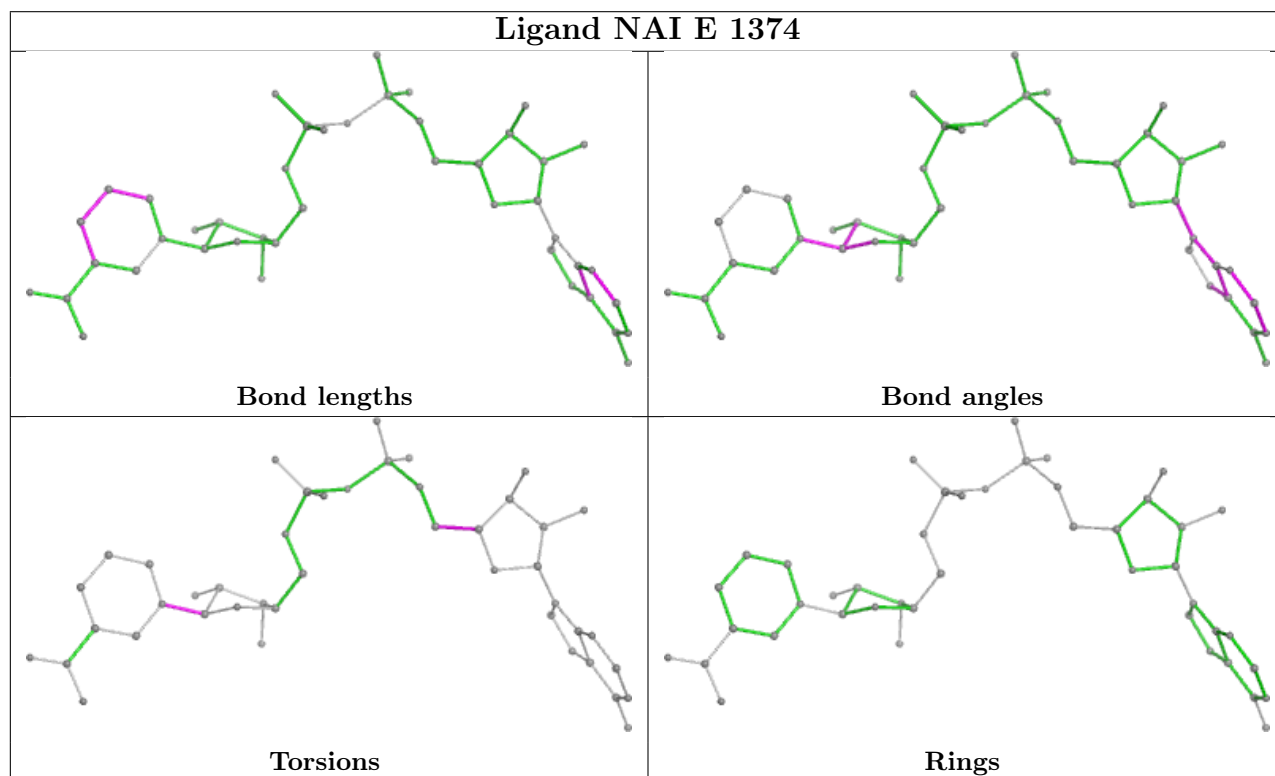
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1374	NAI	2	0
3	C	1372	NAI	3	0
3	B	1372	NAI	1	0
3	A	1373	NAI	1	0
3	F	1374	NAI	1	0

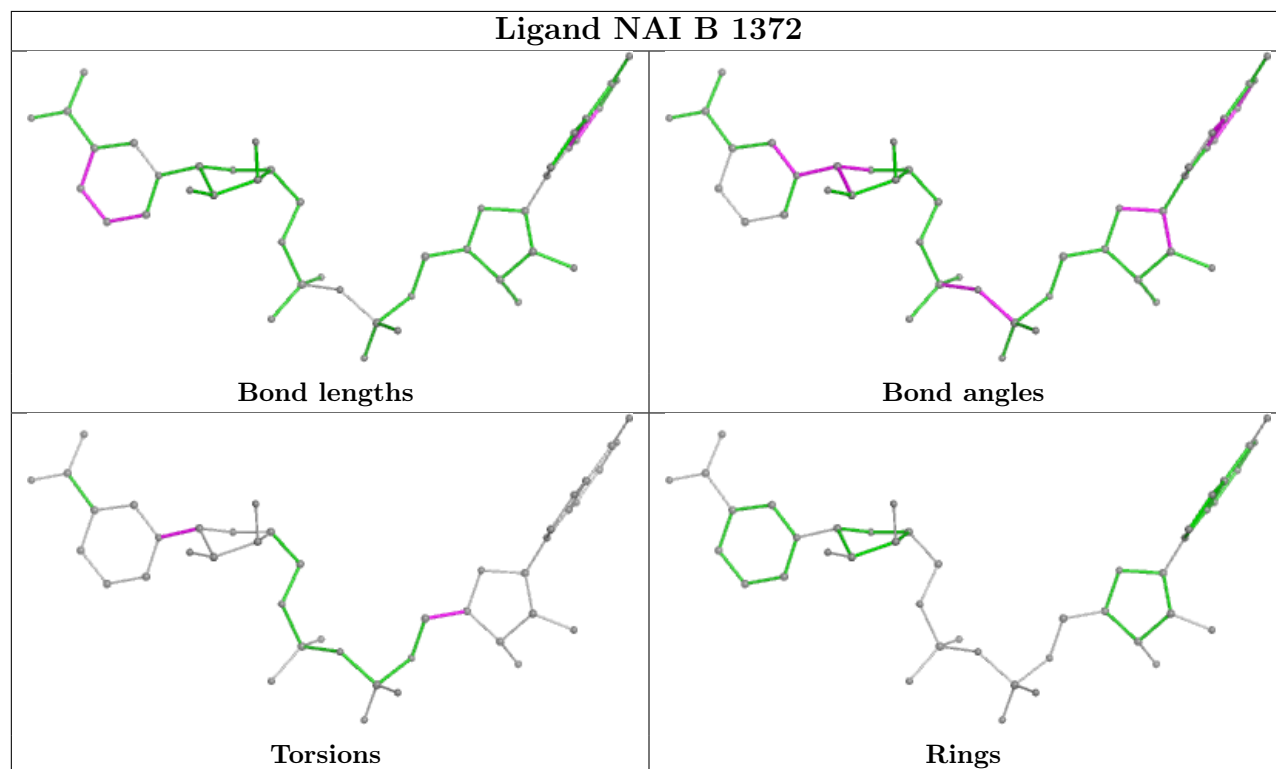
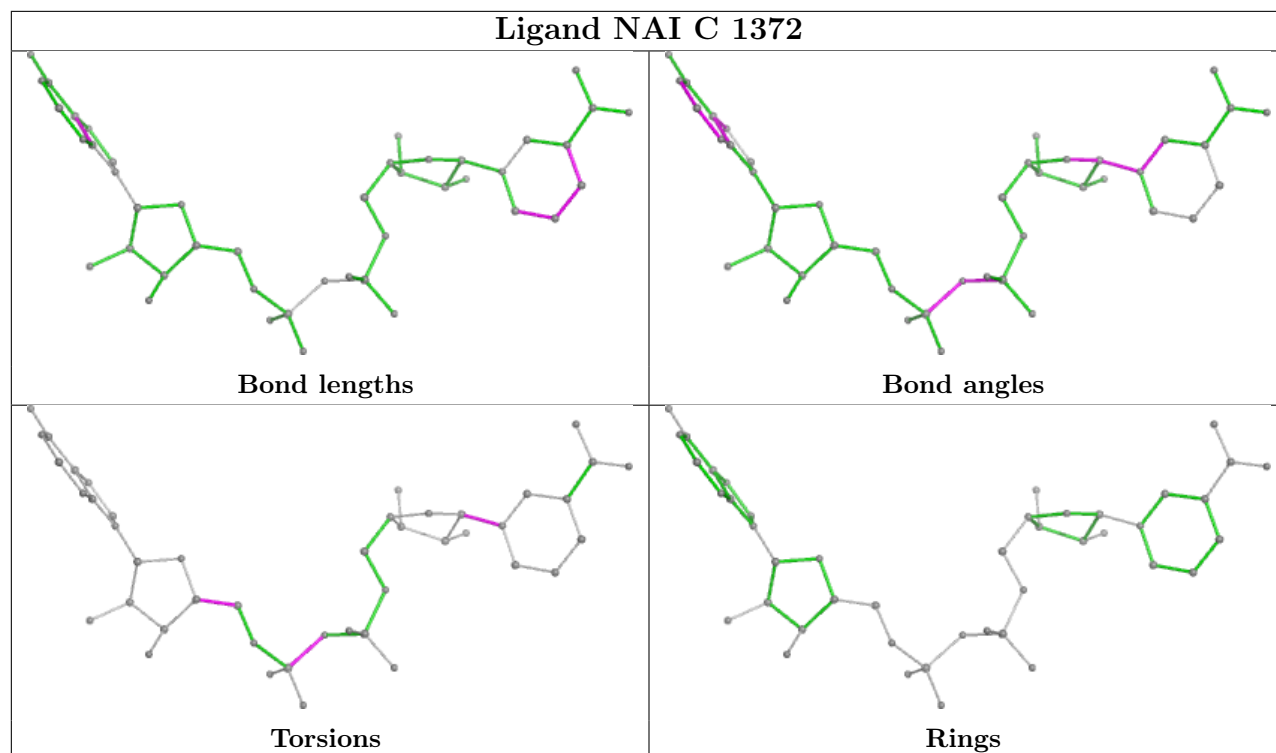
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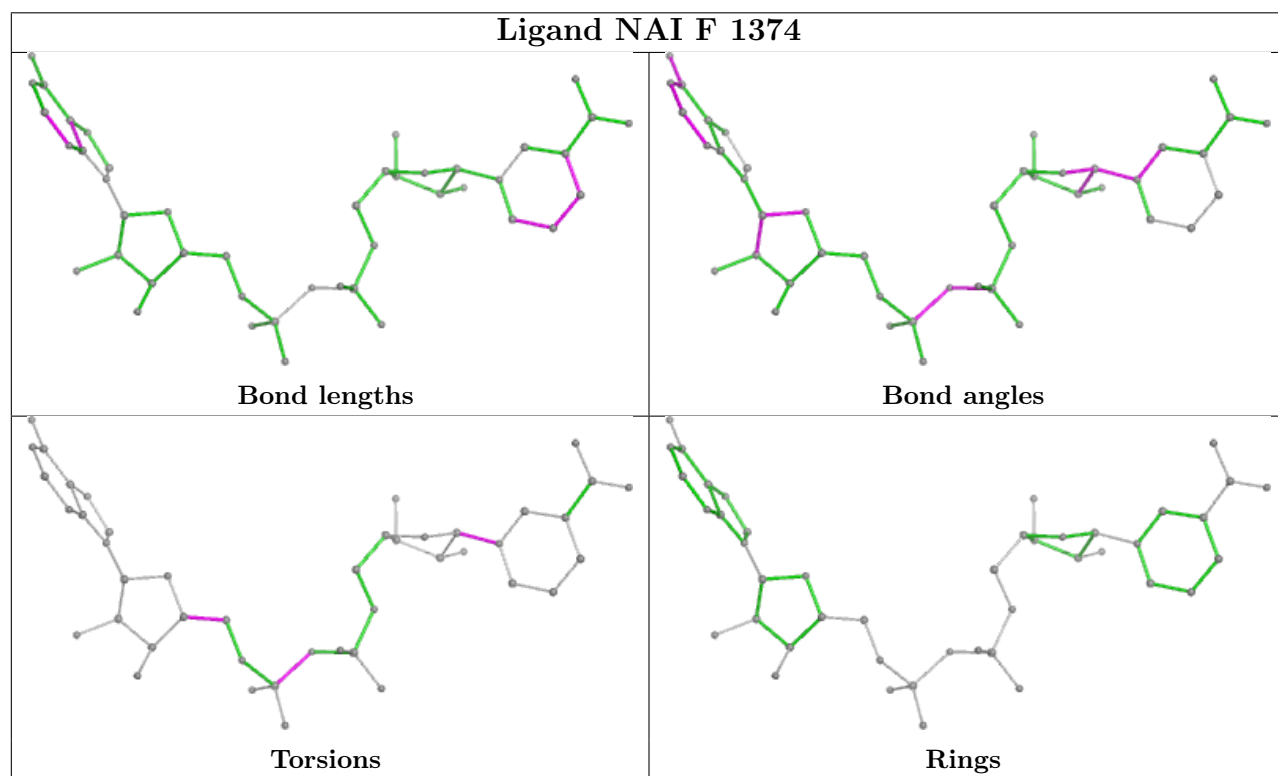
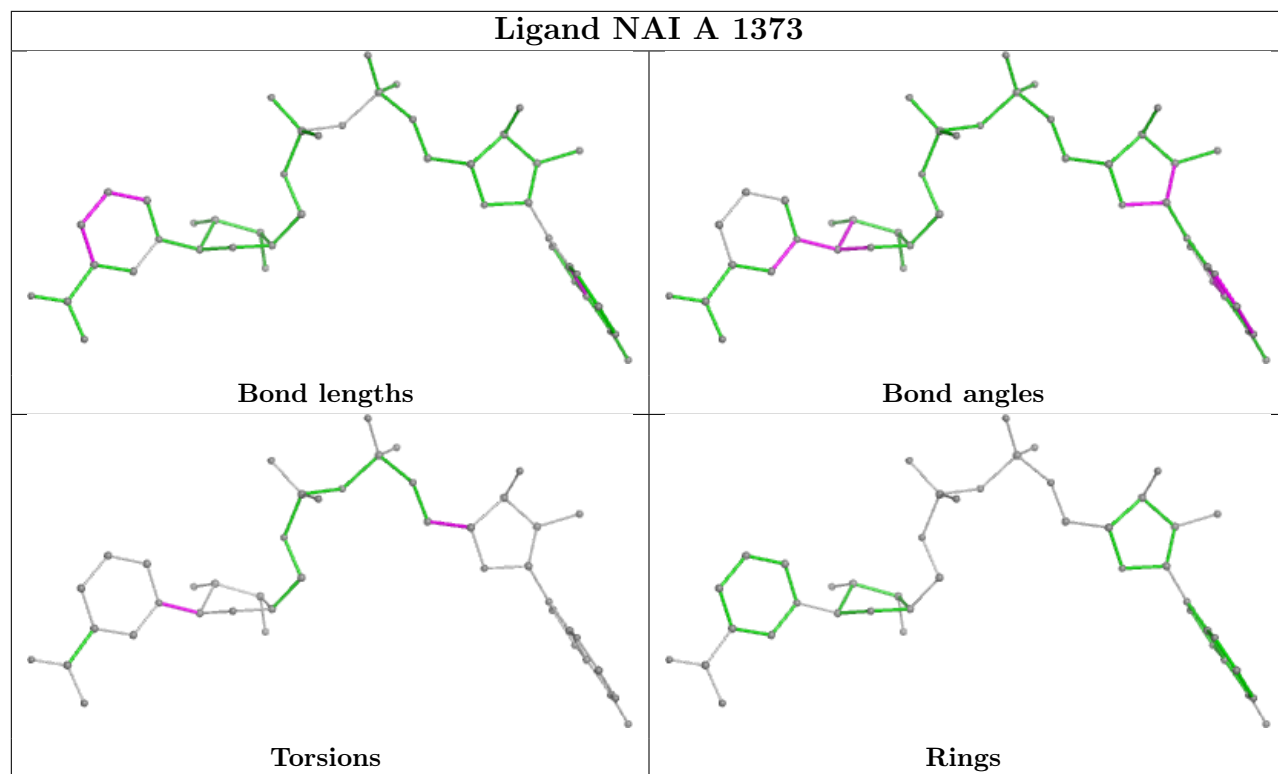
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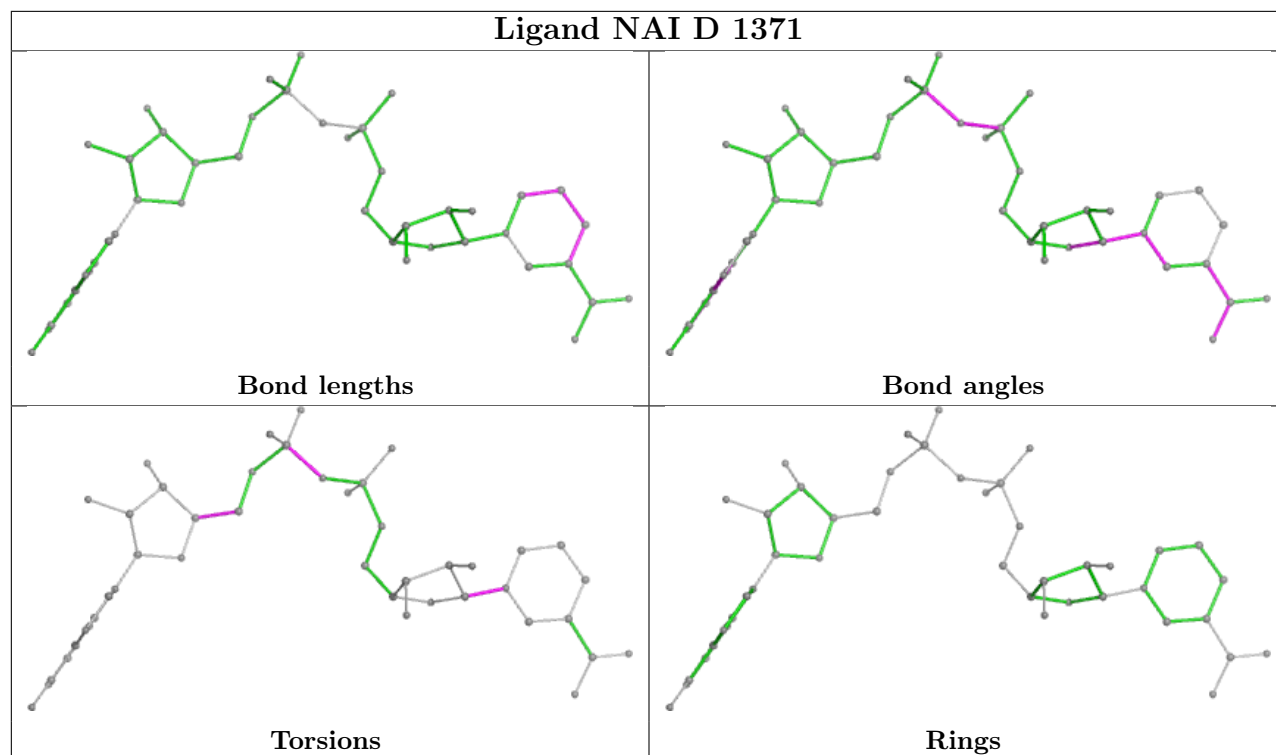
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1371	NAI	3	0

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	371/377 (98%)	0.48	16 (4%) 35 34	26, 46, 56, 68	0
1	B	370/377 (98%)	0.13	6 (1%) 72 70	25, 40, 51, 58	0
1	C	371/377 (98%)	0.56	33 (8%) 9 8	26, 47, 61, 70	0
1	D	370/377 (98%)	0.11	5 (1%) 75 74	25, 40, 52, 57	0
1	E	373/377 (98%)	0.77	47 (12%) 3 3	27, 50, 65, 76	0
1	F	373/377 (98%)	0.43	20 (5%) 25 24	26, 42, 49, 66	0
All	All	2228/2262 (98%)	0.41	127 (5%) 23 23	25, 44, 57, 76	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	372	HIS	5.2
1	C	283	TYR	5.1
1	C	363	PHE	4.4
1	C	368	SER	4.2
1	C	243	GLY	4.1
1	A	57	LEU	4.0
1	F	373	HIS	3.9
1	A	371	ALA	3.7
1	C	362	PRO	3.4
1	C	355	VAL	3.4
1	E	186	ILE	3.4
1	C	357	THR	3.4
1	C	356	ALA	3.4
1	E	366	PRO	3.4
1	F	207	LEU	3.3
1	C	358	ASP	3.3
1	C	354	ARG	3.3
1	F	34	LEU	3.2
1	C	359	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	85	LEU	3.2
1	E	53	ALA	3.1
1	E	34	LEU	3.1
1	A	14	PHE	3.1
1	E	83	GLY	3.0
1	E	373	HIS	3.0
1	E	65	TRP	3.0
1	F	186	ILE	3.0
1	E	46	THR	3.0
1	C	371	ALA	3.0
1	F	194	VAL	2.9
1	E	64	VAL	2.9
1	E	82	TYR	2.9
1	E	183	ALA	2.9
1	C	364	THR	2.9
1	A	51	LYS	2.9
1	C	292	ASP	2.8
1	A	283	TYR	2.8
1	E	187	ALA	2.8
1	E	171	VAL	2.7
1	F	372	HIS	2.7
1	E	215	ILE	2.7
1	B	14	PHE	2.7
1	D	368	SER	2.7
1	C	246	ALA	2.7
1	E	37	ALA	2.7
1	C	257	HIS	2.7
1	C	360	GLY	2.7
1	E	189	GLY	2.7
1	C	30	GLY	2.7
1	E	61	ALA	2.7
1	E	256	ALA	2.7
1	C	215	ILE	2.7
1	F	187	ALA	2.7
1	A	368	SER	2.6
1	E	56	GLN	2.6
1	A	285	HIS	2.6
1	C	256	ALA	2.6
1	C	361	VAL	2.6
1	A	365	GLU	2.6
1	F	181	TYR	2.5
1	F	184	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	283	TYR	2.5
1	A	215	ILE	2.5
1	C	353	GLU	2.5
1	A	53	ALA	2.5
1	C	281	THR	2.5
1	C	365	GLU	2.5
1	E	104	THR	2.4
1	F	57	LEU	2.4
1	E	79	ALA	2.4
1	E	142	ALA	2.4
1	B	212	CYS	2.4
1	D	245	LYS	2.4
1	C	285	HIS	2.4
1	B	281	THR	2.4
1	E	78	ILE	2.4
1	F	215	ILE	2.4
1	C	57	LEU	2.4
1	E	207	LEU	2.4
1	A	363	PHE	2.3
1	C	2	ARG	2.3
1	E	192	ALA	2.3
1	C	282	THR	2.3
1	E	107	LEU	2.3
1	E	194	VAL	2.3
1	A	30	GLY	2.3
1	E	346	HIS	2.2
1	E	234	LEU	2.2
1	E	370	LEU	2.2
1	F	196	VAL	2.2
1	E	176	ALA	2.2
1	E	350	LEU	2.2
1	A	32	GLU	2.2
1	E	360	GLY	2.2
1	F	189	GLY	2.2
1	C	245	LYS	2.2
1	E	51	LYS	2.2
1	B	285	HIS	2.1
1	E	103	CYS	2.1
1	A	58	VAL	2.1
1	D	241	VAL	2.1
1	E	144	VAL	2.1
1	F	173	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	349	ALA	2.1
1	C	369	VAL	2.1
1	B	363	PHE	2.1
1	E	184	ALA	2.1
1	E	140	LEU	2.1
1	F	180	GLY	2.1
1	C	242	PRO	2.1
1	D	209	ALA	2.1
1	F	174	ILE	2.1
1	E	173	VAL	2.1
1	A	209	ALA	2.1
1	E	367	ALA	2.1
1	F	179	ALA	2.1
1	A	360	GLY	2.0
1	F	56	GLN	2.0
1	E	190	MET	2.0
1	C	291	HIS	2.0
1	F	183	ALA	2.0
1	C	370	LEU	2.0
1	E	48	ALA	2.0
1	E	66	ALA	2.0
1	F	212	CYS	2.0
1	D	273	GLY	2.0
1	E	196	VAL	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](#)

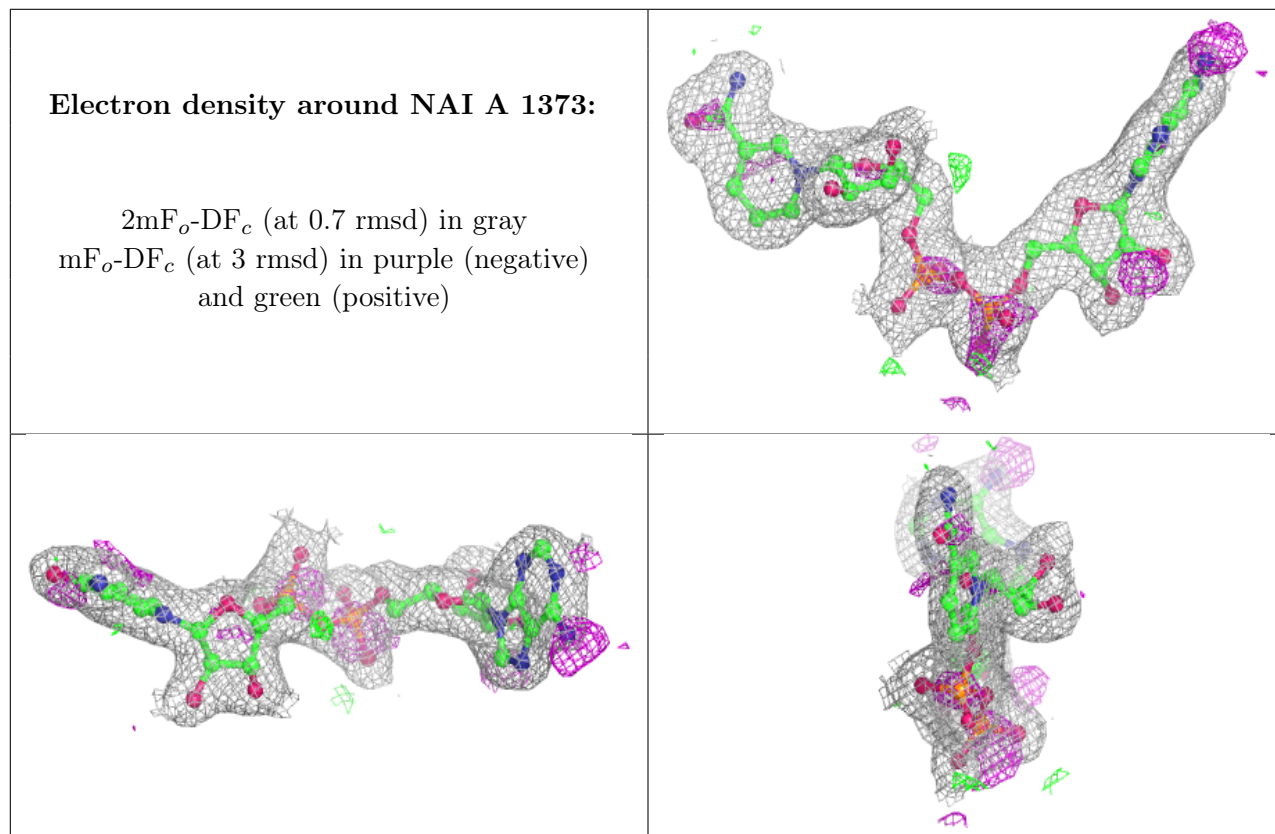
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

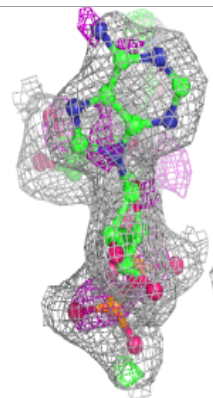
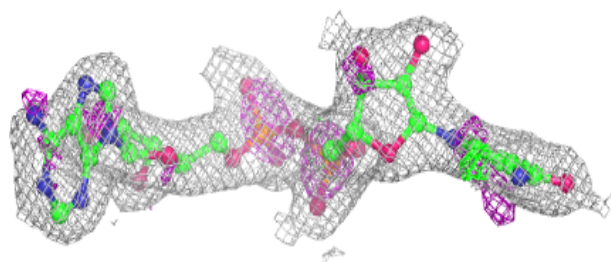
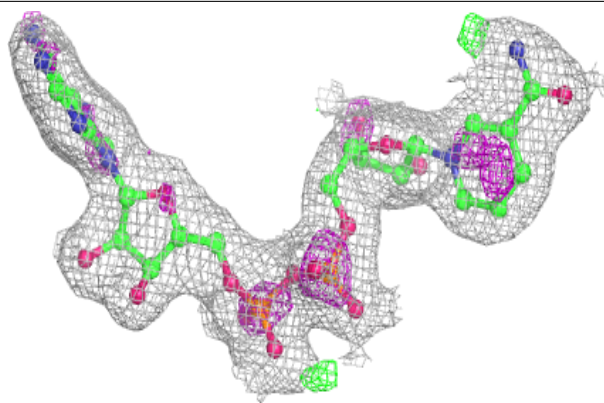
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	A	1372	1/1	0.92	0.12	48,48,48,48	0
3	NAI	A	1373	44/44	0.96	0.09	30,34,39,43	0
3	NAI	C	1372	44/44	0.96	0.13	36,41,46,47	0
3	NAI	D	1371	44/44	0.97	0.10	30,34,39,43	0
3	NAI	E	1374	44/44	0.97	0.10	27,31,40,41	0
3	NAI	B	1372	44/44	0.98	0.07	23,29,33,36	0
2	MG	B	1371	1/1	0.98	0.03	45,45,45,45	0
3	NAI	F	1374	44/44	0.98	0.09	20,24,29,31	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.

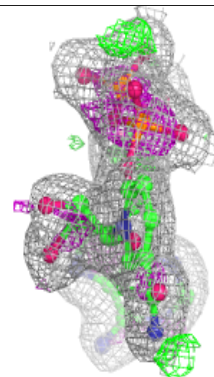
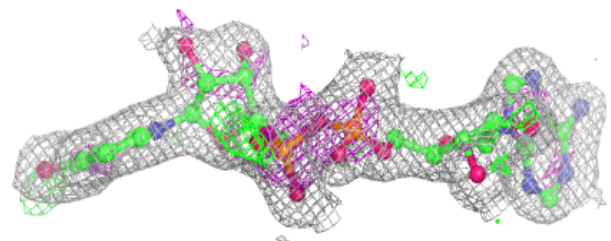
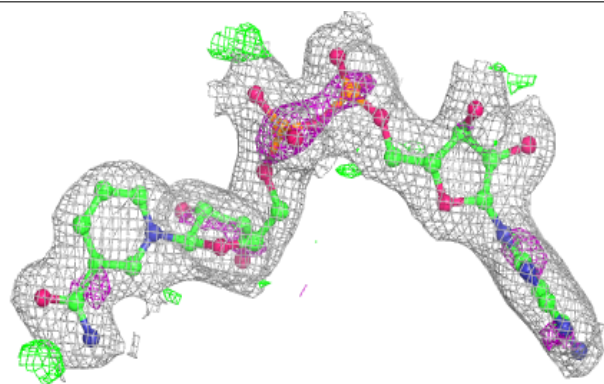


Electron density around NAI C 1372:

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

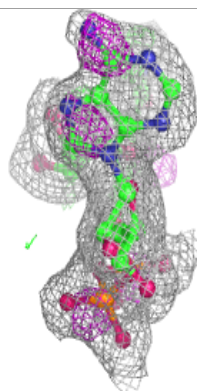
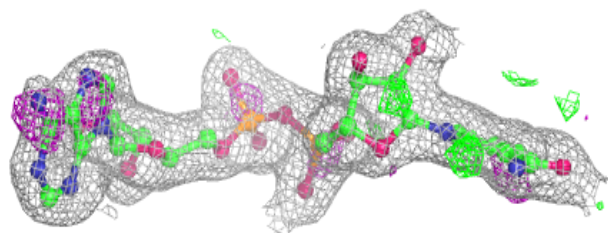
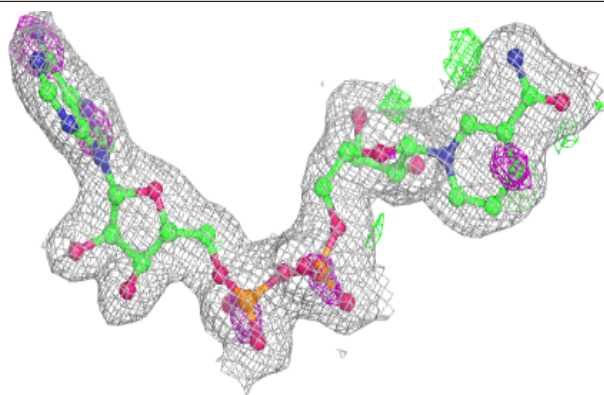
**Electron density around NAI D 1371:**

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

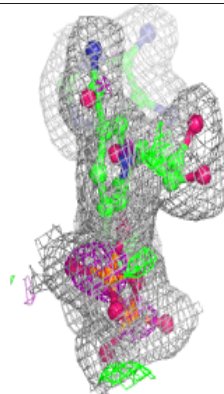
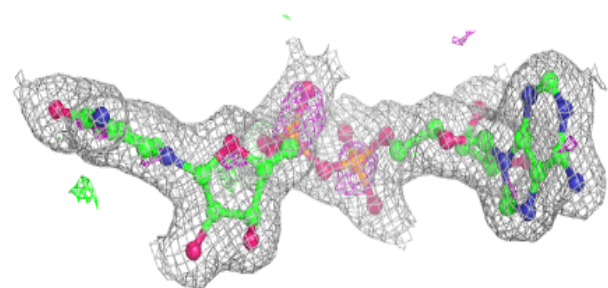
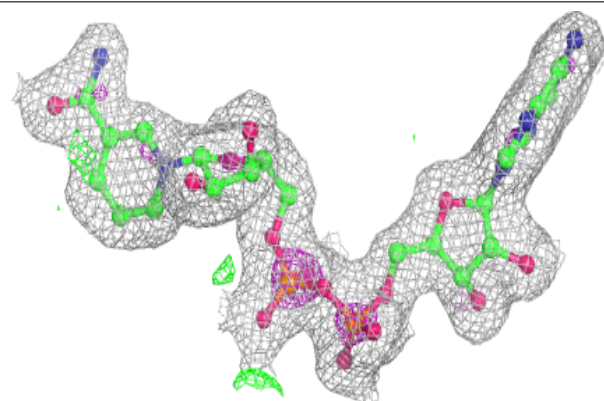


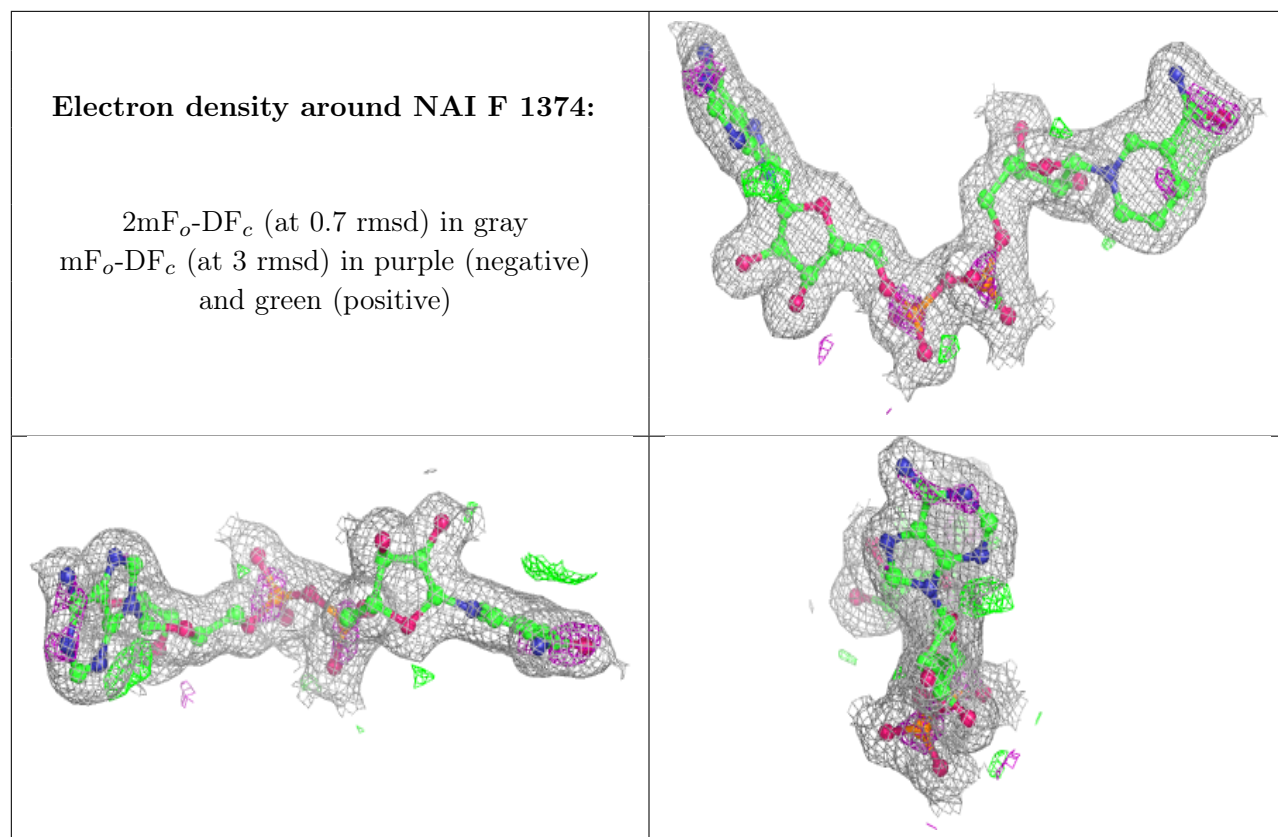
Electron density around NAI E 1374:

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

**Electron density around NAI B 1372:**

$2mF_o-DF_c$ (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.