Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2021 – 05:04 PM GMT

PDB ID	:	6TRY
Title	:	Crystal structure of human Aldehyde dehydrogenase 1A3 in complex with MF13 inhibitor compound
Authors	:	Gelardi, E.L.M.; Garavaglia, S.
Deposited on	:	2019-12-19
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

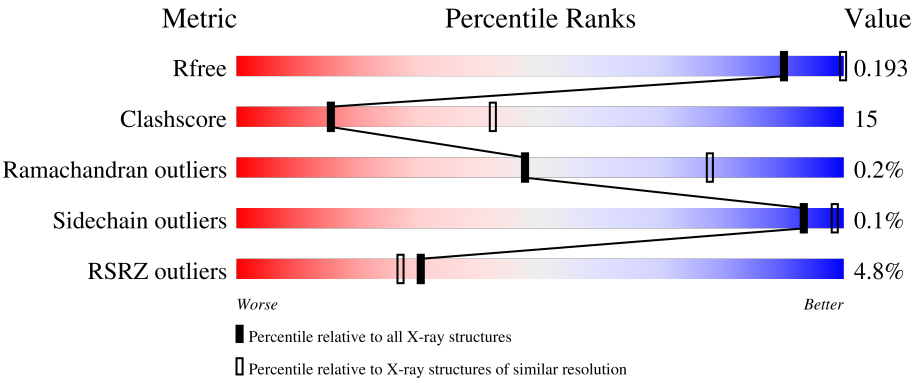
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	512	4% 66% 27% · 7%
1	B	512	5% 71% 22% · 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NW8	A	702	-	-	-	X

2 Entry composition

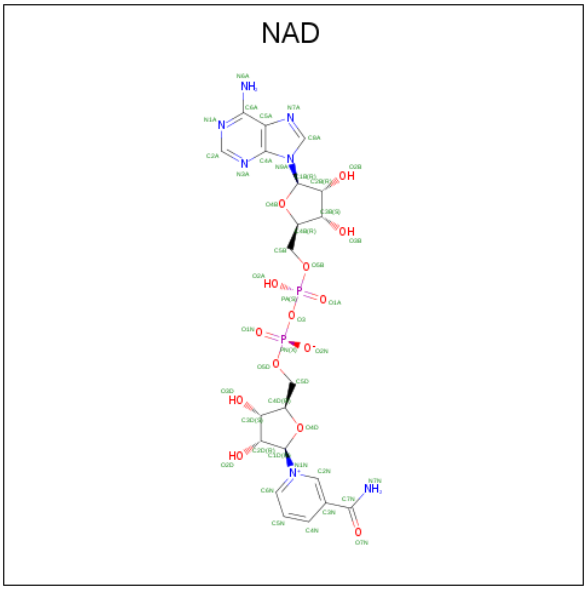
There are 5 unique types of molecules in this entry. The entry contains 7557 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aldehyde dehydrogenase family 1 member A3.

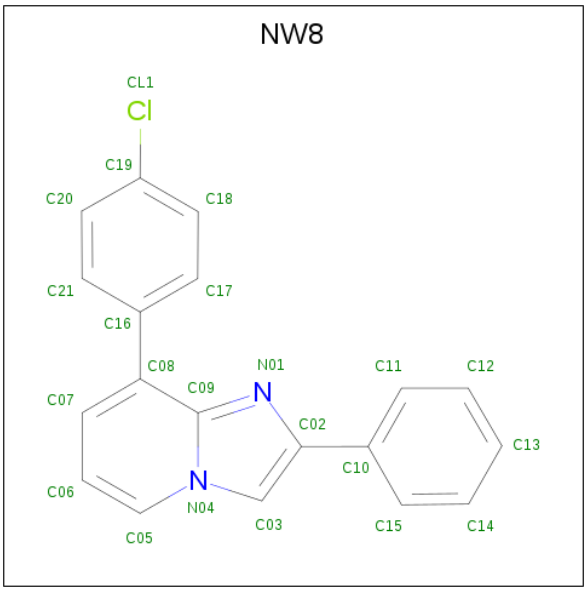
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3689	2352	628	689	20			
1	B	482	Total	C	N	O	S	0	0	0
			3719	2371	632	696	20			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



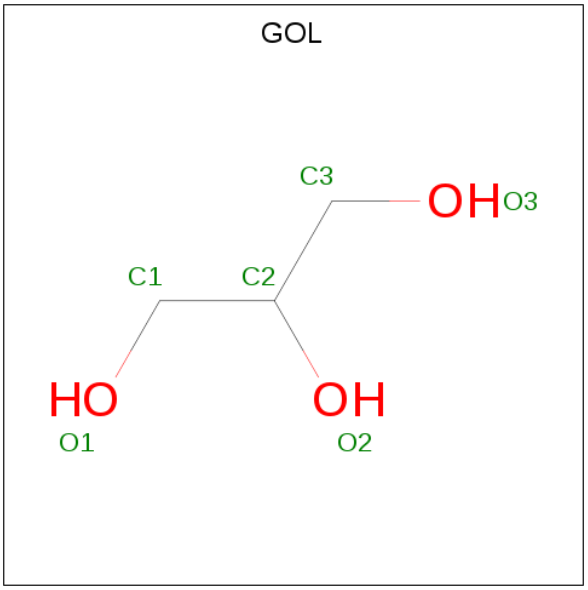
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 8-(4-chlorophenyl)-2-phenyl-imidazo[1,2-a]pyridine (three-letter code: NW8) (formula: $C_{19}H_{13}ClN_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			22	19	1	2		
3	B	1	Total	C	Cl	N	0	0
			22	19	1	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

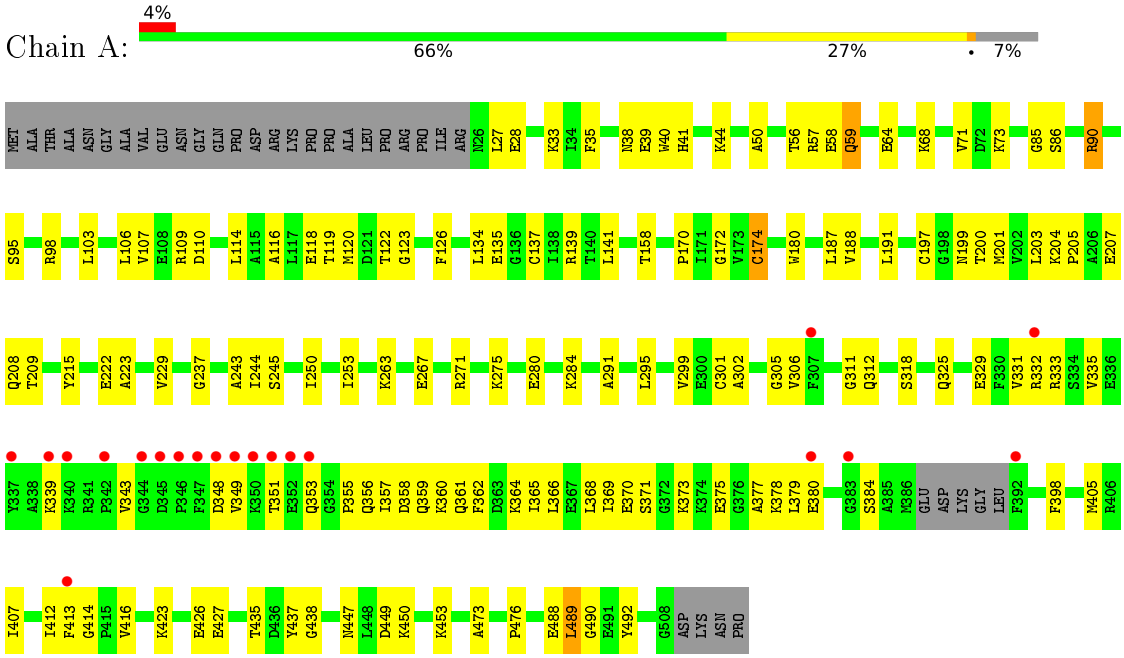
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	B	6	Total O 6 6	0	0

3 Residue-property plots (i)

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

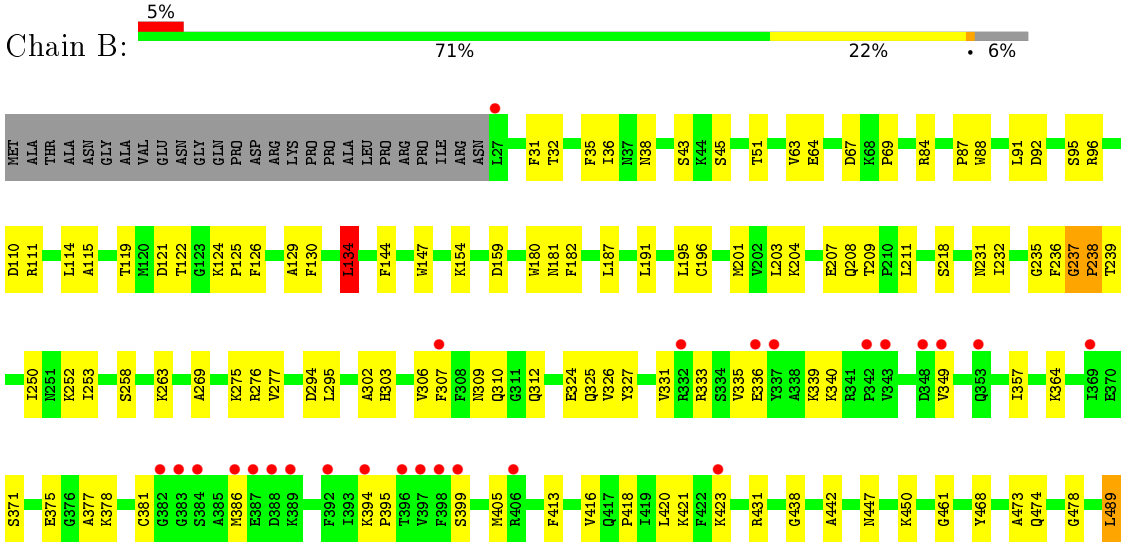
- Molecule 1: Aldehyde dehydrogenase family 1 member A3

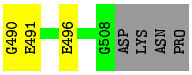
Chain A:



- Molecule 1: Aldehyde dehydrogenase family 1 member A3

Chain B:




G490
E491
E496
G508
ASP
LYS
ASN
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	81.30Å 89.18Å 159.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.96 – 2.90 47.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.96-2.90) 98.5 (47.96-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.191 , 0.273 0.203 , 0.193	Depositor DCC
R_{free} test set	1347 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	60.4	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7557	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NW8, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.83	2/3763 (0.1%)	0.89	10/5089 (0.2%)
1	B	0.53	2/3795 (0.1%)	0.71	9/5134 (0.2%)
All	All	0.70	4/7558 (0.1%)	0.80	19/10223 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLN	C-N	-40.45	0.41	1.34
1	B	238	PRO	N-CA	12.15	1.68	1.47
1	B	237	GLY	C-N	5.33	1.44	1.34
1	A	174	CYS	CB-SG	-5.05	1.73	1.81

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	59	GLN	O-C-N	25.33	163.22	122.70
1	A	59	GLN	C-N-CA	-21.70	67.45	121.70
1	A	59	GLN	CA-C-N	-18.57	76.33	117.20
1	B	489	LEU	N-CA-C	7.62	131.59	111.00
1	B	489	LEU	CB-CA-C	-7.33	96.27	110.20
1	B	294	ASP	N-CA-C	-7.14	91.72	111.00
1	A	489	LEU	N-CA-C	6.92	129.70	111.00
1	A	90	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	B	238	PRO	CA-N-CD	-6.67	102.17	111.50
1	A	490	GLY	N-CA-C	-6.52	96.80	113.10
1	B	159	ASP	N-CA-CB	6.36	122.05	110.60
1	B	490	GLY	N-CA-C	-6.32	97.30	113.10
1	B	349	VAL	CB-CA-C	6.10	122.98	111.40
1	A	489	LEU	CB-CA-C	-6.07	98.66	110.20
1	A	349	VAL	CB-CA-C	5.65	122.14	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	294	ASP	CB-CA-C	5.64	121.68	110.40
1	B	134	LEU	CA-CB-CG	-5.47	102.71	115.30
1	A	489	LEU	CA-C-N	5.24	126.68	116.20
1	A	158	THR	N-CA-C	5.12	124.83	111.00

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	3689	0	3708	130	4
1	B	3719	0	3743	90	4
2	A	44	0	24	3	0
2	B	44	0	24	5	0
3	A	22	0	0	0	0
3	B	22	0	0	0	0
4	A	6	0	8	1	0
5	A	5	0	0	0	0
5	B	6	0	0	2	0
All	All	7557	0	7507	222	4

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 15.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLN:NE2	1:A:413:PHE:CE2	1.81	1.40
1:B:238:PRO:CA	1:B:238:PRO:N	1.67	1.39
1:B:386:MET:SD	1:B:394:LYS:HB2	1.72	1.30
1:A:180:TRP:CH2	1:A:413:PHE:HZ	1.53	1.26
1:A:180:TRP:CH2	1:A:413:PHE:CZ	2.22	1.25
1:A:180:TRP:HH2	1:A:413:PHE:CZ	1.55	1.24
2:B:801:NAD:C1D	2:B:801:NAD:O4D	1.64	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:701:NAD:C1D	2:A:701:NAD:O4D	1.63	1.16
1:A:58:GLU:C	1:A:59:GLN:N	2.10	1.04
1:B:473:ALA:O	1:B:489:LEU:O	1.77	1.01
1:A:473:ALA:O	1:A:489:LEU:O	1.80	1.00
1:A:180:TRP:CZ2	1:A:413:PHE:CZ	2.51	0.98
1:A:361:GLN:NE2	1:A:413:PHE:HE2	1.32	0.96
1:A:180:TRP:CH2	1:A:413:PHE:CE1	2.56	0.93
1:A:295:LEU:HD23	1:A:333:ARG:NH1	1.85	0.90
1:A:435:THR:HG22	1:A:437:TYR:H	1.38	0.89
1:B:386:MET:SD	1:B:394:LYS:CB	2.63	0.86
1:A:180:TRP:CZ2	1:A:413:PHE:HZ	1.90	0.85
1:A:361:GLN:NE2	1:A:413:PHE:CZ	2.45	0.84
1:B:87:PRO:O	1:B:91:LEU:HD13	1.75	0.84
1:A:180:TRP:HH2	1:A:413:PHE:CE1	1.95	0.83
1:A:348:ASP:HB2	1:A:351:THR:OG1	1.78	0.82
1:B:327:TYR:O	1:B:331:VAL:HG23	1.81	0.80
1:B:51:THR:HG21	1:B:211:LEU:HD21	1.64	0.79
1:A:291:ALA:CB	1:A:325:GLN:OE1	2.32	0.77
1:A:361:GLN:HG3	1:A:413:PHE:CD2	2.19	0.77
1:A:245:SER:HA	1:A:253:ILE:HD11	1.68	0.76
1:B:236:PHE:HB2	1:B:239:THR:HG22	1.69	0.75
1:A:295:LEU:HD23	1:A:333:ARG:HH12	1.49	0.75
1:B:121:ASP:OD1	5:B:901:HOH:O	2.05	0.74
1:B:144:PHE:O	1:B:196:CYS:SG	2.42	0.73
1:A:86:SER:O	1:A:90:ARG:HG3	1.88	0.72
1:A:119:THR:HG21	1:A:126:PHE:HA	1.72	0.71
1:B:124:LYS:NZ	1:B:181:ASN:O	2.23	0.71
1:A:280:GLU:OE1	1:A:488:GLU:HG3	1.90	0.71
1:B:447:ASN:OD1	1:B:450:LYS:HG3	1.91	0.71
1:A:187:LEU:HD21	1:A:203:LEU:HD13	1.73	0.71
1:B:331:VAL:O	1:B:335:VAL:HG23	1.91	0.70
1:A:335:VAL:HG12	1:A:339:LYS:HE3	1.73	0.70
1:A:103:LEU:HD23	1:A:103:LEU:O	1.92	0.70
1:B:180:TRP:CH2	1:B:413:PHE:HE2	2.10	0.70
1:A:426:GLU:OE2	1:B:84:ARG:NH1	2.25	0.69
1:A:331:VAL:O	1:A:335:VAL:HG23	1.92	0.69
1:B:238:PRO:C	1:B:238:PRO:N	2.47	0.67
1:A:370:GLU:HA	1:A:373:LYS:HD3	1.74	0.67
1:B:36:ILE:HA	1:B:231:ASN:OD1	1.95	0.66
1:B:35:PHE:CZ	1:B:38:ASN:HA	2.31	0.66
1:B:312:GLN:HB3	1:B:413:PHE:CE2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:TYR:OH	1:B:399:SER:O	2.14	0.65
1:B:336:GLU:O	1:B:340:LYS:HG2	1.97	0.65
1:B:302:ALA:O	1:B:306:VAL:HG23	1.97	0.65
1:A:378:LYS:HE3	1:A:380:GLU:HB2	1.79	0.65
1:B:119:THR:HG21	1:B:126:PHE:HA	1.78	0.64
1:B:378:LYS:HB3	1:B:399:SER:HB3	1.79	0.64
1:A:366:LEU:HD12	1:A:384:SER:HA	1.80	0.64
1:B:115:ALA:O	1:B:119:THR:HG23	1.99	0.62
1:A:447:ASN:HB3	1:A:450:LYS:HB2	1.82	0.62
1:A:57:ARG:O	1:A:58:GLU:HG2	1.99	0.62
1:B:335:VAL:HG13	1:B:381:CYS:HB2	1.82	0.62
1:A:368:LEU:O	1:A:371:SER:OG	2.18	0.61
1:A:361:GLN:HG3	1:A:413:PHE:HD2	1.65	0.61
1:A:103:LEU:HD22	1:A:141:LEU:HD13	1.82	0.60
1:B:416:VAL:O	1:B:418:PRO:HD3	2.01	0.60
1:A:413:PHE:O	1:A:413:PHE:CD2	2.55	0.60
1:A:361:GLN:HB2	1:A:364:LYS:HE2	1.84	0.60
1:A:291:ALA:HB1	1:A:325:GLN:OE1	2.02	0.59
1:A:35:PHE:CZ	1:A:38:ASN:HA	2.37	0.59
1:B:386:MET:SD	1:B:394:LYS:HD2	2.43	0.59
1:A:180:TRP:CZ2	1:A:413:PHE:CE1	2.85	0.59
1:A:361:GLN:HE21	1:A:413:PHE:HE2	0.59	0.59
1:B:378:LYS:HB3	1:B:399:SER:CB	2.33	0.59
1:B:394:LYS:HG3	1:B:395:PRO:HD2	1.85	0.59
1:A:109:ARG:HH22	1:A:222:GLU:CD	2.07	0.58
1:B:110:ASP:O	1:B:114:LEU:HD12	2.03	0.58
2:A:701:NAD:O1N	2:A:701:NAD:H52A	2.03	0.58
1:B:386:MET:SD	1:B:394:LYS:CD	2.92	0.58
1:B:125:PRO:HD3	1:B:310:GLN:NE2	2.18	0.57
1:A:449:ASP:O	1:A:453:LYS:HG3	2.03	0.57
1:A:122:THR:HG22	1:A:209:THR:HG21	1.86	0.57
1:B:121:ASP:OD2	1:B:209:THR:HA	2.03	0.57
1:A:380:GLU:HA	1:A:380:GLU:OE1	2.03	0.57
1:B:180:TRP:CH2	1:B:413:PHE:CE2	2.93	0.57
1:A:103:LEU:HD23	1:A:107:VAL:HG23	1.85	0.57
1:A:180:TRP:HZ2	1:A:413:PHE:CZ	2.19	0.56
1:B:129:ALA:O	1:B:134:LEU:HD12	2.05	0.56
1:B:87:PRO:O	1:B:91:LEU:CD1	2.49	0.56
1:A:103:LEU:HD23	1:A:103:LEU:C	2.26	0.56
1:A:244:ILE:HG23	1:A:250:ILE:HD13	1.87	0.56
1:B:111:ARG:HG2	1:B:130:PHE:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:HB3	1:B:69:PRO:HD2	1.87	0.55
1:A:366:LEU:HA	1:A:369:ILE:HG13	1.87	0.55
1:B:203:LEU:HD12	1:B:232:ILE:HG12	1.87	0.55
1:A:204:LYS:NZ	1:A:205:PRO:O	2.38	0.55
1:A:413:PHE:CG	1:A:413:PHE:O	2.60	0.54
1:A:435:THR:HG22	1:A:437:TYR:N	2.14	0.54
1:A:412:ILE:HG22	1:A:414:GLY:N	2.23	0.54
1:B:335:VAL:HG12	1:B:339:LYS:HD2	1.89	0.54
1:B:181:ASN:OD1	1:B:182:PHE:N	2.41	0.53
1:A:476:PRO:HG3	1:A:492:TYR:CD1	2.43	0.53
1:A:245:SER:HA	1:A:253:ILE:CD1	2.38	0.53
1:A:412:ILE:HG12	1:A:416:VAL:CG2	2.37	0.53
1:B:122:THR:OG1	1:B:124:LYS:HB2	2.09	0.53
1:A:379:LEU:HD11	1:A:398:PHE:CE2	2.43	0.53
1:A:359:GLN:HA	1:A:362:PHE:HB3	1.90	0.53
1:A:253:ILE:HG13	1:A:275:LYS:HD3	1.92	0.52
1:A:71:VAL:HG21	1:A:243:ALA:HB1	1.91	0.52
1:A:412:ILE:HG21	1:A:416:VAL:HG22	1.92	0.52
1:B:252:LYS:HE3	1:B:496:GLU:O	2.10	0.52
1:B:327:TYR:CE2	1:B:421:LYS:HB2	2.44	0.52
1:B:258:SER:HB3	2:B:801:NAD:O1A	2.09	0.52
1:A:412:ILE:HG12	1:A:416:VAL:HG21	1.92	0.52
1:A:377:ALA:HB2	1:A:405:MET:HE1	1.93	0.51
1:B:324:GLU:HB3	1:B:421:LYS:HE3	1.91	0.51
1:A:56:THR:O	1:A:57:ARG:C	2.48	0.51
1:A:180:TRP:CH2	1:A:413:PHE:HE1	2.25	0.51
1:B:92:ASP:HB2	1:B:95:SER:OG	2.10	0.51
1:A:106:LEU:HD12	1:A:223:ALA:HB2	1.93	0.51
1:A:68:LYS:O	1:A:71:VAL:HG22	2.10	0.51
1:B:269:ALA:HB1	1:B:275:LYS:HG3	1.92	0.51
1:A:116:ALA:O	1:A:120:MET:HG3	2.12	0.50
1:A:180:TRP:CE3	1:A:357:ILE:HG12	2.46	0.50
1:A:357:ILE:HD12	1:A:358:ASP:N	2.26	0.50
1:A:365:ILE:O	1:A:369:ILE:HG13	2.12	0.50
1:B:119:THR:CG2	1:B:126:PHE:HA	2.42	0.50
1:B:115:ALA:HB2	1:B:134:LEU:HD13	1.94	0.50
1:A:365:ILE:HD12	1:A:414:GLY:HA3	1.93	0.49
4:A:703:GOL:H12	1:B:276:ARG:HA	1.93	0.49
1:B:306:VAL:HB	1:B:307:PHE:CD1	2.47	0.49
1:A:302:ALA:O	1:A:306:VAL:HG12	2.12	0.49
1:A:368:LEU:HA	1:A:371:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LEU:HD13	1:B:326:VAL:HG11	1.94	0.49
1:A:103:LEU:CD2	1:A:107:VAL:HG23	2.42	0.49
1:A:33:LYS:HB3	1:A:41:HIS:O	2.13	0.48
1:A:85:GLY:O	1:A:90:ARG:HD2	2.13	0.48
1:A:329:GLU:O	1:A:333:ARG:HG2	2.14	0.48
1:A:44:LYS:HA	1:A:44:LYS:HD3	1.61	0.48
1:B:43:SER:HB3	1:B:64:GLU:HB3	1.96	0.48
1:A:356:GLN:H	1:A:356:GLN:CD	2.16	0.48
1:A:359:GLN:HA	1:A:362:PHE:CB	2.44	0.47
1:A:366:LEU:CD1	1:A:384:SER:HA	2.42	0.47
1:A:361:GLN:HB2	1:A:364:LYS:CE	2.44	0.47
1:B:237:GLY:HA3	2:B:801:NAD:C8A	2.44	0.47
1:A:377:ALA:HB2	1:A:405:MET:CE	2.44	0.47
1:A:423:LYS:N	1:A:427:GLU:OE1	2.37	0.47
1:B:377:ALA:HB2	1:B:405:MET:CE	2.44	0.47
1:B:147:TRP:CZ2	1:B:491:GLU:HB2	2.49	0.47
1:A:172:GLY:O	1:A:199:ASN:HB3	2.15	0.47
1:A:301:CYS:O	1:A:305:GLY:N	2.45	0.47
1:B:191:LEU:HA	1:B:201:MET:SD	2.55	0.47
1:A:103:LEU:HD22	1:A:141:LEU:CD1	2.45	0.47
1:B:312:GLN:HA	1:B:413:PHE:CD2	2.50	0.46
1:B:364:LYS:HB2	1:B:364:LYS:HE2	1.54	0.46
1:A:200:THR:HG22	1:A:229:VAL:HA	1.98	0.46
1:B:238:PRO:N	1:B:239:THR:N	2.63	0.46
1:A:137:CYS:HA	1:A:188:VAL:HG21	1.98	0.46
1:A:299:VAL:HG11	1:A:333:ARG:HB2	1.97	0.46
1:A:412:ILE:HG22	1:A:414:GLY:H	1.81	0.46
1:B:125:PRO:HD3	1:B:310:GLN:HE21	1.81	0.45
1:B:207:GLU:HG2	1:B:208:GLN:OE1	2.16	0.45
1:B:32:THR:C	1:B:63:VAL:HG23	2.37	0.45
1:A:103:LEU:CD2	1:A:103:LEU:C	2.84	0.45
1:A:335:VAL:CG1	1:A:339:LYS:HE3	2.46	0.45
1:A:405:MET:HE1	1:A:407:ILE:HD11	1.97	0.45
1:A:50:ALA:CB	1:A:59:GLN:NE2	2.80	0.45
1:B:187:LEU:HD11	1:B:203:LEU:HB3	1.99	0.45
1:B:420:LEU:HD23	1:B:431:ARG:HH21	1.81	0.45
1:A:110:ASP:OD2	1:A:215:TYR:OH	2.30	0.44
1:B:45:SER:HB3	5:B:904:HOH:O	2.16	0.44
1:A:375:GLU:H	1:A:375:GLU:HG3	1.58	0.44
1:B:461:GLY:HA3	1:B:478:GLY:O	2.18	0.44
1:A:284:LYS:NZ	1:A:318:SER:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:HA	1:A:64:GLU:CG	2.48	0.44
1:A:35:PHE:HZ	1:A:38:ASN:HD22	1.64	0.44
1:A:191:LEU:HA	1:A:201:MET:SD	2.58	0.44
1:A:312:GLN:HE22	1:A:356:GLN:HA	1.83	0.44
1:A:56:THR:OG1	1:A:56:THR:O	2.27	0.43
2:B:801:NAD:H6N	2:B:801:NAD:H2D	1.78	0.43
1:A:306:VAL:O	1:A:311:GLY:HA2	2.18	0.43
1:B:371:SER:O	1:B:375:GLU:HG3	2.18	0.43
1:A:237:GLY:HA3	2:A:701:NAD:C8A	2.49	0.43
1:A:271:ARG:O	1:B:263:LYS:HE2	2.18	0.43
1:B:447:ASN:HB3	1:B:450:LYS:HD2	1.99	0.43
2:B:801:NAD:H8A	2:B:801:NAD:H2B	1.84	0.43
1:B:295:LEU:HD23	1:B:333:ARG:CZ	2.49	0.43
1:A:180:TRP:CZ2	1:A:357:ILE:HD11	2.53	0.43
1:A:343:VAL:HB	1:A:353:GLN:HE21	1.84	0.43
1:B:250:ILE:O	1:B:275:LYS:HE3	2.19	0.43
1:A:135:GLU:HG3	1:A:139:ARG:HD2	2.00	0.43
1:B:121:ASP:OD2	1:B:211:LEU:HD23	2.19	0.42
1:A:412:ILE:O	1:A:413:PHE:HB3	2.19	0.42
1:B:180:TRP:CZ2	1:B:357:ILE:HG21	2.54	0.42
1:A:170:PRO:HB3	1:A:197:CYS:O	2.19	0.42
1:B:295:LEU:HD12	1:B:295:LEU:HA	1.73	0.42
1:A:39:GLU:HB2	1:A:41:HIS:HE1	1.84	0.42
1:A:95:SER:HA	1:A:98:ARG:HB2	2.01	0.42
1:B:420:LEU:HD23	1:B:431:ARG:NH2	2.34	0.42
1:B:204:LYS:NZ	1:B:235:GLY:O	2.50	0.42
1:B:88:TRP:CH2	1:B:96:ARG:HG2	2.53	0.42
1:A:174:CYS:O	1:A:201:MET:HA	2.19	0.42
1:A:492:TYR:OH	1:B:154:LYS:HD2	2.20	0.42
1:B:31:PHE:CZ	1:B:218:SER:HB3	2.55	0.42
1:B:303:HIS:O	1:B:307:PHE:HD1	2.03	0.41
1:B:325:GLN:OE1	1:B:325:GLN:N	2.52	0.41
1:B:474:GLN:CD	1:B:474:GLN:H	2.23	0.41
1:A:123:GLY:O	1:A:355:PRO:HD2	2.21	0.41
1:A:118:GLU:HA	1:A:118:GLU:OE1	2.20	0.41
1:B:195:LEU:HD23	1:B:195:LEU:HA	1.74	0.41
1:A:73:LYS:HB3	1:A:73:LYS:NZ	2.35	0.41
1:B:442:ALA:HB2	1:B:468:TYR:CD2	2.56	0.41
1:A:368:LEU:HD23	1:A:371:SER:CB	2.51	0.41
1:A:207:GLU:HG2	1:A:208:GLN:OE1	2.21	0.41
1:A:312:GLN:HB3	1:A:413:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:HD2	1:A:40:TRP:HB3	2.03	0.41
1:B:339:LYS:HG3	1:B:381:CYS:SG	2.61	0.41
1:A:114:LEU:HB2	1:A:134:LEU:HD21	2.03	0.41
1:A:263:LYS:O	1:A:267:GLU:HG3	2.21	0.41
1:A:27:LEU:HD12	1:A:28:GLU:H	1.85	0.41
1:B:253:ILE:HG22	1:B:277:VAL:HG22	2.02	0.41
1:A:358:ASP:CG	1:A:360:LYS:HG3	2.41	0.41
1:B:124:LYS:HE3	1:B:309:ASN:OD1	2.21	0.40
1:A:368:LEU:HD23	1:A:371:SER:HB3	2.02	0.40
1:A:405:MET:CE	1:A:407:ILE:HD11	2.52	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:NH1	1:B:423:LYS:NZ[1_565]	0.53	1.67
1:A:332:ARG:NH1	1:B:423:LYS:CE[1_565]	1.41	0.79
1:A:332:ARG:CZ	1:B:423:LYS:NZ[1_565]	1.76	0.44
1:A:332:ARG:NH2	1:B:423:LYS:CD[1_565]	1.89	0.31

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	472/512 (92%)	449 (95%)	22 (5%)	1 (0%)	47 78
1	B	480/512 (94%)	455 (95%)	24 (5%)	1 (0%)	47 78
All	All	952/1024 (93%)	904 (95%)	46 (5%)	2 (0%)	47 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	GLY
1	B	438	GLY

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	395/422 (94%)	395 (100%)	0	100	100
1	B	398/422 (94%)	397 (100%)	1 (0%)	92	98
All	All	793/844 (94%)	792 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	134	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	59	GLN
1	A	304	GLN
1	A	312	GLN
1	A	353	GLN
1	A	356	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NW8	A	702	-	22,25,25	2.48	4 (18%)	28,35,35	2.18	10 (35%)
2	NAD	B	801	-	42,48,48	5.43	16 (38%)	50,73,73	1.93	8 (16%)
3	NW8	B	802	-	22,25,25	2.31	5 (22%)	28,35,35	2.30	9 (32%)
2	NAD	A	701	1	42,48,48	5.48	19 (45%)	50,73,73	1.82	9 (18%)
4	GOL	A	703	-	5,5,5	1.49	2 (40%)	5,5,5	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NW8	A	702	-	-	0/8/8/8	0/4/4/4
2	NAD	B	801	-	-	11/26/62/62	0/5/5/5
3	NW8	B	802	-	-	0/8/8/8	0/4/4/4
2	NAD	A	701	1	-	8/26/62/62	0/5/5/5
4	GOL	A	703	-	-	1/4/4/4	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	NAD	O4D-C1D	16.50	1.64	1.41
2	B	801	NAD	C2B-C1B	-16.23	1.29	1.53
2	A	701	NAD	C2B-C1B	-16.17	1.29	1.53
2	A	701	NAD	O4D-C1D	16.14	1.63	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	NAD	C2D-C1D	-15.76	1.29	1.53
2	A	701	NAD	C2D-C1D	-15.41	1.30	1.53
2	A	701	NAD	O4B-C1B	14.90	1.61	1.41
2	B	801	NAD	O4B-C1B	13.82	1.60	1.41
3	A	702	NW8	C10-C02	-8.24	1.35	1.48
2	A	701	NAD	C7N-N7N	7.36	1.47	1.33
2	B	801	NAD	C7N-N7N	7.13	1.46	1.33
3	B	802	NW8	C10-C02	-6.52	1.38	1.48
2	A	701	NAD	O4D-C4D	-6.05	1.31	1.45
2	B	801	NAD	O4B-C4B	-5.98	1.31	1.45
2	B	801	NAD	O4D-C4D	-5.79	1.32	1.45
2	A	701	NAD	O4B-C4B	-5.52	1.32	1.45
3	B	802	NW8	C09-N01	4.51	1.37	1.33
3	A	702	NW8	C08-C16	-4.46	1.41	1.49
2	A	701	NAD	O3D-C3D	-4.42	1.32	1.43
3	B	802	NW8	C08-C16	-4.38	1.41	1.49
2	A	701	NAD	C6A-N6A	4.28	1.49	1.34
2	B	801	NAD	C6A-N6A	4.26	1.49	1.34
2	A	701	NAD	O2D-C2D	4.25	1.53	1.43
2	B	801	NAD	O3D-C3D	-4.22	1.33	1.43
2	A	701	NAD	O2B-C2B	4.14	1.52	1.43
2	B	801	NAD	C2A-N3A	3.96	1.38	1.32
2	B	801	NAD	O2B-C2B	3.90	1.52	1.43
2	B	801	NAD	O2D-C2D	3.89	1.52	1.43
3	A	702	NW8	C09-N01	3.71	1.36	1.33
2	A	701	NAD	C2A-N3A	3.31	1.37	1.32
3	B	802	NW8	C19-CL1	3.18	1.81	1.74
2	A	701	NAD	PA-O1A	3.15	1.62	1.50
2	B	801	NAD	C2N-N1N	3.06	1.38	1.35
3	A	702	NW8	C19-CL1	3.03	1.81	1.74
2	B	801	NAD	C5D-C4D	3.00	1.61	1.51
2	A	701	NAD	C5D-C4D	2.94	1.60	1.51
2	B	801	NAD	O3B-C3B	-2.93	1.36	1.43
2	A	701	NAD	O3B-C3B	-2.83	1.36	1.43
2	A	701	NAD	PA-O5B	2.71	1.70	1.59
3	B	802	NW8	C08-C09	2.67	1.46	1.43
2	A	701	NAD	C2N-N1N	2.53	1.38	1.35
4	A	703	GOL	C3-C2	2.25	1.61	1.51
2	A	701	NAD	C5A-C4A	-2.22	1.35	1.40
2	B	801	NAD	C5A-C4A	-2.12	1.35	1.40
4	A	703	GOL	C1-C2	2.07	1.60	1.51
2	A	701	NAD	C3N-C7N	2.02	1.53	1.50

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	NAD	C5A-C6A-N6A	7.15	131.22	120.35
2	A	701	NAD	C5A-C6A-N6A	6.41	130.10	120.35
3	B	802	NW8	C20-C19-C18	-6.35	113.01	121.24
2	A	701	NAD	N3A-C2A-N1A	-5.58	119.95	128.68
3	B	802	NW8	C21-C20-C19	5.53	125.08	119.24
2	B	801	NAD	N3A-C2A-N1A	-5.51	120.07	128.68
3	A	702	NW8	C20-C19-C18	-5.33	114.33	121.24
2	B	801	NAD	N6A-C6A-N1A	-4.94	108.31	118.57
3	A	702	NW8	C21-C20-C19	4.71	124.21	119.24
2	A	701	NAD	N6A-C6A-N1A	-4.13	110.00	118.57
3	B	802	NW8	C20-C19-CL1	3.65	125.07	119.35
2	B	801	NAD	C6N-N1N-C2N	-3.60	118.69	121.97
3	B	802	NW8	C02-N01-C09	3.49	110.70	103.78
2	A	701	NAD	C3D-C2D-C1D	3.16	105.74	100.98
3	A	702	NW8	C15-C10-C11	3.07	123.71	117.59
3	A	702	NW8	C15-C10-C02	-2.93	116.65	121.28
2	A	701	NAD	C5D-C4D-C3D	-2.89	104.34	115.18
3	B	802	NW8	C17-C18-C19	2.86	122.26	119.24
2	B	801	NAD	C5B-C4B-C3B	-2.84	104.55	115.18
2	B	801	NAD	C5D-C4D-C3D	-2.83	104.57	115.18
3	A	702	NW8	C10-C02-N01	2.74	125.38	120.78
3	A	702	NW8	C20-C19-CL1	2.73	123.63	119.35
2	A	701	NAD	O7N-C7N-N7N	-2.69	118.75	122.58
3	A	702	NW8	C17-C18-C19	2.67	122.05	119.24
3	A	702	NW8	C14-C15-C10	-2.65	117.23	120.56
2	B	801	NAD	O7N-C7N-N7N	-2.64	118.83	122.58
3	B	802	NW8	C10-C02-N01	2.63	125.20	120.78
3	A	702	NW8	C02-C03-N04	-2.53	105.30	107.89
2	A	701	NAD	O5B-PA-O1A	2.45	118.63	109.07
3	A	702	NW8	C02-N01-C09	2.39	108.52	103.78
2	A	701	NAD	C1B-N9A-C4A	-2.33	122.55	126.64
2	B	801	NAD	PA-O5B-C5B	-2.25	108.48	121.68
2	A	701	NAD	C3N-C7N-N7N	2.20	120.39	117.75
3	B	802	NW8	C15-C10-C02	-2.20	117.81	121.28
3	B	802	NW8	C21-C16-C08	2.17	124.50	120.86
3	B	802	NW8	C18-C17-C16	2.09	124.14	121.13

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	NAD	C5B-O5B-PA-O3
2	B	801	NAD	O4D-C1D-N1N-C2N
2	B	801	NAD	O4D-C1D-N1N-C6N
2	B	801	NAD	C2D-C1D-N1N-C2N
2	B	801	NAD	C2D-C1D-N1N-C6N
2	A	701	NAD	C5B-O5B-PA-O1A
2	A	701	NAD	C5B-O5B-PA-O3
2	A	701	NAD	C5D-O5D-PN-O3
2	A	701	NAD	O4B-C4B-C5B-O5B
2	B	801	NAD	O4B-C4B-C5B-O5B
2	A	701	NAD	C3B-C4B-C5B-O5B
2	A	701	NAD	C3D-C4D-C5D-O5D
2	B	801	NAD	PA-O3-PN-O5D
4	A	703	GOL	O2-C2-C3-O3
2	A	701	NAD	O4D-C4D-C5D-O5D
2	B	801	NAD	C5B-O5B-PA-O1A
2	B	801	NAD	C5B-O5B-PA-O2A
2	A	701	NAD	C5B-O5B-PA-O2A
2	B	801	NAD	C3B-C4B-C5B-O5B
2	B	801	NAD	O4D-C4D-C5D-O5D

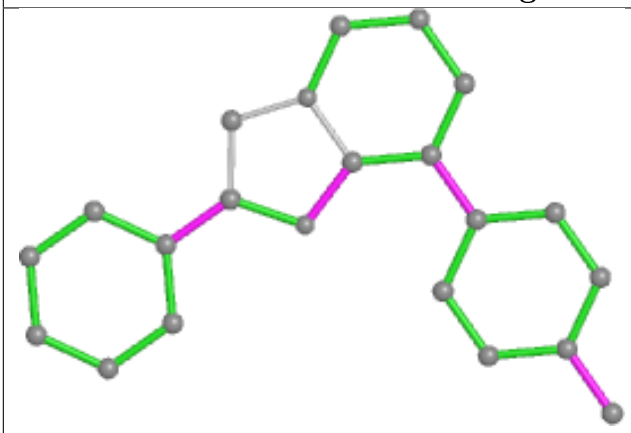
There are no ring outliers.

3 monomers are involved in 9 short contacts:

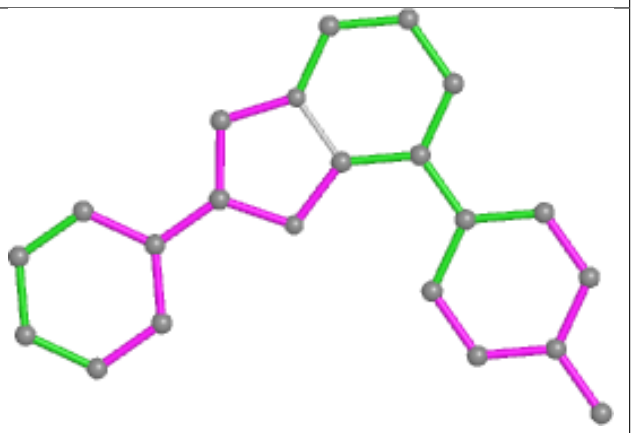
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	NAD	5	0
2	A	701	NAD	3	0
4	A	703	GOL	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

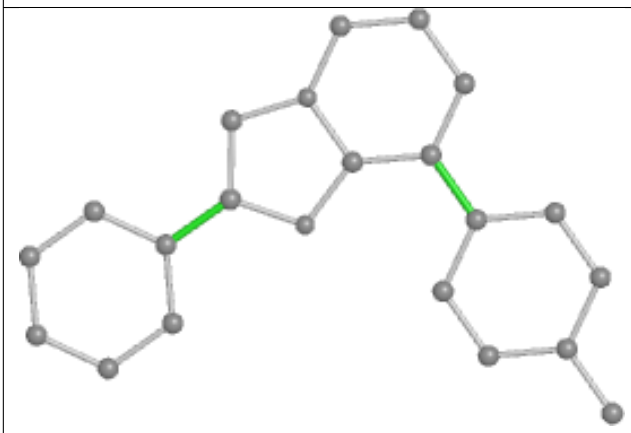
Ligand NW8 A 702



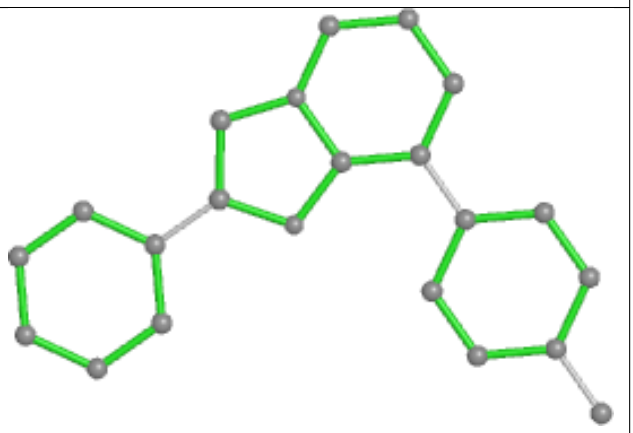
Bond lengths



Bond angles

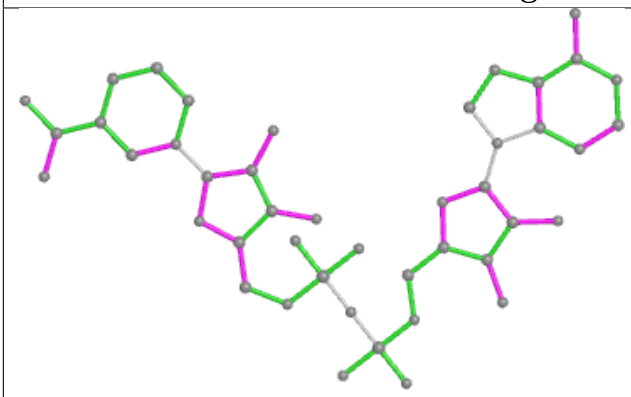


Torsions

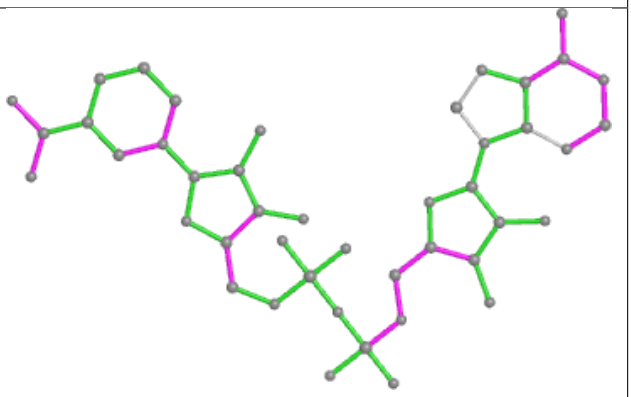


Rings

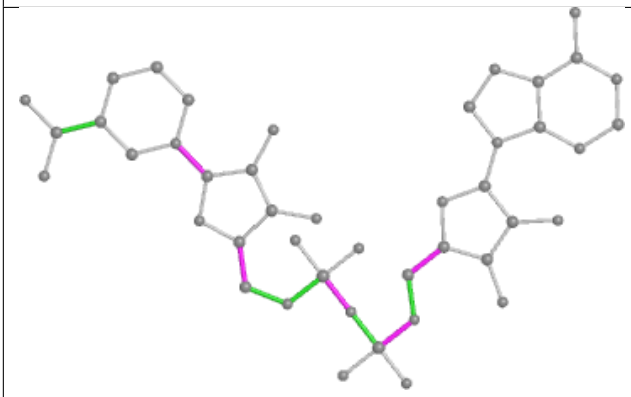
Ligand NAD B 801



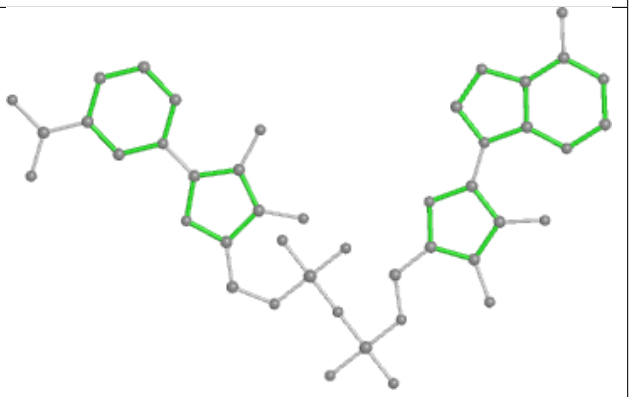
Bond lengths



Bond angles

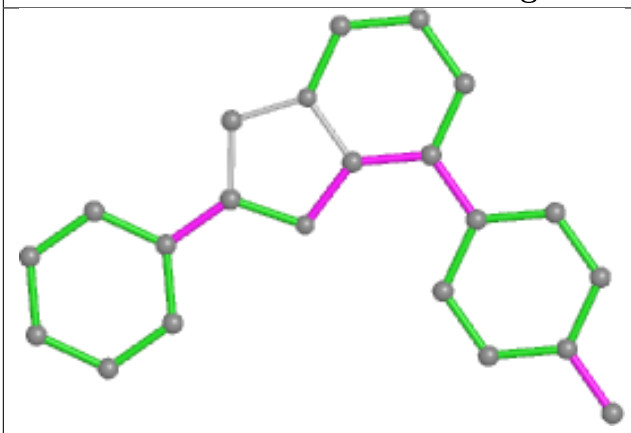


Torsions

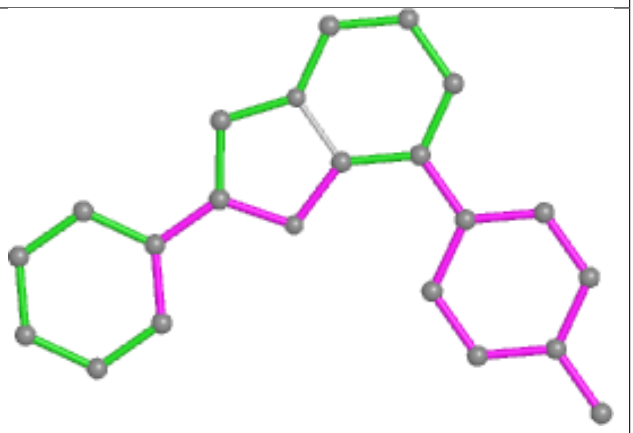


Rings

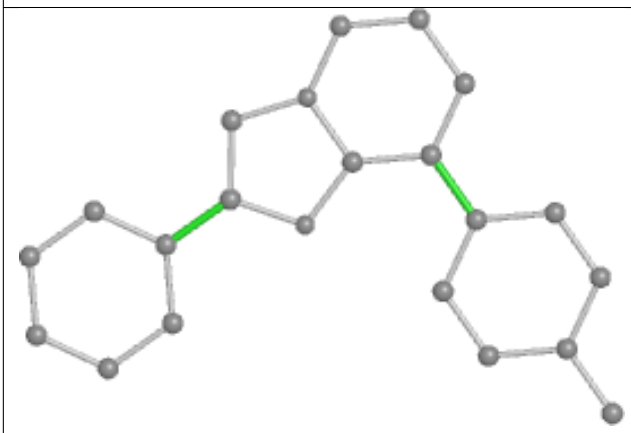
Ligand NW8 B 802



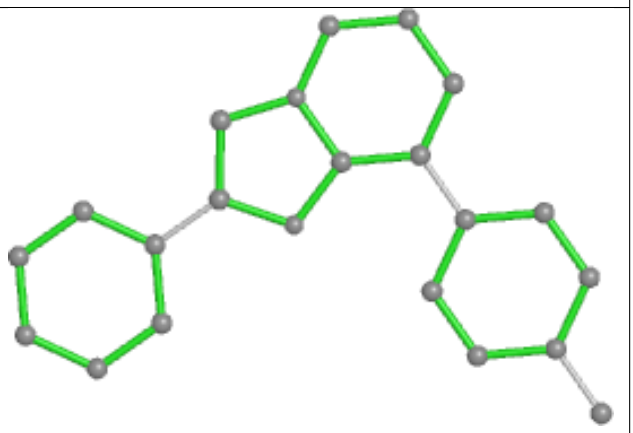
Bond lengths



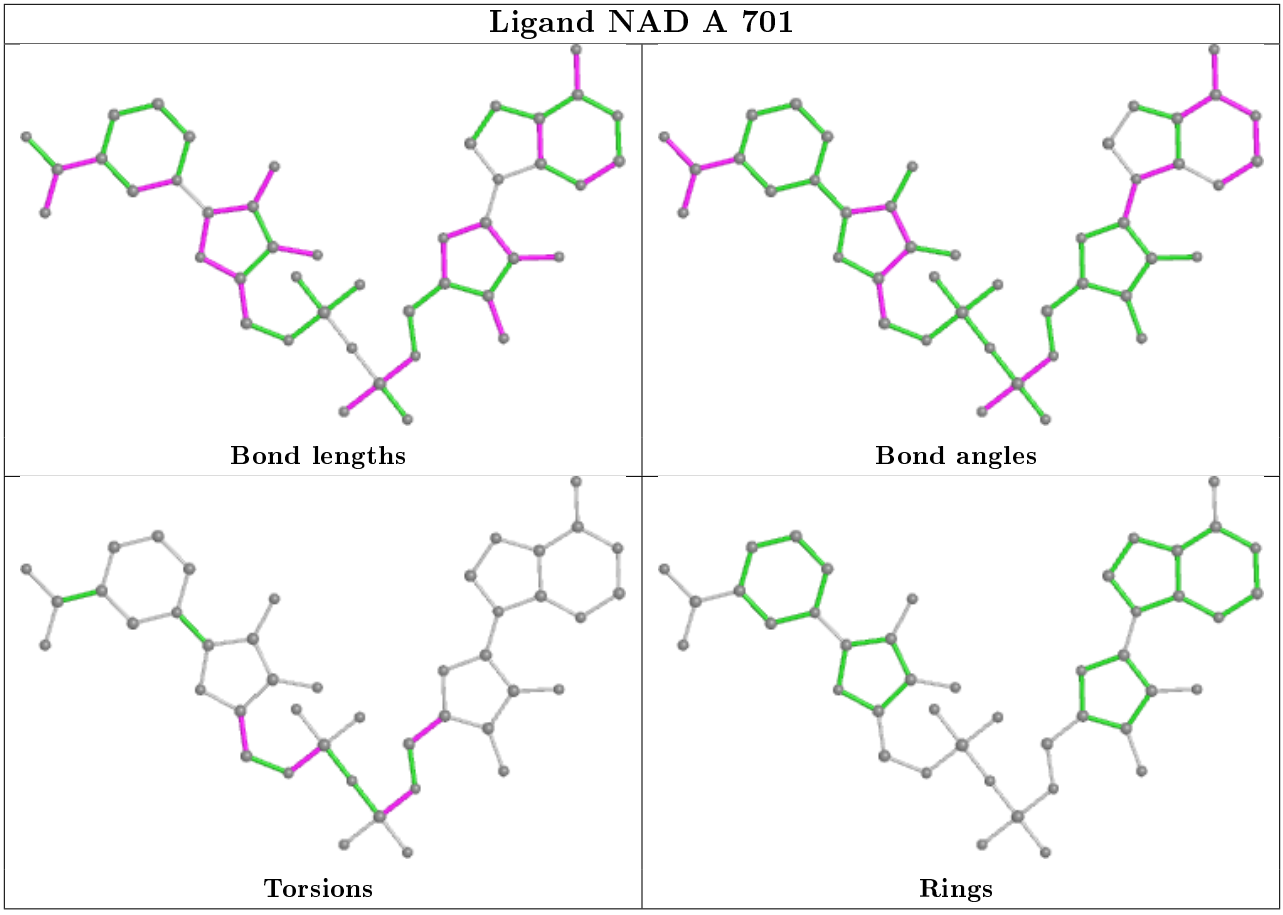
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	58:GLU	C	59:GLN	N	2.10
1	A	59:GLN	C	60:ILE	N	0.41

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, 95^{th} 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	478/512 (93%)	0.10	20 (4%)	36	32	31, 53, 114, 134	0
1	B	482/512 (94%)	0.08	26 (5%)	25	22	30, 54, 91, 135	0
All	All	960/1024 (93%)	0.09	46 (4%)	30	27	30, 54, 103, 135	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	346	PRO	6.5
1	A	350	LYS	5.7
1	A	349	VAL	5.4
1	B	386	MET	5.4
1	A	413	PHE	4.9
1	B	388	ASP	4.7
1	A	348	ASP	4.2
1	A	353	GLN	3.7
1	A	351	THR	3.7
1	A	345	ASP	3.4
1	A	344	GLY	3.2
1	A	347	PHE	3.2
1	B	389	LYS	3.1
1	A	340	LYS	3.1
1	B	394	LYS	3.1
1	B	336	GLU	3.0
1	B	383	GLY	3.0
1	B	387	GLU	2.9
1	B	384	SER	2.8
1	B	27	LEU	2.8
1	A	352	GLU	2.7
1	B	349	VAL	2.7
1	B	399	SER	2.7
1	B	369	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	343	VAL	2.6
1	B	342	PRO	2.6
1	B	332	ARG	2.5
1	B	348	ASP	2.5
1	B	382	GLY	2.5
1	B	398	PHE	2.4
1	B	396	THR	2.4
1	A	342	PRO	2.4
1	A	392	PHE	2.3
1	B	353	GLN	2.3
1	A	339	LYS	2.3
1	B	392	PHE	2.3
1	B	307	PHE	2.3
1	A	337	TYR	2.2
1	B	423	LYS	2.2
1	A	380	GLU	2.2
1	B	406	ARG	2.2
1	A	307	PHE	2.2
1	B	337	TYR	2.2
1	A	383	GLY	2.1
1	B	397	VAL	2.1
1	A	332	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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
3	NW8	A	702	22/22	0.77	0.64	55,86,96,111	0

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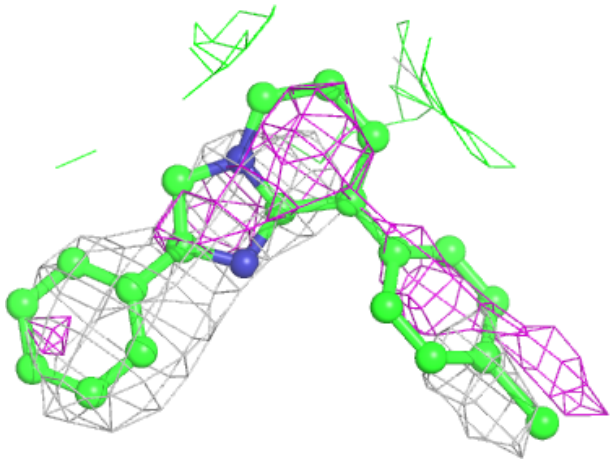
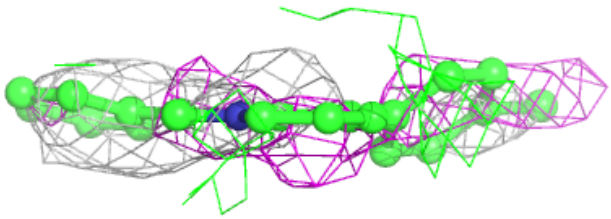
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NW8	B	802	22/22	0.81	0.34	55,73,86,94	0
4	GOL	A	703	6/6	0.88	0.26	47,54,56,59	0
2	NAD	A	701	44/44	0.89	0.21	37,65,127,130	0
2	NAD	B	801	44/44	0.94	0.19	46,63,150,154	0

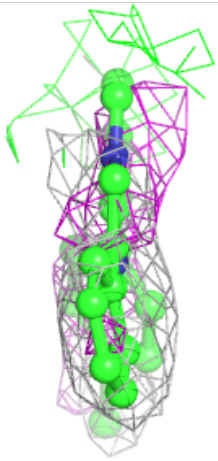
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NW8 A 702:

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

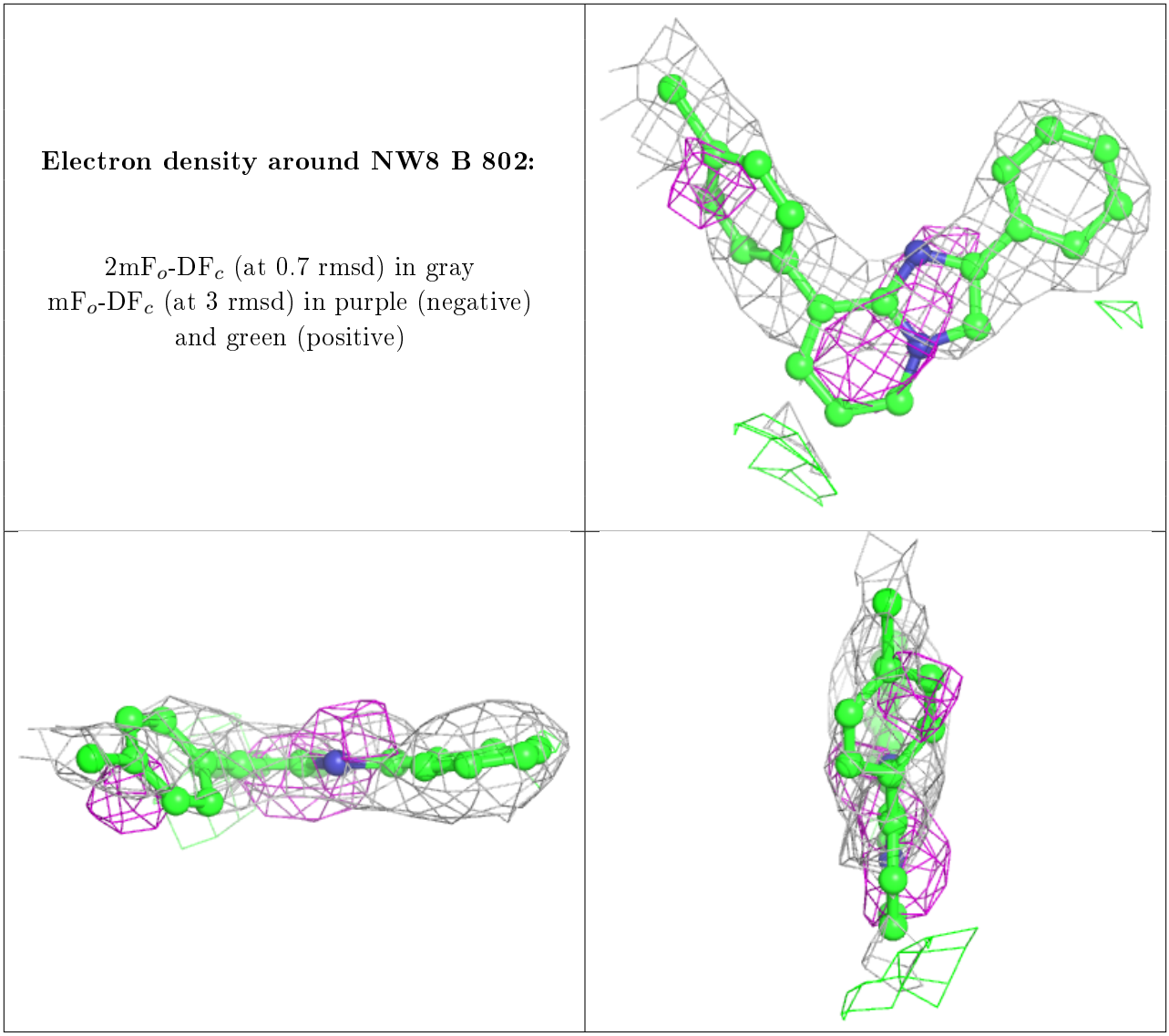






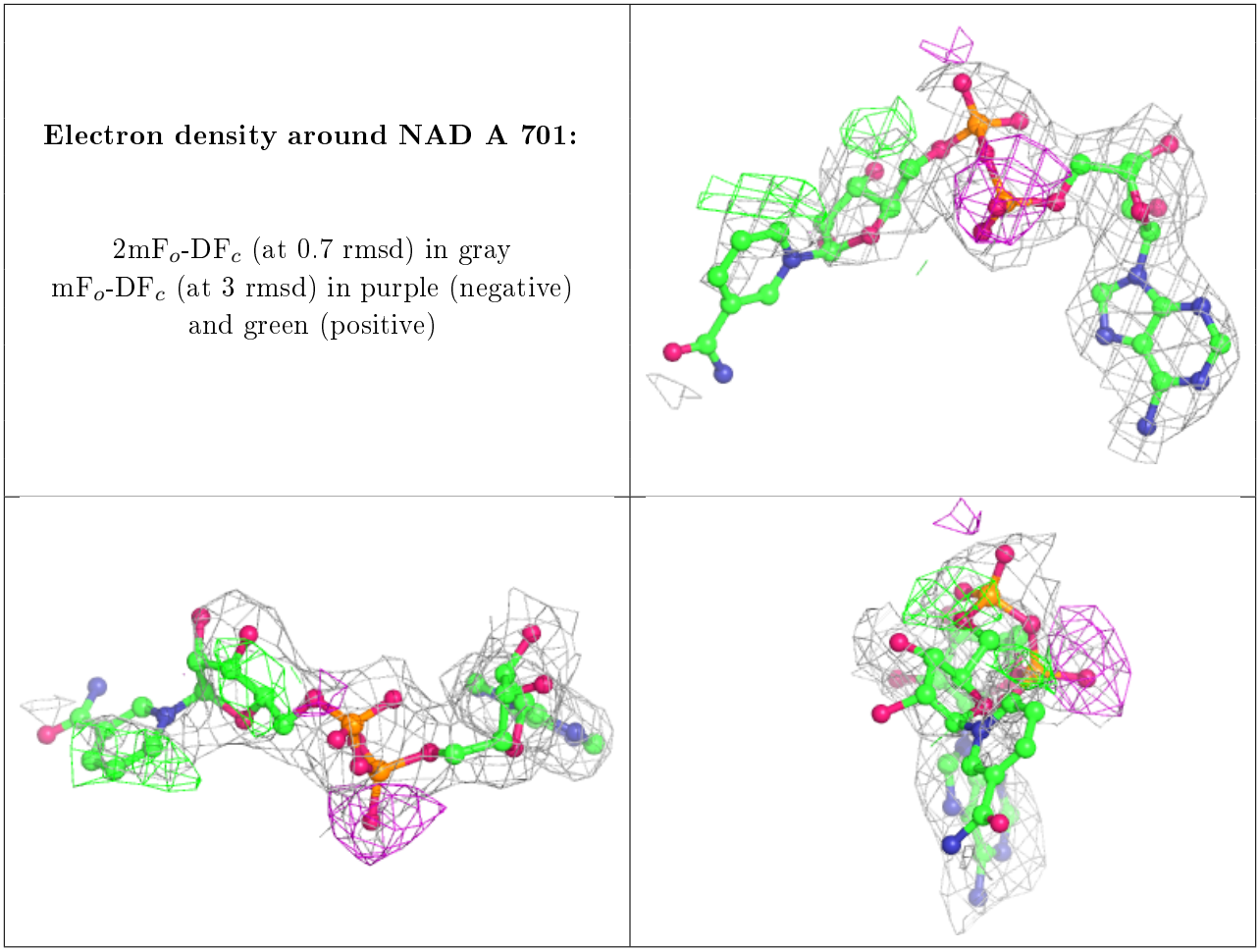
Electron density around NW8 B 802:

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



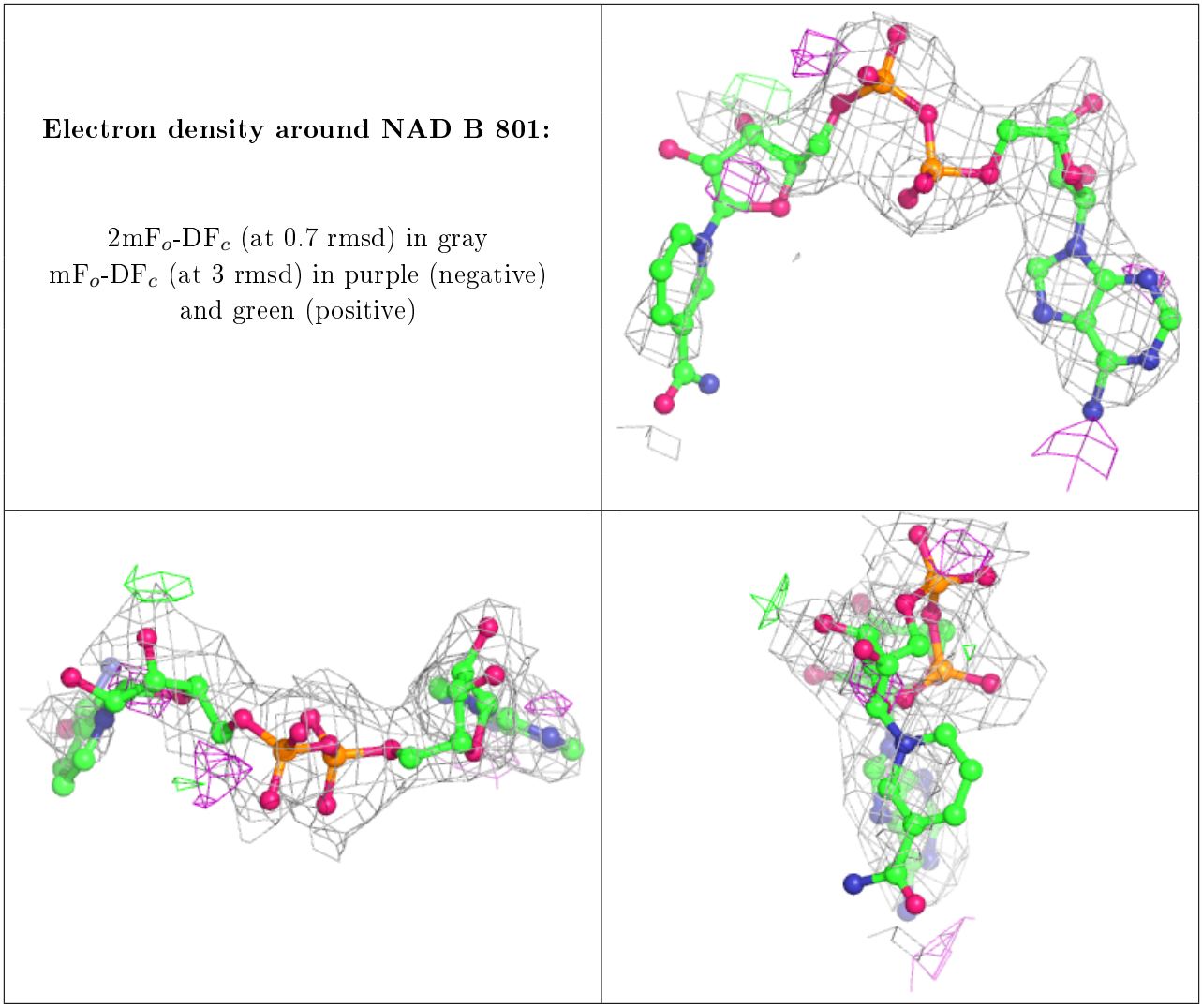
Electron density around NAD A 701:

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



Electron density around NAD B 801:

$2mF_o$-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

There are no such residues in this entry.