



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 05:34 AM EDT

PDB ID : 6TE5
Title : Crystal structure of human Aldehyde dehydrogenase 1A3 in complex with LQ43 inhibitor compound
Authors : Gelardi, E.L.M.; Garavaglia, S.
Deposited on : 2019-11-11
Resolution : 3.25 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

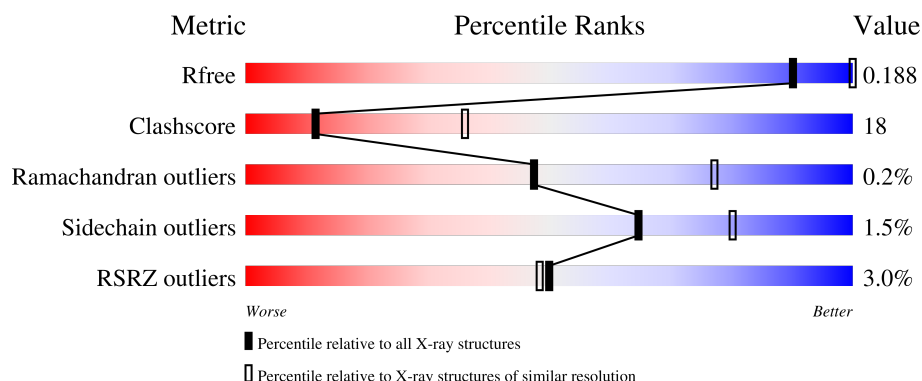
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	512	<div> <div>3%</div> <div>65%</div> <div>28%</div> <div>• 5%</div> </div>
1	B	512	<div> <div>3%</div> <div>64%</div> <div>27%</div> <div>• 6%</div> </div>

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

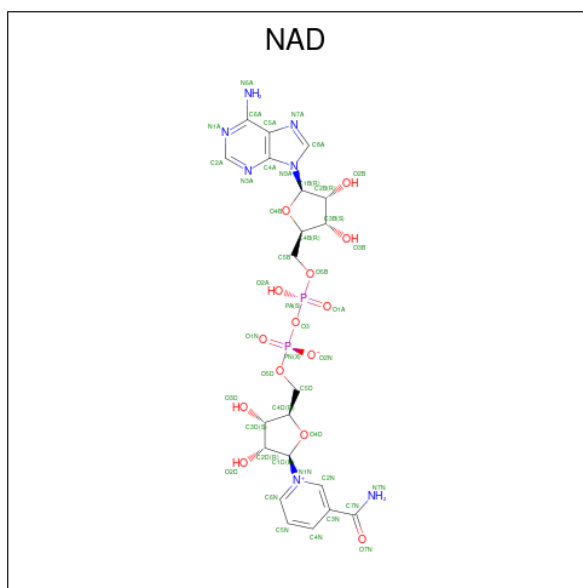
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	N4Q	A	602	-	-	-	X
3	N4Q	B	702	-	X	-	X

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.

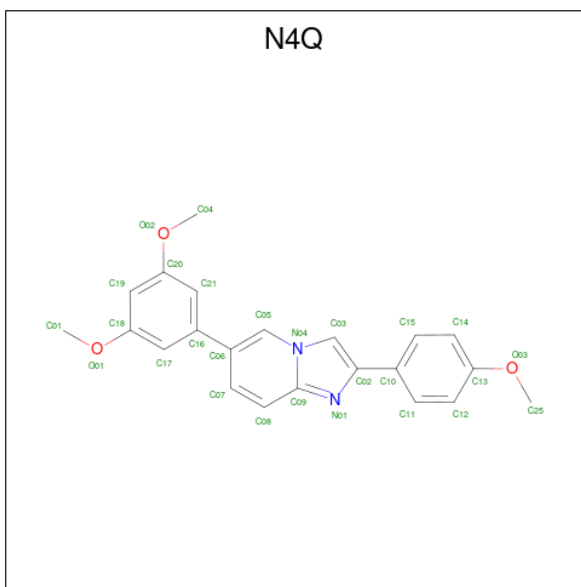
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total 3746	C 2387	N 639	O 700	S 20	0	0	0
1	B	479	Total 3700	C 2358	N 632	O 690	S 20	0	0	0

- 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 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is 6-(3,5-dimethoxyphenyl)-2-(4-methoxyphenyl)imidazo[1,2-a]pyridine (three-letter code: N4Q) (formula: C₂₂H₂₀N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	22	2	3		
3	B	1	Total	C	N	O	0	0
			27	22	2	3		

- 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		

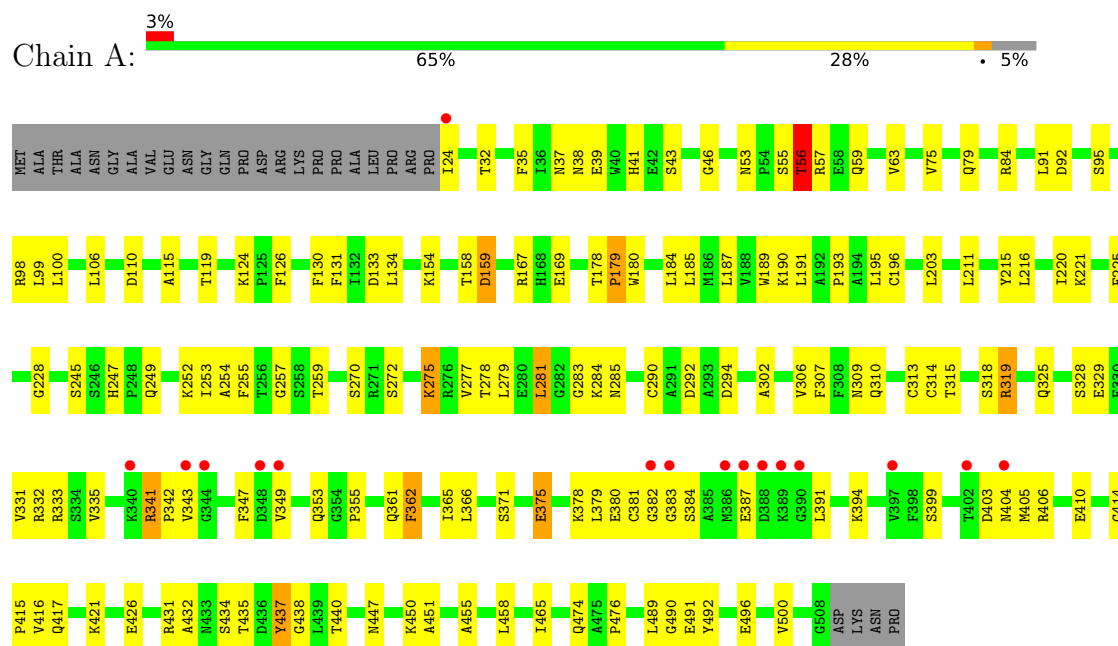
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	O 7	0	0
5	B	13	Total 13	O 13	0	0

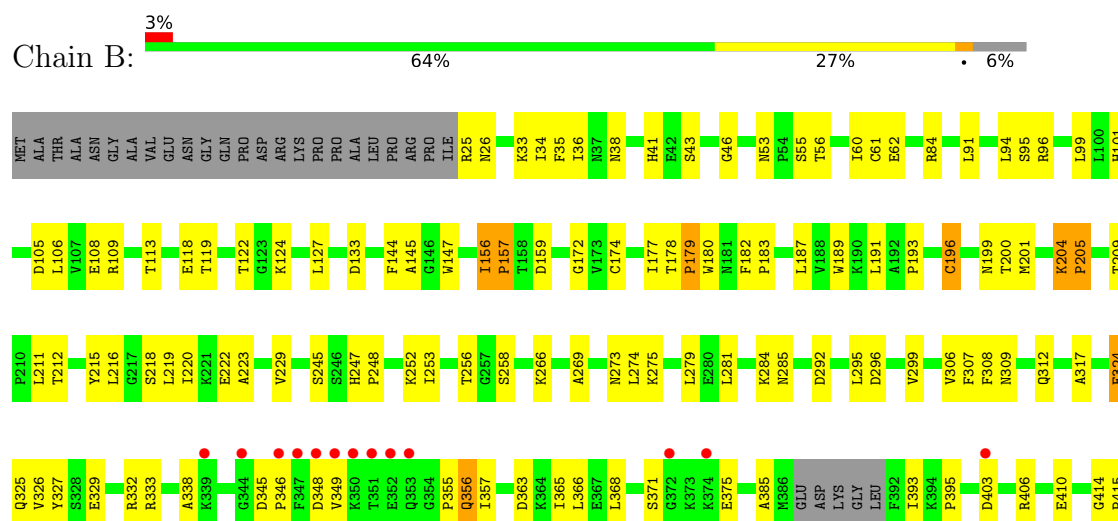
3 Residue-property plots [i](#)

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



• Molecule 1: Aldehyde dehydrogenase family 1 member A3



V416	Q417	P418	K421	F422	K423	S424	I425	E426	E427	R431	T435	D436	Y437	G438	K446	N447	K450	A457	A473	Q474	A475	P476	M485	G486	R487	E488	L489	G490	E491	E496	G508	ASP	LYS	ASN	PRD
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	81.18Å 89.34Å 159.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.96 – 3.25 47.96 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.96-3.25) 99.9 (47.96-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.14-3260-000	Depositor
R, R_{free}	0.187 , 0.238 0.187 , 0.188	Depositor DCC
R_{free} test set	926 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7614	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, GOL, N4Q

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	0.63	2/3822 (0.1%)	0.84	13/5170 (0.3%)
1	B	0.81	8/3775 (0.2%)	0.80	9/5106 (0.2%)
All	All	0.72	10/7597 (0.1%)	0.82	22/10276 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	PRO	N-CD	28.18	1.87	1.47
1	A	179	PRO	N-CD	-13.96	1.28	1.47
1	B	157	PRO	N-CA	12.46	1.68	1.47
1	B	179	PRO	N-CA	10.94	1.65	1.47
1	A	341	ARG	C-N	8.32	1.50	1.34
1	B	285	ASN	C-N	8.24	1.49	1.34
1	B	204	LYS	C-N	6.95	1.47	1.34
1	B	179	PRO	N-CD	-6.89	1.38	1.47
1	B	156	ILE	C-N	5.28	1.44	1.34
1	B	174	CYS	CB-SG	-5.10	1.73	1.81

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	PRO	CA-N-CD	-14.03	91.86	111.50
1	B	205	PRO	N-CA-CB	12.75	118.59	103.30
1	A	405	MET	N-CA-CB	12.53	133.15	110.60
1	B	159	ASP	N-CA-CB	11.00	130.40	110.60
1	A	405	MET	N-CA-C	-8.29	88.62	111.00
1	A	404	ASN	N-CA-C	-8.19	88.89	111.00
1	A	179	PRO	CA-N-CD	7.51	122.22	111.70
1	A	179	PRO	N-CA-CB	-7.33	94.51	103.30
1	B	157	PRO	CA-N-CD	-7.28	101.31	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	ASP	N-CA-C	-7.09	91.86	111.00
1	A	318	SER	CB-CA-C	-7.05	96.71	110.10
1	B	159	ASP	N-CA-C	-6.75	92.77	111.00
1	B	94	LEU	CA-CB-CG	6.48	130.20	115.30
1	A	275	LYS	CB-CA-C	-6.07	98.26	110.40
1	A	56	THR	N-CA-C	-5.79	95.37	111.00
1	A	319	ARG	N-CA-C	-5.79	95.37	111.00
1	B	204	LYS	C-N-CA	5.57	145.39	122.00
1	A	318	SER	N-CA-C	5.35	125.43	111.00
1	B	179	PRO	N-CD-CG	5.31	111.17	103.20
1	A	434	SER	N-CA-CB	5.22	118.33	110.50
1	A	159	ASP	N-CA-CB	5.06	119.71	110.60
1	B	179	PRO	CA-N-CD	-5.02	104.47	111.50

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	3746	0	3771	133	1
1	B	3700	0	3724	134	4
2	A	44	0	25	3	3
2	B	44	0	26	8	0
3	A	27	0	0	0	0
3	B	27	0	0	0	0
4	A	6	0	8	2	0
5	A	7	0	0	2	0
5	B	13	0	0	8	0
All	All	7614	0	7554	267	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 18.

All (267) 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:B:157:PRO:N	1:B:157:PRO:CA	1.68	1.40
1:B:205:PRO:N	1:B:205:PRO:CD	1.87	1.32
1:A:500:VAL:O	1:B:487:ARG:NH2	1.67	1.24
2:B:701:NAD:H51N	5:B:806:HOH:O	1.52	1.09
1:A:362:PHE:CE2	1:A:366:LEU:HD12	1.93	1.04
1:B:118:GLU:OE2	1:B:183:PRO:HD2	1.59	1.01
1:B:365:ILE:HD12	1:B:414:GLY:HA3	1.42	0.98
1:B:248:PRO:O	1:B:273:ASN:ND2	1.97	0.98
1:B:248:PRO:HA	1:B:273:ASN:HD22	1.26	0.97
1:B:324:GLU:OE2	1:B:421:LYS:NZ	1.98	0.97
1:A:32:THR:O	1:A:63:VAL:HG13	1.65	0.96
1:A:362:PHE:CE2	1:A:366:LEU:CD1	2.49	0.95
1:B:258:SER:HB3	2:B:701:NAD:O1A	1.68	0.94
1:B:179:PRO:HD3	1:B:256:THR:O	1.69	0.93
1:A:362:PHE:HE2	1:A:366:LEU:CD1	1.83	0.91
1:B:53:ASN:HB2	1:B:60:ILE:HD11	1.52	0.90
1:B:416:VAL:O	1:B:418:PRO:HD3	1.70	0.90
1:B:473:ALA:O	1:B:489:LEU:O	1.92	0.88
1:B:284:LYS:HD2	1:B:435:THR:HG21	1.52	0.88
1:A:178:THR:HB	1:A:179:PRO:HD2	1.55	0.87
1:A:380:GLU:OE2	1:A:399:SER:HB2	1.77	0.85
1:A:43:SER:HB2	1:A:46:GLY:H	1.40	0.85
1:B:248:PRO:CA	1:B:273:ASN:HD22	1.92	0.83
1:A:378:LYS:HB3	1:A:399:SER:HB3	1.61	0.82
1:A:53:ASN:O	1:A:56:THR:O	1.96	0.82
1:B:248:PRO:C	1:B:273:ASN:ND2	2.32	0.82
2:A:601:NAD:O2A	2:A:601:NAD:H3D	1.80	0.80
2:B:701:NAD:H3D	5:B:806:HOH:O	1.82	0.80
1:B:307:PHE:CD1	1:B:415:PRO:HB3	2.18	0.78
1:B:211:LEU:N	5:B:801:HOH:O	2.17	0.77
1:A:362:PHE:CD2	1:A:366:LEU:HD12	2.21	0.76
1:A:362:PHE:CD1	1:A:391:LEU:HD23	2.21	0.75
1:B:258:SER:CB	2:B:701:NAD:O1A	2.35	0.75
1:A:361:GLN:O	1:A:365:ILE:HG22	1.87	0.74
1:A:380:GLU:OE2	1:A:399:SER:CB	2.35	0.74
1:B:147:TRP:CZ2	1:B:491:GLU:HG3	2.22	0.74
1:B:403:ASP:OD1	1:B:431:ARG:NH1	2.20	0.74
2:B:701:NAD:O2A	2:B:701:NAD:O3D	2.04	0.73
1:B:327:TYR:CE1	1:B:421:LYS:HB2	2.24	0.73
1:A:55:SER:HA	1:A:355:PRO:HG3	1.69	0.73
1:A:406:ARG:NH1	1:A:410:GLU:OE2	2.22	0.73
1:A:403:ASP:OD1	1:A:431:ARG:NH1	2.22	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLU:CD	1:A:387:GLU:O	2.27	0.72
1:B:118:GLU:OE2	1:B:183:PRO:CD	2.38	0.71
1:B:55:SER:HB2	1:B:346:PRO:HG2	1.71	0.71
1:B:189:TRP:CD2	1:B:489:LEU:HD11	2.26	0.71
1:A:307:PHE:HB3	1:A:341:ARG:NH2	2.05	0.70
1:A:187:LEU:HD21	1:A:203:LEU:HD23	1.73	0.70
2:B:701:NAD:C5D	5:B:806:HOH:O	2.22	0.70
1:B:179:PRO:HG3	1:B:256:THR:HG22	1.74	0.70
1:A:387:GLU:O	1:A:387:GLU:OE1	2.10	0.69
1:B:284:LYS:HE3	1:B:437:TYR:HD2	1.58	0.69
1:A:365:ILE:HD12	1:A:414:GLY:HA3	1.74	0.68
1:B:248:PRO:C	1:B:273:ASN:HD22	1.97	0.68
1:B:292:ASP:O	1:B:446:LYS:HE3	1.95	0.67
1:B:157:PRO:N	1:B:157:PRO:C	2.45	0.67
1:A:187:LEU:HD11	1:A:203:LEU:HG	1.77	0.67
1:B:284:LYS:HD2	1:B:435:THR:CG2	2.26	0.66
1:A:252:LYS:HE2	1:A:278:THR:HG23	1.78	0.66
1:A:362:PHE:HD1	1:A:391:LEU:HD23	1.59	0.65
1:A:245:SER:HA	1:A:253:ILE:HD11	1.77	0.65
1:A:353:GLN:HE22	1:A:415:PRO:HG3	1.61	0.65
1:B:91:LEU:HD22	1:B:95:SER:HB2	1.77	0.64
1:A:189:TRP:CE2	1:A:489:LEU:HD11	2.33	0.63
1:A:371:SER:O	1:A:375:GLU:HB2	1.97	0.63
1:A:178:THR:CB	1:A:179:PRO:HD2	2.27	0.63
1:B:365:ILE:CD1	1:B:414:GLY:HA3	2.23	0.62
1:A:35:PHE:CE1	1:A:38:ASN:HA	2.35	0.61
1:A:39:GLU:HB2	1:A:41:HIS:HE1	1.63	0.61
1:A:319:ARG:HH22	1:A:432:ALA:HA	1.65	0.61
1:A:180:TRP:HE1	2:A:601:NAD:H51N	1.65	0.61
1:A:189:TRP:CZ2	1:A:489:LEU:HD11	2.36	0.61
1:B:329:GLU:OE2	1:B:332:ARG:NH2	2.35	0.60
1:A:124:LYS:NZ	1:A:133:ASP:OD1	2.32	0.60
1:A:167:ARG:NH1	1:A:169:GLU:OE2	2.34	0.60
1:B:204:LYS:C	1:B:204:LYS:HD2	2.22	0.60
1:A:285:ASN:CG	1:A:440:THR:HG22	2.22	0.60
1:B:212:THR:N	5:B:801:HOH:O	2.06	0.60
1:B:284:LYS:HE3	1:B:437:TYR:CD2	2.37	0.59
1:A:84:ARG:NH1	1:B:426:GLU:OE1	2.35	0.59
1:B:326:VAL:HG22	1:B:326:VAL:O	2.03	0.59
1:A:447:ASN:HB3	1:A:450:LYS:HB2	1.85	0.59
1:B:307:PHE:HD1	1:B:415:PRO:HB3	1.65	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:PHE:CZ	1:A:38:ASN:HA	2.37	0.59
1:A:307:PHE:O	1:A:341:ARG:NH2	2.35	0.59
1:A:110:ASP:OD2	1:A:215:TYR:OH	2.16	0.58
1:B:133:ASP:OD1	1:B:182:PHE:HD1	1.86	0.58
1:A:343:VAL:HG12	1:A:353:GLN:HB3	1.85	0.58
1:B:474:GLN:HB3	5:B:802:HOH:O	2.03	0.58
1:B:307:PHE:CE1	1:B:415:PRO:HB3	2.38	0.58
1:B:296:ASP:OD1	1:B:333:ARG:NH1	2.38	0.57
1:B:56:THR:HG23	1:B:56:THR:O	2.05	0.57
1:A:43:SER:HB2	1:A:46:GLY:N	2.18	0.56
1:A:184:LEU:N	5:A:701:HOH:O	2.38	0.56
1:A:437:TYR:N	1:A:437:TYR:CD1	2.73	0.56
1:B:119:THR:HG23	1:B:124:LYS:O	2.05	0.56
1:B:172:GLY:O	1:B:199:ASN:HB3	2.05	0.56
1:A:92:ASP:HB3	1:A:95:SER:OG	2.06	0.56
1:B:279:LEU:HB3	1:B:281:LEU:HD21	1.87	0.56
1:A:270:SER:HB3	1:B:266:LYS:HB3	1.88	0.55
1:A:384:SER:O	1:A:394:LYS:HB2	2.05	0.55
1:A:38:ASN:HB3	1:A:221:LYS:HG3	1.89	0.55
1:A:319:ARG:NH2	1:A:432:ALA:HA	2.21	0.55
1:A:362:PHE:CE2	1:A:366:LEU:HD11	2.38	0.55
1:B:33:LYS:HB3	1:B:41:HIS:O	2.06	0.55
1:B:338:ALA:HB1	1:B:395:PRO:HB2	1.87	0.55
1:A:421:LYS:O	1:A:431:ARG:NH2	2.40	0.55
1:B:133:ASP:OD1	1:B:182:PHE:CD1	2.59	0.54
1:B:189:TRP:CE2	1:B:489:LEU:HD11	2.43	0.54
1:B:269:ALA:HB1	1:B:275:LYS:HG3	1.90	0.54
1:A:84:ARG:HH21	1:B:457:ALA:HB2	1.73	0.54
1:B:35:PHE:CZ	1:B:38:ASN:HA	2.42	0.54
1:B:147:TRP:CH2	1:B:491:GLU:HG3	2.42	0.54
1:B:106:LEU:HD12	1:B:223:ALA:HB2	1.88	0.54
1:B:157:PRO:O	1:B:157:PRO:HG2	2.08	0.54
1:B:252:LYS:HE3	1:B:496:GLU:O	2.08	0.53
1:B:55:SER:HA	1:B:355:PRO:HG3	1.89	0.53
1:B:295:LEU:CD1	1:B:326:VAL:HG21	2.38	0.53
1:A:245:SER:HA	1:A:253:ILE:CD1	2.38	0.53
1:B:211:LEU:CA	5:B:801:HOH:O	2.54	0.53
1:A:353:GLN:NE2	1:A:415:PRO:HG3	2.24	0.53
1:B:345:ASP:O	1:B:348:ASP:HB2	2.09	0.53
1:B:43:SER:HB2	1:B:46:GLY:N	2.24	0.52
1:B:266:LYS:CE	1:B:485:ASN:HD21	2.22	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ASP:HA	1:B:299:VAL:HG22	1.90	0.52
1:B:25:ARG:HG3	1:B:26:ASN:H	1.75	0.52
1:A:32:THR:O	1:A:63:VAL:CG1	2.51	0.52
1:A:245:SER:O	1:A:275:LYS:HE2	2.10	0.52
1:A:154:LYS:NZ	1:B:491:GLU:OE1	2.41	0.52
1:B:312:GLN:NE2	1:B:356:GLN:HB3	2.25	0.52
1:B:122:THR:HG22	1:B:209:THR:HG21	1.90	0.52
1:A:272:SER:O	1:A:272:SER:OG	2.26	0.52
1:B:189:TRP:CG	1:B:489:LEU:HD11	2.45	0.52
1:A:178:THR:CB	1:A:179:PRO:CD	2.87	0.52
1:B:61:CYS:SG	1:B:62:GLU:N	2.82	0.52
1:A:329:GLU:HG3	1:A:332:ARG:HH12	1.75	0.51
1:B:127:LEU:HD11	1:B:349:VAL:HG12	1.92	0.51
1:A:306:VAL:HG21	1:A:417:GLN:HG3	1.92	0.51
1:A:310:GLN:HG3	1:A:353:GLN:HG3	1.93	0.51
1:A:362:PHE:CD2	1:A:362:PHE:C	2.83	0.51
1:A:259:THR:HA	1:A:281:LEU:HD13	1.91	0.51
1:B:325:GLN:OE1	1:B:325:GLN:N	2.43	0.51
1:A:474:GLN:O	1:B:156:ILE:HD13	2.11	0.51
1:A:283:GLY:HA2	1:A:437:TYR:HB3	1.92	0.50
1:A:381:CYS:SG	1:A:382:GLY:N	2.84	0.50
1:A:185:LEU:N	5:A:701:HOH:O	2.15	0.50
1:B:200:THR:HG22	1:B:229:VAL:HA	1.93	0.50
1:B:327:TYR:HE1	1:B:421:LYS:HB2	1.76	0.50
1:B:423:LYS:N	1:B:427:GLU:OE1	2.42	0.49
1:B:385:ALA:HA	1:B:393:ILE:HA	1.93	0.49
1:B:118:GLU:OE1	1:B:212:THR:HG21	2.13	0.49
1:A:39:GLU:HB2	1:A:41:HIS:CE1	2.44	0.49
1:A:415:PRO:O	1:A:416:VAL:HG23	2.12	0.49
1:A:325:GLN:OE1	1:A:325:GLN:N	2.36	0.49
1:A:331:VAL:O	1:A:335:VAL:HG13	2.12	0.49
1:A:180:TRP:HE1	2:A:601:NAD:C5D	2.25	0.49
1:B:53:ASN:HB2	1:B:60:ILE:CD1	2.34	0.49
1:B:312:GLN:HE22	1:B:356:GLN:HB3	1.77	0.48
1:A:252:LYS:HE3	1:A:496:GLU:O	2.13	0.48
1:B:416:VAL:C	1:B:418:PRO:HD3	2.32	0.48
1:B:485:ASN:OD1	1:B:485:ASN:O	2.31	0.48
1:B:424:SER:OG	1:B:426:GLU:N	2.47	0.48
1:B:447:ASN:HB3	1:B:450:LYS:HB2	1.94	0.48
1:A:191:LEU:HD21	1:A:195:LEU:HD12	1.95	0.48
1:A:437:TYR:N	1:A:437:TYR:HD1	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:TRP:CE3	1:B:357:ILE:HD12	2.49	0.48
1:A:292:ASP:OD1	1:A:292:ASP:N	2.43	0.48
1:A:24:ILE:O	1:A:347:PHE:HE2	1.96	0.48
1:B:245:SER:HA	1:B:253:ILE:HD11	1.95	0.48
1:A:426:GLU:OE2	1:B:84:ARG:NH2	2.46	0.47
1:A:310:GLN:O	1:A:415:PRO:HD3	2.14	0.47
1:B:324:GLU:OE2	1:B:421:LYS:CE	2.63	0.47
1:A:302:ALA:O	1:A:306:VAL:HG23	2.15	0.47
1:A:455:ALA:HB2	1:A:465:ILE:HD11	1.97	0.47
1:B:109:ARG:NH2	1:B:222:GLU:OE1	2.45	0.47
1:B:327:TYR:CD1	1:B:421:LYS:HG3	2.50	0.47
1:B:245:SER:HA	1:B:253:ILE:CD1	2.45	0.47
1:B:144:PHE:CE1	1:B:193:PRO:HB3	2.51	0.46
1:B:266:LYS:NZ	1:B:485:ASN:ND2	2.62	0.46
1:B:306:VAL:HG22	1:B:317:ALA:HB3	1.96	0.46
1:A:37:ASN:HA	1:A:228:GLY:N	2.30	0.46
1:A:451:ALA:HB1	1:A:465:ILE:HD13	1.97	0.46
1:A:307:PHE:HB3	1:A:341:ARG:CZ	2.45	0.46
1:B:216:LEU:O	1:B:220:ILE:HG13	2.16	0.46
1:A:290:CYS:SG	1:A:450:LYS:HE2	2.55	0.46
1:B:191:LEU:HA	1:B:201:MET:SD	2.56	0.46
1:A:284:LYS:HG3	1:A:435:THR:HG21	1.97	0.45
1:A:379:LEU:HD11	1:A:383:GLY:CA	2.46	0.45
1:A:491:GLU:HG2	1:A:491:GLU:O	2.17	0.45
1:A:329:GLU:HG3	1:A:332:ARG:NH1	2.31	0.45
1:A:99:LEU:HB3	1:A:225:PHE:CE1	2.50	0.45
1:B:178:THR:HG21	1:B:187:LEU:HD13	1.99	0.45
1:B:365:ILE:HG23	1:B:366:LEU:H	1.81	0.45
1:B:43:SER:HB2	1:B:46:GLY:H	1.82	0.45
1:B:295:LEU:HD12	1:B:295:LEU:HA	1.66	0.45
1:A:193:PRO:HA	1:A:196:CYS:SG	2.56	0.45
1:A:216:LEU:O	1:A:220:ILE:HG13	2.17	0.45
1:A:476:PRO:HG3	1:A:492:TYR:CD1	2.52	0.45
1:A:191:LEU:O	1:A:195:LEU:HB2	2.17	0.45
1:A:100:LEU:HD12	1:A:196:CYS:HB3	1.99	0.45
1:B:215:TYR:O	1:B:218:SER:N	2.48	0.45
1:B:101:HIS:CE1	1:B:145:ALA:HB3	2.52	0.45
1:B:105:ASP:O	1:B:108:GLU:HB3	2.17	0.45
1:A:75:VAL:HG11	1:A:247:HIS:CE1	2.52	0.44
1:A:278:THR:HG21	1:A:496:GLU:HB3	1.99	0.44
1:B:96:ARG:HD2	1:B:196:CYS:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:NAD:H8A	2:B:701:NAD:H51A	1.99	0.44
1:A:255:PHE:HB3	1:A:279:LEU:HD23	1.98	0.44
1:A:362:PHE:C	1:A:362:PHE:HD2	2.19	0.44
1:B:113:THR:HG21	1:B:215:TYR:CE2	2.53	0.44
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.58	0.44
1:B:101:HIS:ND1	1:B:145:ALA:HB1	2.32	0.44
1:B:371:SER:O	1:B:375:GLU:OE1	2.36	0.44
1:B:247:HIS:ND1	1:B:248:PRO:HD2	2.32	0.44
1:B:406:ARG:HG2	1:B:410:GLU:OE2	2.17	0.44
1:A:115:ALA:HB2	1:A:134:LEU:HD12	2.00	0.44
1:A:255:PHE:CZ	1:A:257:GLY:HA3	2.53	0.44
1:B:295:LEU:HD11	1:B:326:VAL:HG21	1.98	0.44
1:A:277:VAL:H	4:A:603:GOL:C3	2.31	0.44
1:B:204:LYS:C	1:B:204:LYS:CD	2.85	0.44
1:B:204:LYS:O	1:B:204:LYS:HG3	2.18	0.44
1:B:312:GLN:HE22	1:B:356:GLN:HA	1.83	0.44
1:A:130:PHE:HD2	1:A:131:PHE:CE1	2.36	0.44
1:A:341:ARG:HA	1:A:342:PRO:HD2	1.83	0.43
1:B:101:HIS:ND1	1:B:145:ALA:CB	2.81	0.43
1:B:106:LEU:HB3	1:B:219:LEU:HD22	1.99	0.43
1:B:476:PRO:HA	1:B:488:GLU:O	2.18	0.43
1:A:329:GLU:O	1:A:333:ARG:HG3	2.18	0.43
1:A:98:ARG:HA	1:A:98:ARG:HD2	1.83	0.43
1:B:211:LEU:HB2	5:B:801:HOH:O	2.18	0.43
1:A:490:GLY:C	1:A:492:TYR:N	2.68	0.43
1:A:319:ARG:HH22	1:A:432:ALA:CA	2.30	0.42
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.78	0.42
1:B:425:ILE:HD13	1:B:425:ILE:HA	1.85	0.42
2:B:701:NAD:H51A	2:B:701:NAD:C8A	2.49	0.42
1:A:315:THR:O	1:A:315:THR:OG1	2.36	0.42
1:A:79:GLN:NE2	1:A:249:GLN:HB3	2.35	0.42
1:B:124:LYS:HG2	1:B:309:ASN:OD1	2.20	0.42
1:B:178:THR:HB	1:B:179:PRO:HD2	2.01	0.42
1:A:91:LEU:HD12	1:A:92:ASP:H	1.84	0.42
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.81	0.42
1:B:34:ILE:HG22	1:B:36:ILE:HG13	2.02	0.42
1:A:253:ILE:HG13	1:A:275:LYS:HD3	2.01	0.42
1:A:313:CYS:SG	1:A:314:CYS:N	2.92	0.42
1:B:365:ILE:O	1:B:368:LEU:N	2.53	0.42
1:A:332:ARG:O	1:A:335:VAL:HG22	2.20	0.42
1:B:211:LEU:HA	1:B:211:LEU:HD23	1.71	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LYS:HE3	1:B:133:ASP:OD2	2.20	0.41
1:B:403:ASP:OD2	1:B:431:ARG:HD2	2.19	0.41
1:B:177:ILE:HA	1:B:204:LYS:O	2.20	0.41
1:A:124:LYS:HE2	1:A:309:ASN:OD1	2.21	0.41
1:A:277:VAL:H	4:A:603:GOL:H31	1.85	0.41
1:B:308:PHE:CD1	1:B:309:ASN:N	2.89	0.41
1:A:57:ARG:HD2	1:A:391:LEU:HG	2.03	0.41
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.82	0.41
1:B:189:TRP:CD2	1:B:489:LEU:CD1	3.01	0.41
1:B:266:LYS:HE3	1:B:485:ASN:HD21	1.85	0.41
1:A:190:LYS:HE3	1:A:254:ALA:HB1	2.03	0.41
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.94	0.40
1:B:99:LEU:HA	1:B:99:LEU:HD23	1.81	0.40
1:A:119:THR:OG1	1:A:126:PHE:HA	2.21	0.40
1:A:158:THR:OG1	1:A:159:ASP:N	2.53	0.40
1:A:319:ARG:NH2	1:A:432:ALA:O	2.50	0.40
1:A:38:ASN:O	1:A:221:LYS:HE3	2.21	0.40
1:A:435:THR:HB	1:A:437:TYR:H	1.85	0.40
1:A:314:CYS:SG	1:A:315:THR:HG23	2.61	0.40
1:B:416:VAL:HG12	1:B:418:PRO:HG3	2.03	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:B:363:ASP:OD1	2:A:601:NAD:N7N[3_555]	0.92	1.28
1:B:363:ASP:OD1	2:A:601:NAD:O7N[3_555]	2.00	0.20
1:A:328:SER:OG	1:B:324:GLU:OE1[1_565]	2.01	0.19
1:B:363:ASP:OD2	2:A:601:NAD:N7N[3_555]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	483/512 (94%)	453 (94%)	29 (6%)	1 (0%)	47	77
1	B	475/512 (93%)	430 (90%)	44 (9%)	1 (0%)	47	77
All	All	958/1024 (94%)	883 (92%)	73 (8%)	2 (0%)	47	77

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	401/422 (95%)	394 (98%)	7 (2%)	60	78
1	B	396/422 (94%)	391 (99%)	5 (1%)	69	82
All	All	797/844 (94%)	785 (98%)	12 (2%)	65	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	59	GLN
1	A	281	LEU
1	A	349	VAL
1	A	362	PHE
1	A	375	GLU
1	A	437	TYR
1	B	196	CYS
1	B	274	LEU
1	B	324	GLU
1	B	356	GLN
1	B	474	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	A	304	GLN
1	B	273	ASN
1	B	312	GLN
1	B	485	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](#)

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	$\# Z > 2$
2	NAD	B	701	-	42,48,48	0.84	2 (4%)	50,73,73	1.24	7 (14%)
3	N4Q	B	702	-	27,30,30	2.24	7 (25%)	34,42,42	3.90	19 (55%)
4	GOL	A	603	-	5,5,5	1.19	0	5,5,5	0.83	0
3	N4Q	A	602	-	27,30,30	2.28	6 (22%)	34,42,42	3.65	17 (50%)
2	NAD	A	601	1	42,48,48	0.92	2 (4%)	50,73,73	1.37	5 (10%)

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
2	NAD	B	701	-	-	12/26/62/62	0/5/5/5
3	N4Q	B	702	-	-	10/14/14/14	0/4/4/4
4	GOL	A	603	-	-	2/4/4/4	-
3	N4Q	A	602	-	-	12/14/14/14	0/4/4/4
2	NAD	A	601	1	-	3/26/62/62	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	N4Q	C10-C02	-6.75	1.38	1.48
3	A	602	N4Q	C10-C02	-6.33	1.39	1.48
3	A	602	N4Q	C16-C06	-5.00	1.36	1.49
3	A	602	N4Q	O01-C18	4.91	1.47	1.37
3	B	702	N4Q	C16-C06	-4.40	1.38	1.49
3	B	702	N4Q	C09-N01	4.15	1.37	1.33
3	B	702	N4Q	O01-C18	3.73	1.45	1.37
3	A	602	N4Q	C19-C18	3.17	1.44	1.38
3	A	602	N4Q	C19-C20	3.14	1.44	1.38
2	A	601	NAD	C2N-N1N	3.09	1.38	1.35
2	B	701	NAD	C2N-N1N	2.69	1.38	1.35
3	A	602	N4Q	C09-N01	2.62	1.35	1.33
3	B	702	N4Q	C08-C09	2.54	1.44	1.40
2	A	601	NAD	C8A-N7A	-2.36	1.30	1.34
3	B	702	N4Q	C05-N04	-2.33	1.33	1.37
3	B	702	N4Q	C19-C20	2.29	1.42	1.38
2	B	701	NAD	C8A-N7A	-2.26	1.30	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	N4Q	C17-C16-C06	-11.65	101.59	120.86
3	A	602	N4Q	C17-C16-C06	-9.37	105.37	120.86
3	A	602	N4Q	C15-C10-C02	-8.87	107.28	121.28
3	B	702	N4Q	C21-C16-C06	8.82	135.45	120.86
3	B	702	N4Q	C15-C10-C02	-7.05	110.15	121.28
3	A	602	N4Q	C11-C10-C02	6.97	132.29	121.28
3	A	602	N4Q	C19-C18-C17	-6.21	111.09	120.98
3	A	602	N4Q	C21-C16-C17	6.08	127.31	118.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	N4Q	C19-C18-C17	-5.84	111.67	120.98
3	B	702	N4Q	C16-C21-C20	-5.72	112.48	119.94
2	A	601	NAD	O4D-C1D-C2D	-5.66	98.66	106.93
3	A	602	N4Q	C20-C19-C18	5.34	126.52	118.48
3	B	702	N4Q	C16-C17-C18	5.28	126.81	119.94
3	A	602	N4Q	C16-C21-C20	-5.00	113.43	119.94
3	B	702	N4Q	C11-C10-C02	4.80	128.87	121.28
3	A	602	N4Q	C01-O01-C18	4.68	127.68	117.51
3	B	702	N4Q	C04-O02-C20	-4.34	108.10	117.51
3	A	602	N4Q	C21-C16-C06	3.89	127.29	120.86
3	B	702	N4Q	C02-C03-N04	-3.84	103.97	107.89
3	B	702	N4Q	C10-C02-N01	3.68	126.96	120.78
3	B	702	N4Q	C05-C06-C16	-3.68	112.62	120.53
3	A	602	N4Q	C02-C03-N04	-3.63	104.19	107.89
2	A	601	NAD	C6N-N1N-C2N	-3.46	118.81	121.97
2	B	701	NAD	O3B-C3B-C2B	-3.32	101.09	111.82
3	B	702	N4Q	C21-C16-C17	3.15	122.96	118.31
3	B	702	N4Q	C08-C07-C06	-3.12	115.93	121.00
3	B	702	N4Q	C07-C06-C16	3.11	126.75	121.36
2	B	701	NAD	C3D-C2D-C1D	2.99	105.48	100.98
2	B	701	NAD	C6N-N1N-C2N	-2.91	119.32	121.97
3	A	602	N4Q	C12-C11-C10	-2.81	117.09	121.13
2	A	601	NAD	O3B-C3B-C4B	-2.78	103.03	111.05
3	A	602	N4Q	C05-C06-C07	2.74	122.56	117.39
3	B	702	N4Q	C20-C19-C18	2.71	122.56	118.48
3	B	702	N4Q	C12-C11-C10	-2.71	117.23	121.13
2	A	601	NAD	C3B-C2B-C1B	2.65	104.97	100.98
3	A	602	N4Q	C04-O02-C20	-2.64	111.78	117.51
2	B	701	NAD	PN-O3-PA	-2.59	123.92	132.83
3	A	602	N4Q	C08-C07-C06	-2.46	117.00	121.00
3	B	702	N4Q	O01-C18-C19	2.43	131.56	119.94
2	A	601	NAD	C5A-C6A-N6A	2.32	123.87	120.35
2	B	701	NAD	O4D-C1D-C2D	-2.27	103.61	106.93
3	A	602	N4Q	C05-C06-C16	-2.26	115.66	120.53
2	B	701	NAD	C5A-C6A-N6A	2.26	123.79	120.35
3	A	602	N4Q	C02-N01-C09	2.19	109.00	104.33
2	B	701	NAD	PA-O5B-C5B	-2.19	108.86	121.68
3	B	702	N4Q	C03-C02-C10	-2.12	124.37	129.15
3	B	702	N4Q	C02-N01-C09	2.06	108.74	104.33
3	A	602	N4Q	C07-C08-C09	-2.06	117.27	119.76

There are no chirality outliers.

All (39) torsion outliers are listed below:

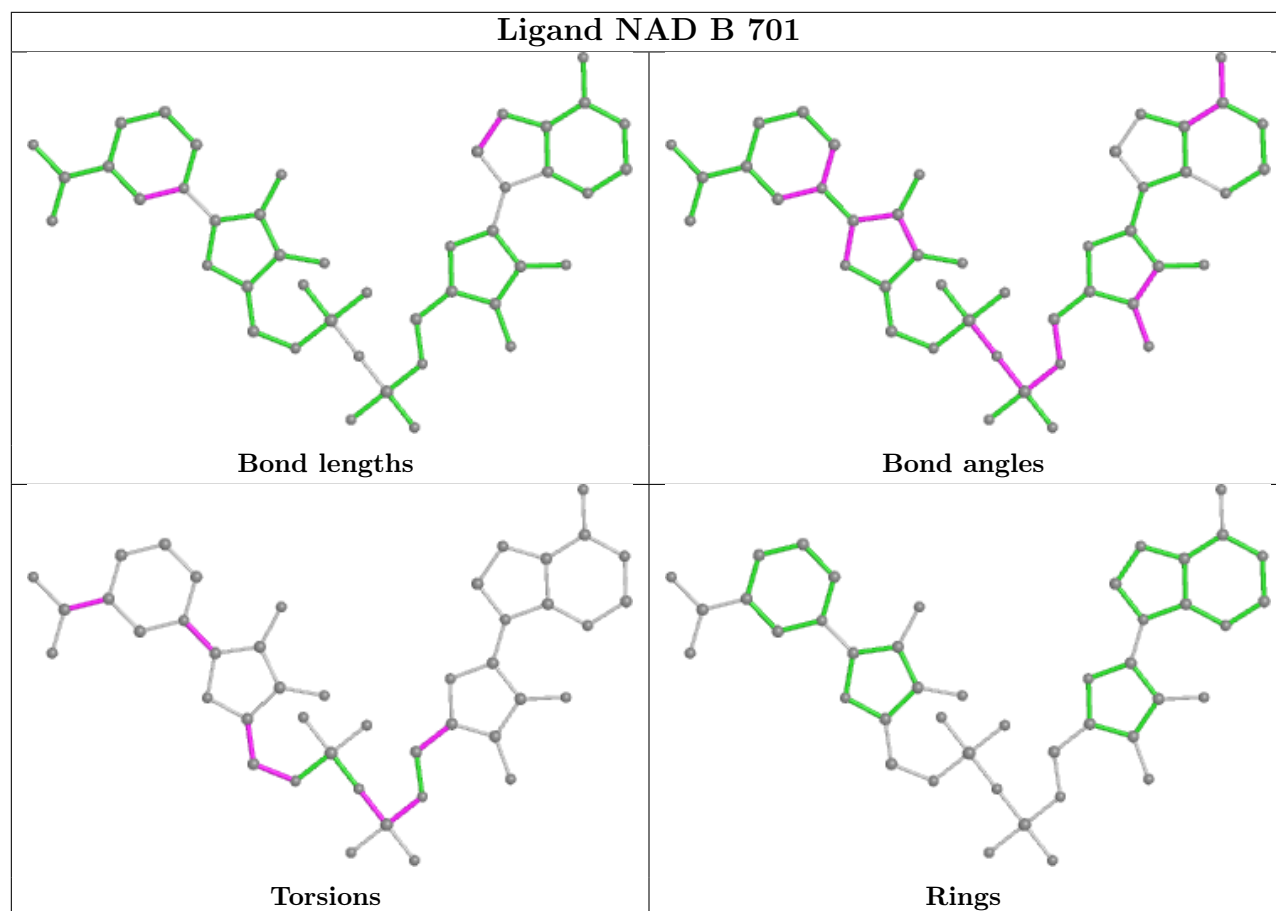
Mol	Chain	Res	Type	Atoms
2	A	601	NAD	PA-O3-PN-O5D
2	A	601	NAD	O4D-C4D-C5D-O5D
2	B	701	NAD	C2D-C1D-N1N-C2N
2	B	701	NAD	C2D-C1D-N1N-C6N
3	A	602	N4Q	C03-C02-C10-C11
3	A	602	N4Q	C03-C02-C10-C15
3	A	602	N4Q	N01-C02-C10-C11
3	A	602	N4Q	N01-C02-C10-C15
3	B	702	N4Q	N01-C02-C10-C15
3	B	702	N4Q	C14-C13-O03-C25
2	B	701	NAD	O4B-C4B-C5B-O5B
3	B	702	N4Q	C12-C13-O03-C25
3	B	702	N4Q	C19-C20-O02-C04
2	B	701	NAD	C3B-C4B-C5B-O5B
3	B	702	N4Q	C21-C20-O02-C04
3	B	702	N4Q	C03-C02-C10-C15
3	B	702	N4Q	N01-C02-C10-C11
3	A	602	N4Q	C07-C06-C16-C21
3	A	602	N4Q	C05-C06-C16-C21
4	A	603	GOL	C1-C2-C3-O3
3	A	602	N4Q	C17-C18-O01-C01
3	A	602	N4Q	C19-C18-O01-C01
3	A	602	N4Q	C07-C06-C16-C17
3	B	702	N4Q	C19-C18-O01-C01
3	B	702	N4Q	C17-C18-O01-C01
3	B	702	N4Q	C03-C02-C10-C11
2	B	701	NAD	C4N-C3N-C7N-N7N
2	B	701	NAD	C4D-C5D-O5D-PN
3	A	602	N4Q	C05-C06-C16-C17
3	A	602	N4Q	C19-C20-O02-C04
3	A	602	N4Q	C21-C20-O02-C04
2	B	701	NAD	C4N-C3N-C7N-O7N
2	B	701	NAD	C2N-C3N-C7N-N7N
4	A	603	GOL	O2-C2-C3-O3
2	B	701	NAD	PN-O3-PA-O5B
2	A	601	NAD	C3D-C4D-C5D-O5D
2	B	701	NAD	O4D-C4D-C5D-O5D
2	B	701	NAD	C5B-O5B-PA-O1A
2	B	701	NAD	C2N-C3N-C7N-O7N

There are no ring outliers.

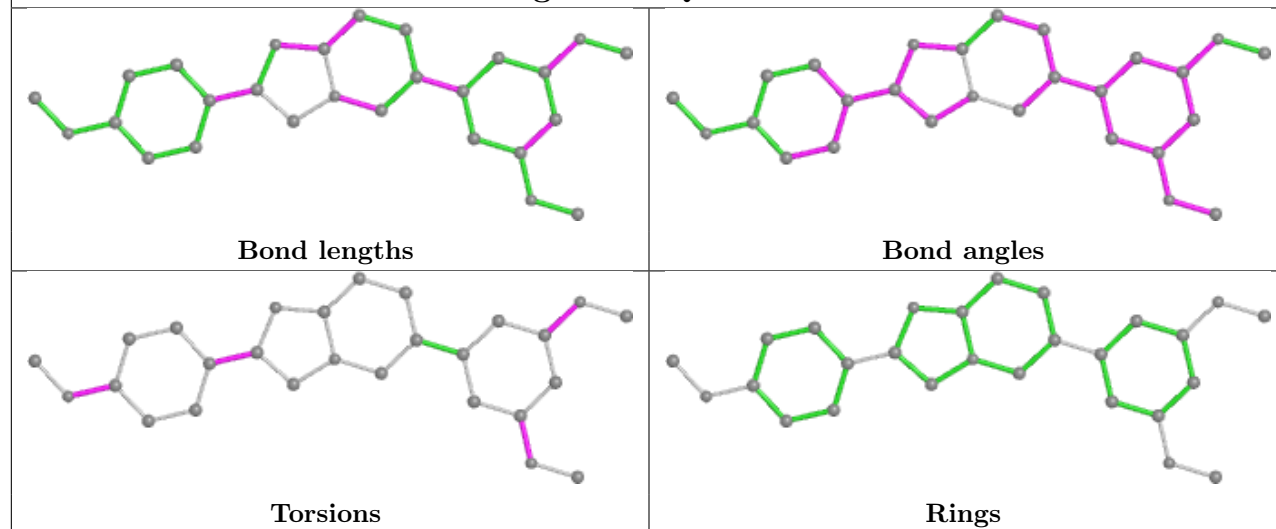
3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	NAD	8	0
4	A	603	GOL	2	0
2	A	601	NAD	3	3

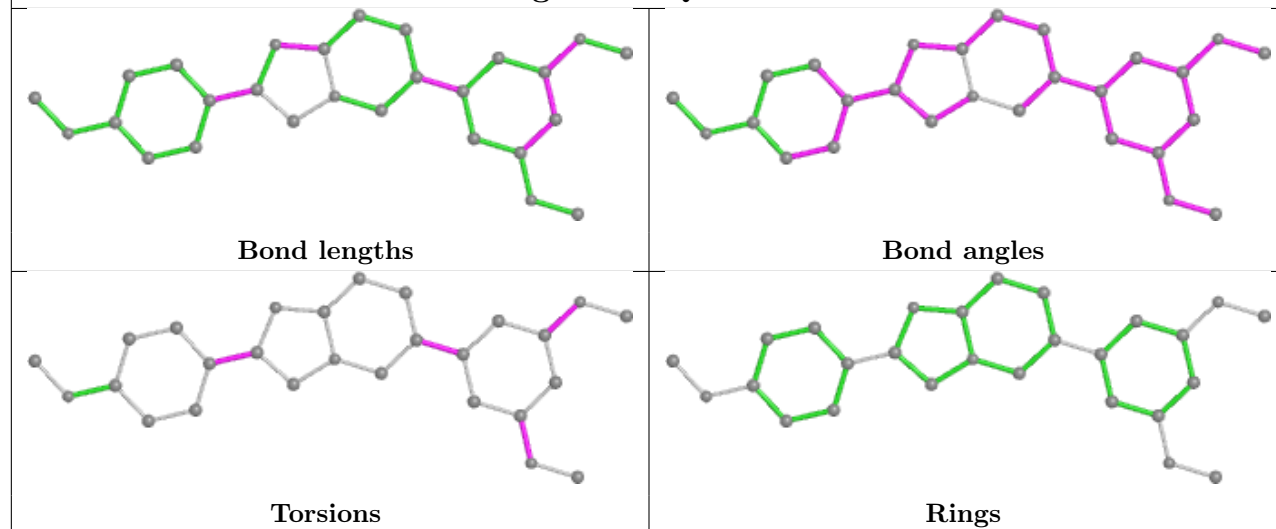
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

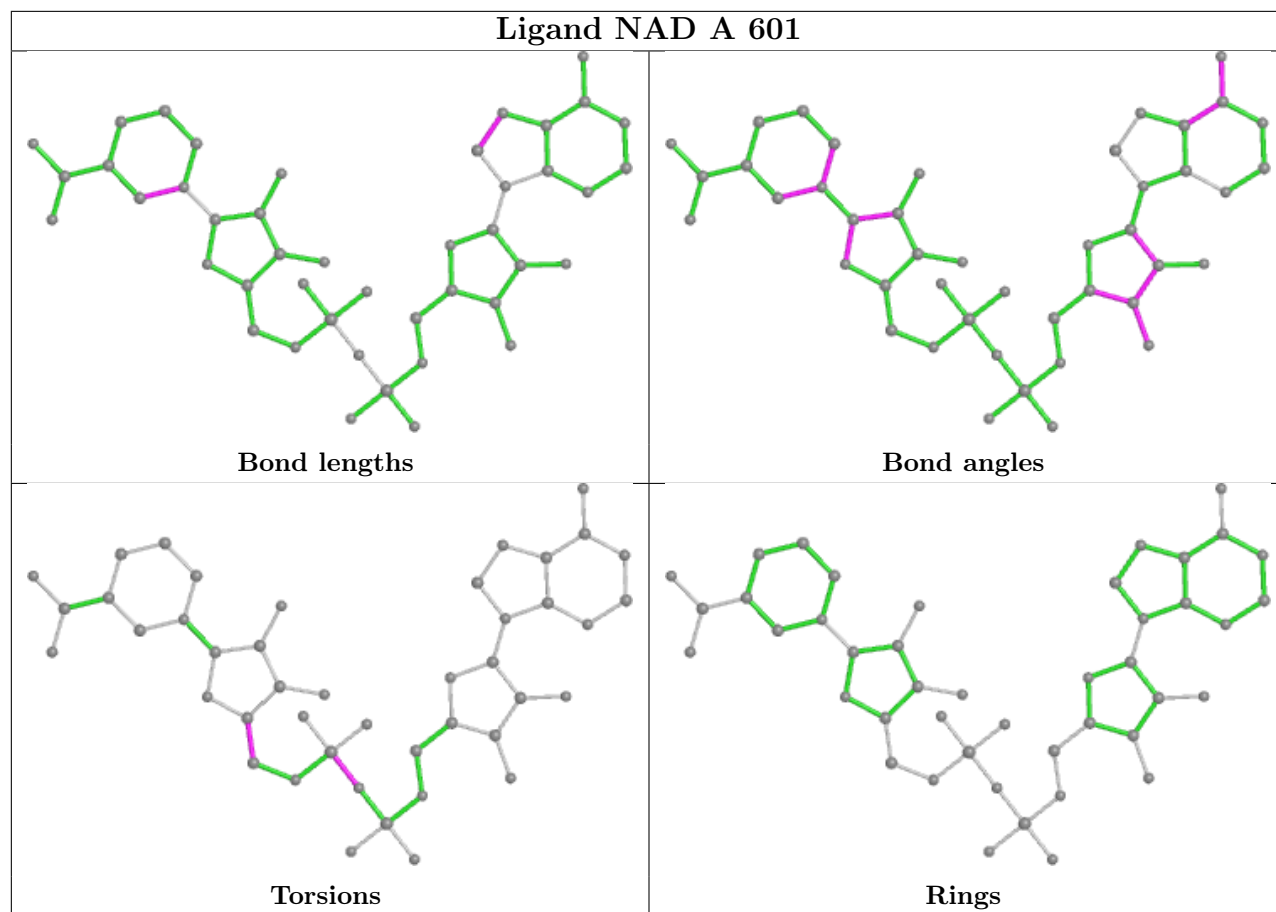


Ligand N4Q B 702



Ligand N4Q A 602





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	485/512 (94%)	-0.14	16 (3%) 46 43	27, 49, 85, 119	0
1	B	479/512 (93%)	-0.08	13 (2%) 54 51	29, 49, 104, 123	0
All	All	964/1024 (94%)	-0.11	29 (3%) 50 48	27, 49, 99, 123	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	349	VAL	5.2
1	B	346	PRO	5.1
1	A	348	ASP	3.7
1	B	344	GLY	3.6
1	A	386	MET	3.5
1	A	343	VAL	3.5
1	A	389	LYS	3.4
1	B	352	GLU	3.3
1	B	348	ASP	3.1
1	B	350	LYS	3.1
1	B	374	LYS	3.0
1	B	372	GLY	2.8
1	B	347	PHE	2.6
1	A	24	ILE	2.5
1	A	397	VAL	2.5
1	A	383	GLY	2.5
1	B	353	GLN	2.4
1	A	404	ASN	2.4
1	B	403	ASP	2.3
1	A	382	GLY	2.3
1	A	388	ASP	2.2
1	B	339	LYS	2.2
1	A	390	GLY	2.2
1	A	349	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	351	THR	2.1
1	A	387	GLU	2.0
1	A	340	LYS	2.0
1	A	344	GLY	2.0
1	A	402	THR	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](#)

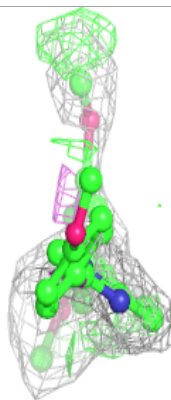
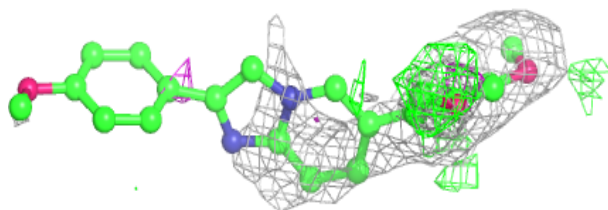
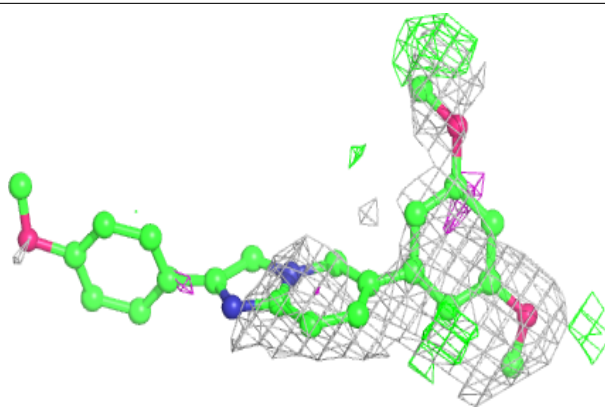
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	N4Q	A	602	27/27	0.65	0.46	52,100,129,137	0
3	N4Q	B	702	27/27	0.75	0.51	61,96,126,134	0
2	NAD	A	601	44/44	0.90	0.25	44,59,113,119	0
4	GOL	A	603	6/6	0.92	0.20	45,46,50,50	0
2	NAD	B	701	44/44	0.93	0.19	38,56,116,118	0

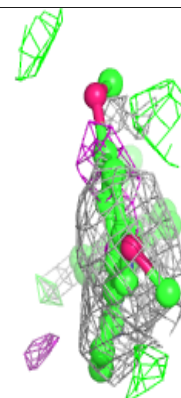
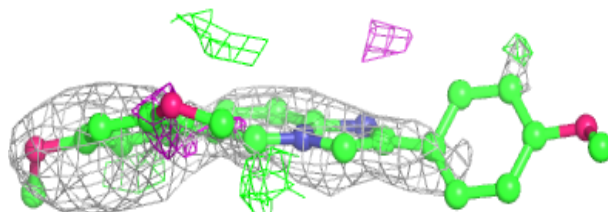
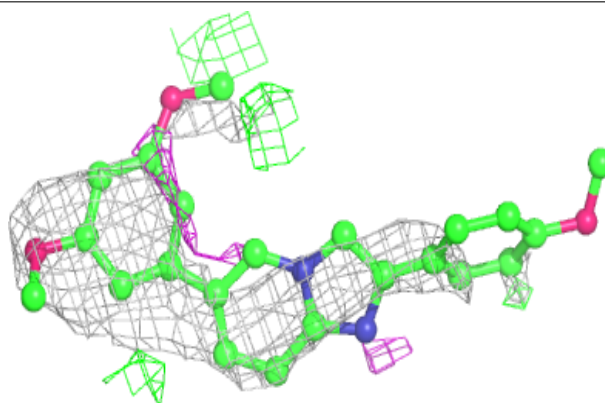
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around N4Q A 602:

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

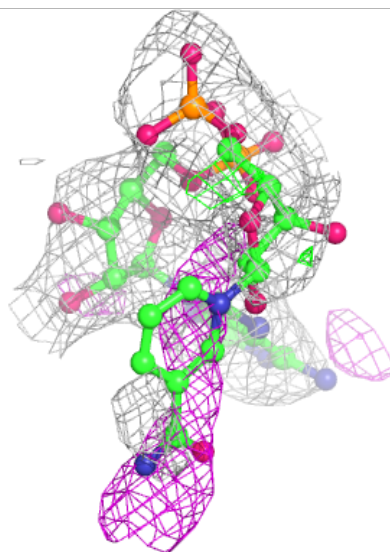
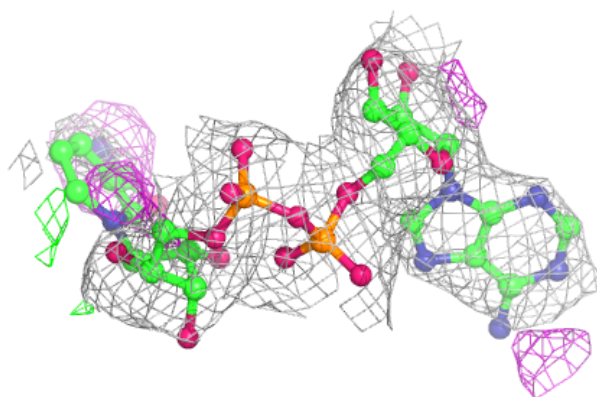
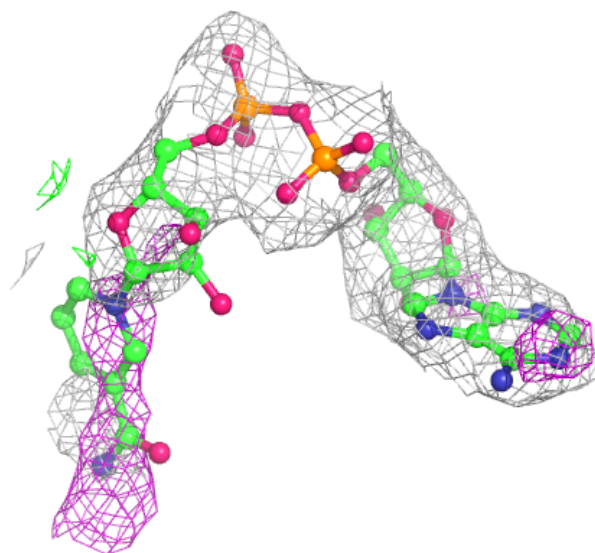
**Electron density around N4Q B 702:**

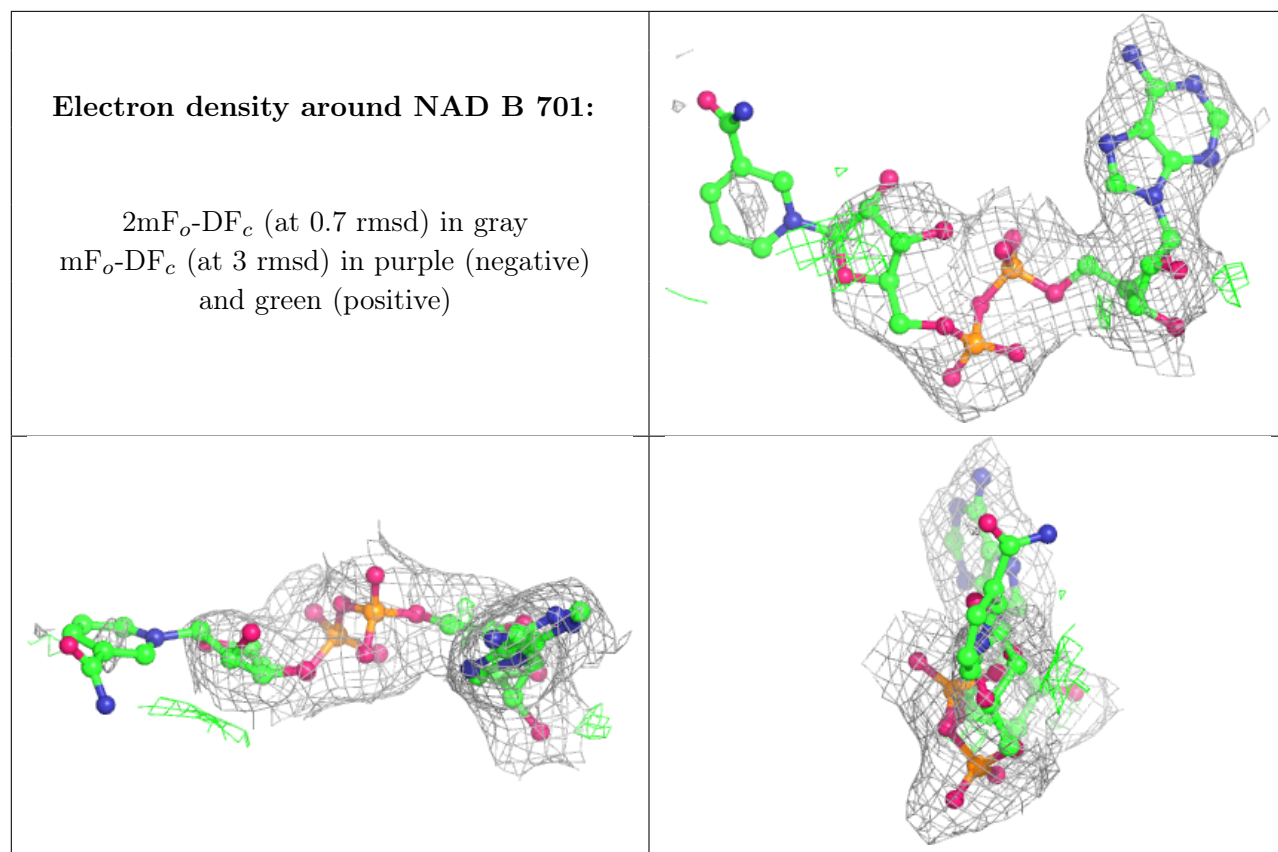
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAD A 601:

$2mF_o-DF_c$ (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.