



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2021 – 05:11 PM GMT

PDB ID : 7A6Q  
Title : Crystal structure of human aldehyde dehydrogenase 1A3 in complex with selective NR6 inhibitor compound  
Authors : Gelardi, E.L.M.; Garavaglia, S.  
Deposited on : 2020-08-26  
Resolution : 2.95 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](mailto: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.

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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

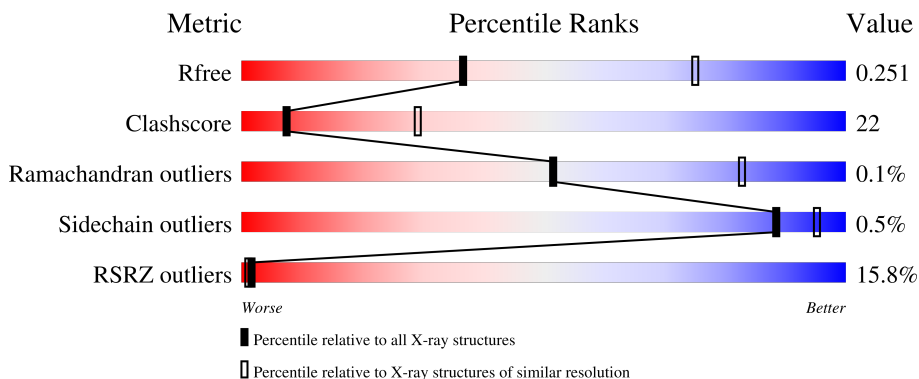
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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  $\geq 3$ , 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	
1	B	512	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	NA	A	603	-	-	-	X
4	NA	B	607	-	-	-	X
6	R2K	B	604	-	-	-	X

## 2 Entry composition [i](#)

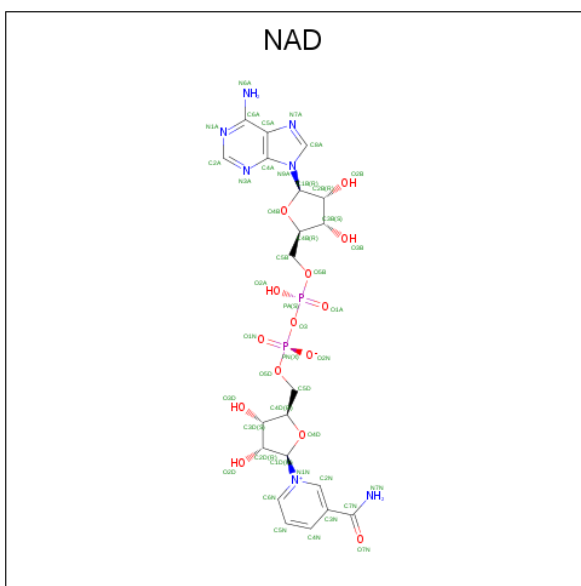
There are 7 unique types of molecules in this entry. The entry contains 7871 atoms, of which 84 are hydrogens and 0 are deuteriums.

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.

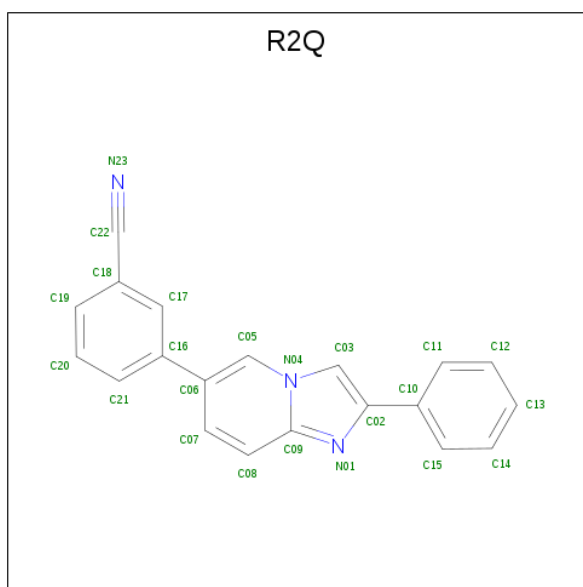
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	489	Total 3780	2410	646	704	20	0	0	0
1	B	489	Total 3780	2410	646	704	20	0	0	0

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

- Molecule 3 is 3-(2-phenylimidazo[1,2-a]pyridin-6-yl)benzenecarbonitrile (three-letter code: R2Q) (formula:  $C_{20}H_{13}N_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
3	A	1	36	20	13	3	0	0
3	B	1	36	20	13	3	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

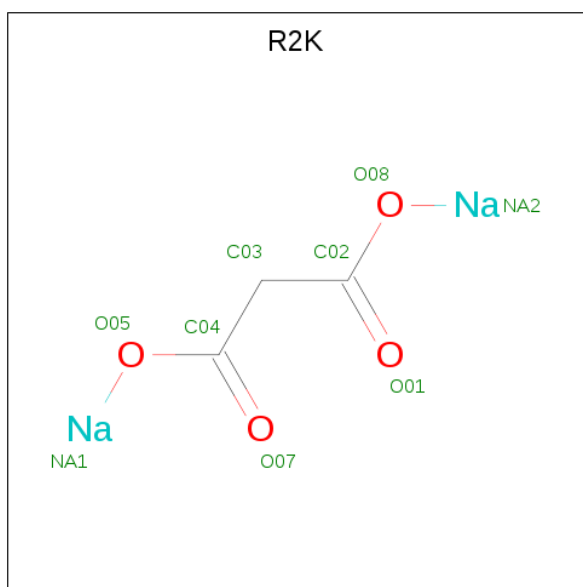
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	B	2	2	2	0	0
4	A	2	2	2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	14	3	8	3	0	0
5	A	1	14	3	8	3	0	0
5	A	1	14	3	8	3	0	0
5	A	1	14	3	8	3	0	0
5	A	1	14	3	8	3	0	0
5	B	1	14	3	8	3	0	0
5	B	1	14	3	8	3	0	0

- Molecule 6 is (3-oxidanylidene-3-sodiooxy-propanoyl)oxysodium (three-letter code: R2K) (formula:  $C_3H_2Na_2O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	Na	O		
6	B	1	11	3	2	2	4	0	0

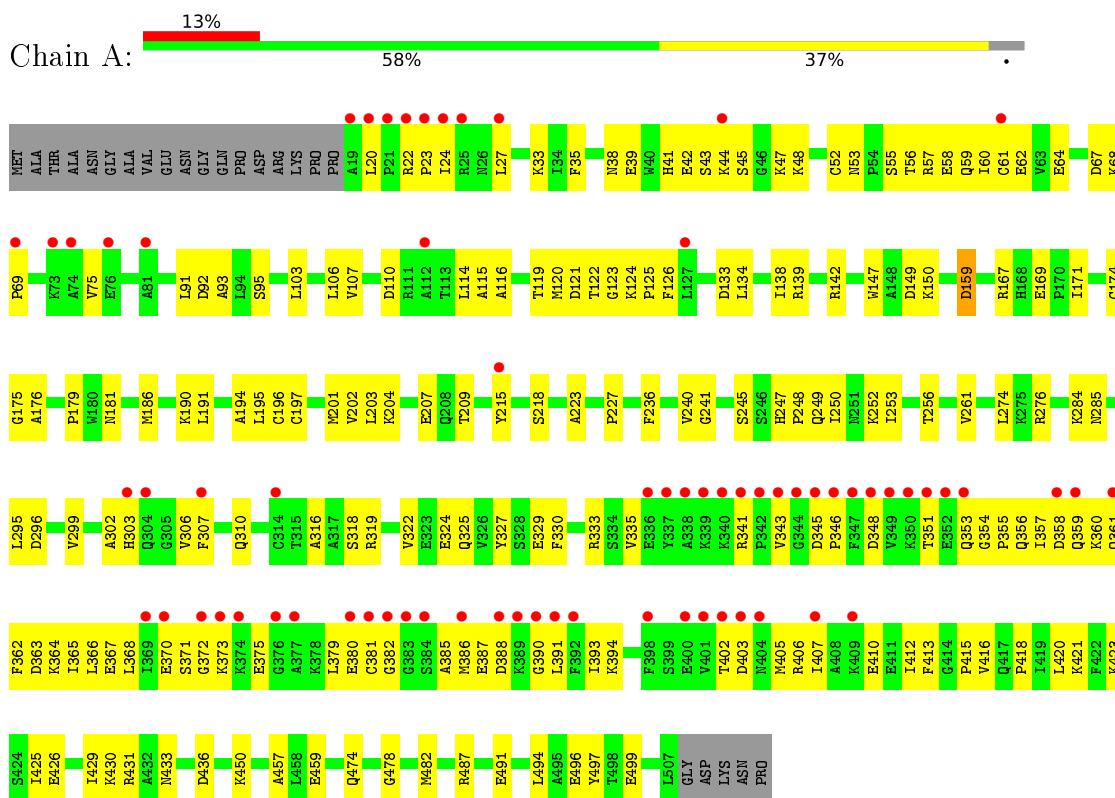
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	23	Total	O	0	0
			23	23		
7	B	15	Total	O	0	0
			15	15		

### 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.

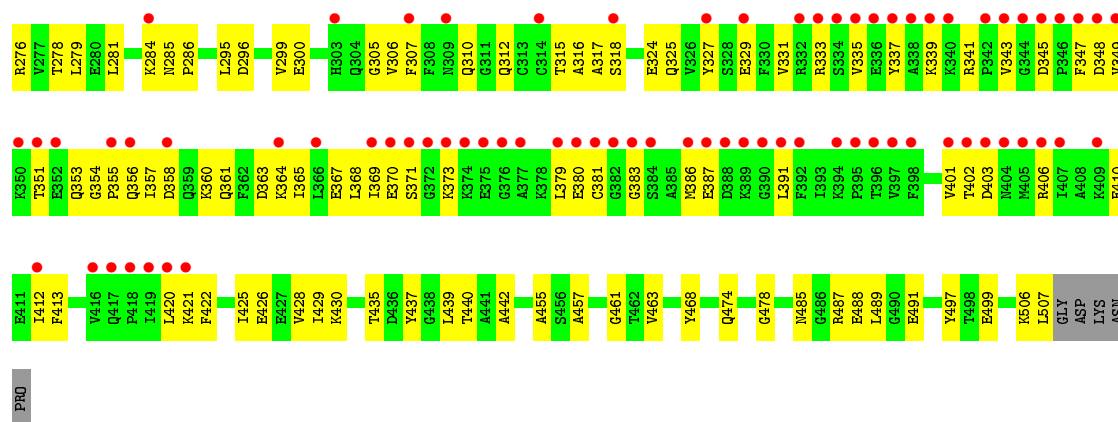
- Molecule 1: Aldehyde dehydrogenase family 1 member A3



- Molecule 1: Aldehyde dehydrogenase family 1 member A3







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.16Å 89.51Å 158.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.32 – 2.95 48.32 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.32-2.95) 99.6 (48.32-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.96Å)	Xtrriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, $R_{free}$	0.194 , 0.250 0.194 , 0.251	Depositor DCC
$R_{free}$ test set	1306 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.4	Xtrriage
Anisotropy	0.361	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 75.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7871	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, R2K, R2Q, NAD, NA

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	0.32	0/3858	0.49	0/5221
1	B	0.32	0/3858	0.48	0/5221
All	All	0.32	0/7716	0.49	0/10442

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3780	0	3813	181	3
1	B	3780	0	3813	154	0
2	A	44	0	24	10	0
2	B	44	0	24	3	2
3	A	23	13	0	1	0
3	B	23	13	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	30	40	40	3	0
5	B	12	16	16	1	0
6	B	9	2	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	23	0	0	1	0
7	B	15	0	0	8	0
All	All	7787	84	7730	343	3

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 22.

All (343) 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)
2:A:601:NAD:C1D	2:A:601:NAD:O4D	1.63	1.20
1:A:382:GLY:HA2	1:A:394:LYS:HD2	1.34	1.08
1:A:119:THR:HG21	1:A:126:PHE:HA	1.39	1.05
1:A:341:ARG:HH12	1:A:353:GLN:HB2	1.28	0.97
1:A:121:ASP:OD2	1:A:209:THR:HA	1.66	0.95
1:A:44:LYS:HD3	1:A:69:PRO:HG2	1.50	0.94
1:A:44:LYS:CD	1:A:69:PRO:CB	2.50	0.89
1:A:310:GLN:HE21	1:A:354:GLY:H	1.17	0.88
1:A:24:ILE:HG23	1:A:27:LEU:HD13	1.54	0.87
1:B:178:THR:HG22	1:B:190:LYS:HE2	1.55	0.87
1:A:406:ARG:NH1	1:A:410:GLU:OE2	2.10	0.85
1:A:412:ILE:HG21	1:A:416:VAL:HG12	1.58	0.85
1:A:44:LYS:HD3	1:A:69:PRO:CG	2.06	0.84
1:A:44:LYS:HD2	1:A:69:PRO:CB	2.06	0.84
1:A:412:ILE:HG21	1:A:416:VAL:CG1	2.09	0.83
1:B:127:LEU:HD11	1:B:349:VAL:HG13	1.60	0.82
1:B:339:LYS:HE2	1:B:381:CYS:HA	1.61	0.81
1:A:284:LYS:HG3	1:A:319:ARG:HD2	1.62	0.80
1:B:363:ASP:O	1:B:367:GLU:HG2	1.82	0.80
1:A:44:LYS:HD3	1:A:69:PRO:CB	2.12	0.79
1:A:363:ASP:O	1:A:367:GLU:HG2	1.84	0.78
1:B:122:THR:HG22	1:B:209:THR:HG21	1.63	0.78
1:B:180:TRP:CE3	1:B:357:ILE:HD13	2.20	0.77
1:B:23:PRO:HB2	1:B:347:PHE:HD2	1.49	0.76
1:B:341:ARG:NH1	1:B:353:GLN:HB2	2.00	0.76
1:A:44:LYS:HD2	1:A:69:PRO:HB3	1.66	0.76
1:A:364:LYS:HE3	1:A:413:PHE:CZ	2.21	0.76
1:A:24:ILE:HG21	1:A:27:LEU:HD22	1.68	0.75
1:B:30:LYS:NZ	7:B:702:HOH:O	2.18	0.75
1:A:91:LEU:HD22	1:A:95:SER:HB2	1.70	0.74
1:A:124:LYS:NZ	1:A:133:ASP:OD2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HD13	1:A:27:LEU:HD22	1.71	0.72
1:A:119:THR:CG2	1:A:126:PHE:HA	2.18	0.72
1:A:348:ASP:O	1:A:351:THR:HG22	1.90	0.72
1:B:296:ASP:OD1	1:B:333:ARG:NH2	2.21	0.72
1:A:425:ILE:HD11	1:A:450:LYS:HD2	1.71	0.71
1:A:360:LYS:O	1:A:364:LYS:HG2	1.91	0.71
1:A:299:VAL:HG12	1:A:330:PHE:CD1	2.26	0.71
1:A:412:ILE:HD13	1:A:416:VAL:HG13	1.73	0.71
1:A:284:LYS:HE2	1:A:410:GLU:O	1.91	0.70
1:A:245:SER:HA	1:A:253:ILE:HD12	1.72	0.70
1:A:382:GLY:CA	1:A:394:LYS:HD2	2.17	0.70
1:B:348:ASP:O	1:B:351:THR:HG22	1.92	0.70
1:B:35:PHE:CZ	1:B:38:ASN:HA	2.27	0.70
1:A:122:THR:HG22	1:A:209:THR:HG21	1.73	0.69
1:B:71:VAL:HG21	1:B:243:ALA:HB1	1.75	0.68
1:A:310:GLN:HE21	1:A:354:GLY:N	1.91	0.68
1:B:401:VAL:HG23	1:B:420:LEU:HG	1.74	0.68
1:A:119:THR:HG21	1:A:126:PHE:CA	2.19	0.68
1:A:299:VAL:HG12	1:A:330:PHE:CE1	2.30	0.67
1:A:44:LYS:CD	1:A:69:PRO:HB2	2.25	0.67
1:B:22:ARG:HB2	1:B:23:PRO:HD2	1.76	0.67
1:A:310:GLN:HG3	1:A:353:GLN:HG3	1.75	0.67
1:A:44:LYS:HD2	1:A:69:PRO:HB2	1.76	0.67
1:A:295:LEU:O	1:A:299:VAL:HG13	1.95	0.66
1:B:343:VAL:HG22	1:B:353:GLN:HB3	1.76	0.66
1:A:176:ALA:HB3	1:A:203:LEU:HD22	1.78	0.66
1:B:167:ARG:NH1	1:B:169:GLU:OE2	2.29	0.66
1:B:178:THR:CG2	1:B:190:LYS:HE2	2.25	0.65
1:B:345:ASP:O	1:B:351:THR:HG21	1.95	0.65
1:A:252:LYS:HE3	1:A:496:GLU:O	1.97	0.65
1:A:35:PHE:CZ	1:A:38:ASN:HA	2.32	0.65
1:B:187:LEU:HD11	1:B:203:LEU:HD13	1.79	0.64
1:A:91:LEU:HD22	1:A:95:SER:CB	2.27	0.64
1:A:24:ILE:CG2	1:A:27:LEU:HD22	2.29	0.63
1:A:44:LYS:CD	1:A:69:PRO:HB3	2.22	0.63
1:B:402:THR:HG22	1:B:403:ASP:H	1.63	0.63
1:B:68:LYS:O	1:B:71:VAL:HG22	1.98	0.63
1:B:44:LYS:NZ	1:B:73:LYS:HE3	2.13	0.63
1:B:360:LYS:O	1:B:364:LYS:HG2	1.99	0.62
1:A:307:PHE:O	1:A:341:ARG:NH2	2.31	0.62
1:A:341:ARG:NH1	1:A:353:GLN:HB2	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ALA:O	1:A:119:THR:HG23	2.01	0.61
1:A:335:VAL:HG13	1:A:381:CYS:SG	2.41	0.60
1:A:379:LEU:HD23	1:A:380:GLU:N	2.15	0.60
1:B:103:LEU:O	1:B:107:VAL:HG23	2.01	0.60
1:B:295:LEU:O	1:B:299:VAL:HG23	2.02	0.60
1:A:116:ALA:O	1:A:120:MET:HG3	2.01	0.60
1:B:115:ALA:O	1:B:119:THR:HG22	2.02	0.60
1:A:24:ILE:CG2	1:A:27:LEU:HD13	2.31	0.59
1:B:178:THR:HG22	1:B:190:LYS:CE	2.31	0.59
1:B:75:VAL:HG22	1:B:250:ILE:HD11	1.84	0.59
1:B:27:LEU:HD21	7:B:702:HOH:O	2.00	0.59
1:A:207:GLU:CG	1:A:236:PHE:HA	2.31	0.59
1:B:327:TYR:CE2	1:B:421:LYS:HB2	2.37	0.59
1:A:20:LEU:HD12	1:A:20:LEU:O	2.03	0.59
1:B:341:ARG:HH12	1:B:353:GLN:HB2	1.67	0.59
1:B:39:GLU:HB2	1:B:41:HIS:HE1	1.67	0.59
1:B:402:THR:HG22	1:B:403:ASP:N	2.18	0.59
1:B:499:GLU:OE2	5:B:603:GOL:O2	2.21	0.58
1:A:121:ASP:OD2	1:A:209:THR:CA	2.47	0.58
1:B:285:ASN:HB2	1:B:316:ALA:O	2.03	0.58
1:B:91:LEU:HD22	1:B:95:SER:HB2	1.85	0.58
1:B:55:SER:HB3	1:B:355:PRO:HG3	1.84	0.58
1:A:285:ASN:HB2	1:A:316:ALA:O	2.04	0.57
1:A:478:GLY:HA3	1:A:487:ARG:HD3	1.84	0.57
1:A:207:GLU:HG2	1:A:236:PHE:CD2	2.39	0.57
1:A:48:LYS:HE3	1:A:64:GLU:OE2	2.05	0.57
1:B:23:PRO:CB	1:B:347:PHE:HD2	2.14	0.57
1:A:372:GLY:HA3	1:A:407:ILE:HG21	1.86	0.57
1:B:360:LYS:HG2	2:B:601:NAD:H5N	1.85	0.56
1:A:121:ASP:CG	1:A:209:THR:HA	2.24	0.56
1:B:284:LYS:NZ	1:B:318:SER:HB3	2.19	0.56
1:A:303:HIS:CE1	1:A:341:ARG:HD2	2.41	0.56
1:A:284:LYS:CG	1:A:319:ARG:HD2	2.33	0.56
1:B:252:LYS:HG2	1:B:253:ILE:N	2.20	0.56
1:B:335:VAL:HG13	1:B:381:CYS:SG	2.46	0.56
1:A:360:LYS:CG	2:A:601:NAD:H5N	2.36	0.56
1:A:366:LEU:HG	1:A:370:GLU:OE2	2.05	0.56
1:B:20:LEU:HD12	1:B:20:LEU:O	2.06	0.55
1:B:318:SER:OG	1:B:412:ILE:HG12	2.06	0.55
1:A:361:GLN:O	1:A:365:ILE:HG13	2.07	0.55
1:A:39:GLU:HB2	1:A:41:HIS:HE1	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:CYS:HA	1:A:60:ILE:H	1.70	0.55
5:A:608:GOL:H32	5:A:609:GOL:O3	2.06	0.55
1:A:67:ASP:OD1	1:A:68:LYS:N	2.34	0.55
1:B:118:GLU:OE2	1:B:183:PRO:HD2	2.07	0.55
1:A:35:PHE:HZ	1:A:38:ASN:HD22	1.55	0.55
1:B:116:ALA:O	1:B:120:MET:HG3	2.07	0.55
1:B:91:LEU:HD22	1:B:95:SER:CB	2.37	0.55
1:B:325:GLN:OE1	1:B:325:GLN:N	2.39	0.54
1:B:478:GLY:HA3	1:B:487:ARG:HD3	1.90	0.54
1:A:403:ASP:OD1	1:A:431:ARG:NH2	2.39	0.54
1:B:259:THR:HA	1:B:281:LEU:HD13	1.90	0.54
1:A:362:PHE:CD1	1:A:393:ILE:HD11	2.43	0.54
1:A:57:ARG:HH11	1:A:390:GLY:HA2	1.72	0.54
1:B:29:VAL:HG21	1:B:61:CYS:SG	2.48	0.54
1:A:426:GLU:OE1	1:B:84:ARG:NH2	2.40	0.53
1:B:147:TRP:CZ2	1:B:491:GLU:HB2	2.43	0.53
1:B:124:LYS:HE3	1:B:133:ASP:OD2	2.08	0.53
1:A:325:GLN:N	1:A:325:GLN:OE1	2.37	0.53
1:B:426:GLU:HG3	1:B:430:LYS:HE3	1.90	0.53
1:A:249:GLN:HA	1:A:249:GLN:OE1	2.09	0.53
1:B:176:ALA:HB3	1:B:203:LEU:HD22	1.90	0.53
1:B:357:ILE:HG23	1:B:361:GLN:HB2	1.90	0.53
1:A:402:THR:HG22	1:A:403:ASP:N	2.23	0.53
1:B:259:THR:O	1:B:263:LYS:HG3	2.09	0.52
1:B:185:LEU:HD11	7:B:704:HOH:O	2.08	0.52
1:A:345:ASP:O	1:A:351:THR:HG21	2.09	0.52
1:A:360:LYS:HG2	2:A:601:NAD:C5N	2.40	0.52
1:A:167:ARG:NH1	1:A:169:GLU:OE2	2.43	0.52
1:B:506:LYS:O	1:B:507:LEU:HD23	2.10	0.52
1:A:296:ASP:O	1:A:299:VAL:HG22	2.10	0.52
1:B:207:GLU:CG	1:B:236:PHE:HA	2.40	0.52
1:A:364:LYS:HE3	1:A:413:PHE:CE1	2.45	0.52
1:B:357:ILE:CG2	1:B:361:GLN:HB2	2.39	0.52
1:B:361:GLN:O	1:B:365:ILE:HG13	2.10	0.52
1:B:138:ILE:O	1:B:142:ARG:HG2	2.10	0.52
1:B:386:MET:O	1:B:387:GLU:HG3	2.10	0.51
1:A:429:ILE:HD13	1:A:457:ALA:CB	2.40	0.51
1:A:245:SER:HA	1:A:253:ILE:CD1	2.38	0.51
1:A:356:GLN:HG2	1:A:391:LEU:O	2.10	0.51
3:A:602:R2Q:C22	7:A:705:HOH:O	2.59	0.51
1:A:147:TRP:CZ2	1:A:491:GLU:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:O	1:B:220:ILE:HG13	2.10	0.51
1:B:285:ASN:ND2	1:B:315:THR:HA	2.25	0.51
1:B:442:ALA:HB2	1:B:468:TYR:CD1	2.45	0.51
1:B:327:TYR:CD2	1:B:421:LYS:HB2	2.46	0.51
1:A:345:ASP:HB3	1:A:348:ASP:HB2	1.92	0.51
1:A:420:LEU:HD23	1:A:431:ARG:NH2	2.25	0.51
1:B:71:VAL:HG21	1:B:243:ALA:CB	2.40	0.51
1:A:360:LYS:HG2	2:A:601:NAD:H5N	1.92	0.51
1:B:207:GLU:HG2	1:B:236:PHE:CD2	2.46	0.51
1:B:51:THR:HA	6:B:604:R2K:O01	2.11	0.50
1:A:45:SER:OG	1:A:47:LYS:HG3	2.11	0.50
1:B:310:GLN:HE21	1:B:354:GLY:H	1.60	0.50
1:A:171:ILE:HG13	1:A:497:TYR:C	2.32	0.50
1:B:485:ASN:HB2	7:B:701:HOH:O	2.11	0.50
1:A:204:LYS:HD2	1:A:240:VAL:HG12	1.92	0.50
1:A:284:LYS:NZ	1:A:318:SER:HB3	2.26	0.50
1:A:362:PHE:HZ	1:A:385:ALA:HB2	1.77	0.50
1:B:139:ARG:NH2	1:B:474:GLN:HE22	2.09	0.50
1:B:67:ASP:OD1	1:B:68:LYS:N	2.37	0.50
1:A:138:ILE:O	1:A:142:ARG:HG2	2.12	0.50
1:A:139:ARG:HH21	1:A:474:GLN:HE22	1.59	0.50
2:A:601:NAD:H62A	5:A:605:GOL:H32	1.75	0.50
1:A:93:ALA:HB1	1:A:149:ASP:HA	1.94	0.50
1:B:27:LEU:HD11	7:B:702:HOH:O	2.11	0.50
1:B:179:PRO:HG3	1:B:256:THR:HG22	1.94	0.49
1:B:39:GLU:HB2	1:B:41:HIS:CE1	2.46	0.49
1:A:261:VAL:HG21	2:A:601:NAD:O1A	2.12	0.49
1:B:284:LYS:HE2	1:B:410:GLU:O	2.12	0.49
1:B:329:GLU:HA	1:B:329:GLU:OE1	2.12	0.49
1:B:53:ASN:HB3	1:B:56:THR:OG1	2.12	0.49
1:A:191:LEU:HD21	1:A:195:LEU:HD12	1.93	0.49
1:B:247:HIS:HB3	1:B:250:ILE:CG1	2.42	0.49
1:B:215:TYR:O	1:B:218:SER:OG	2.22	0.49
1:B:327:TYR:O	1:B:331:VAL:HG23	2.11	0.49
1:A:33:LYS:HB3	1:A:41:HIS:O	2.13	0.49
1:A:61:CYS:SG	1:A:62:GLU:N	2.85	0.49
1:B:356:GLN:HG2	1:B:391:LEU:O	2.12	0.49
1:A:174:CYS:O	1:A:201:MET:HA	2.12	0.49
1:B:179:PRO:HG2	1:B:181:ASN:OD1	2.12	0.49
1:B:439:LEU:HG	1:B:440:THR:HG23	1.94	0.49
1:B:111:ARG:HG2	1:B:130:PHE:CE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:VAL:HG13	1:B:307:PHE:CD2	2.47	0.48
1:B:171:ILE:HG13	1:B:497:TYR:C	2.32	0.48
1:A:357:ILE:HG23	1:A:358:ASP:H	1.78	0.48
1:B:379:LEU:HD23	1:B:380:GLU:N	2.28	0.48
1:A:343:VAL:O	1:A:343:VAL:HG13	2.13	0.48
1:B:357:ILE:HG23	1:B:358:ASP:H	1.78	0.48
1:A:436:ASP:HB3	1:A:482:MET:CE	2.43	0.48
1:B:247:HIS:HB3	1:B:250:ILE:HG12	1.95	0.48
1:B:61:CYS:SG	1:B:62:GLU:N	2.87	0.48
1:B:44:LYS:HZ2	1:B:73:LYS:HE3	1.79	0.48
1:A:284:LYS:HD2	1:A:318:SER:CB	2.43	0.48
1:B:406:ARG:NH1	1:B:410:GLU:OE2	2.47	0.48
1:B:278:THR:HA	7:B:701:HOH:O	2.15	0.47
1:B:305:GLY:HA3	1:B:468:TYR:CD2	2.49	0.47
1:A:420:LEU:HD12	1:A:420:LEU:N	2.28	0.47
1:B:43:SER:N	1:B:64:GLU:OE2	2.32	0.47
1:A:24:ILE:HG23	1:A:27:LEU:CD1	2.37	0.47
1:A:386:MET:O	1:A:387:GLU:HG3	2.14	0.47
1:A:75:VAL:HG21	1:A:247:HIS:CD2	2.49	0.47
1:A:329:GLU:HG3	1:A:333:ARG:HD2	1.97	0.47
1:A:368:LEU:HD12	1:A:371:SER:HB3	1.97	0.47
1:A:247:HIS:ND1	1:A:248:PRO:HD2	2.30	0.47
1:B:420:LEU:N	1:B:420:LEU:HD12	2.29	0.47
1:B:261:VAL:O	1:B:265:VAL:HG23	2.14	0.47
1:B:286:PRO:HD2	1:B:440:THR:O	2.15	0.47
1:A:179:PRO:HG2	1:A:181:ASN:OD1	2.15	0.46
1:A:412:ILE:O	1:A:413:PHE:CG	2.67	0.46
1:B:33:LYS:O	1:B:214:LEU:HD22	2.15	0.46
1:B:461:GLY:HA3	1:B:478:GLY:O	2.16	0.46
1:A:60:ILE:HD11	1:A:120:MET:O	2.14	0.46
1:A:284:LYS:HG3	1:A:319:ARG:CD	2.40	0.46
1:A:56:THR:HG22	1:A:58:GLU:HB3	1.98	0.46
1:A:92:ASP:HB2	1:A:95:SER:OG	2.15	0.46
1:B:149:ASP:OD1	1:B:150:LYS:HG3	2.14	0.46
1:A:186:MET:HE2	1:A:256:THR:HG21	1.97	0.46
1:A:207:GLU:HG3	1:A:236:PHE:HA	1.98	0.46
1:A:368:LEU:HA	1:A:371:SER:HB3	1.97	0.46
1:B:184:LEU:O	1:B:188:VAL:HG23	2.16	0.46
1:A:247:HIS:HB3	1:A:250:ILE:HG13	1.98	0.46
1:A:22:ARG:HB2	1:A:23:PRO:HD2	1.98	0.46
1:A:402:THR:HG22	1:A:403:ASP:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:CYS:SG	1:A:494:LEU:HD22	2.56	0.46
1:B:324:GLU:HG3	1:B:325:GLN:OE1	2.16	0.46
1:B:368:LEU:HA	1:B:371:SER:HB3	1.97	0.46
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.84	0.45
1:A:362:PHE:HD1	1:A:393:ILE:HD11	1.78	0.45
1:B:357:ILE:HG21	1:B:361:GLN:HG2	1.98	0.45
1:A:302:ALA:O	1:A:306:VAL:HG23	2.15	0.45
1:A:364:LYS:CE	1:A:413:PHE:CZ	2.96	0.45
1:B:412:ILE:O	1:B:413:PHE:CG	2.70	0.45
1:A:329:GLU:O	1:A:333:ARG:HG3	2.16	0.45
1:A:318:SER:O	1:A:418:PRO:HG2	2.17	0.45
1:A:124:LYS:HG2	1:A:125:PRO:HD2	1.98	0.45
1:A:194:ALA:HB2	1:A:497:TYR:CE1	2.52	0.45
1:A:103:LEU:O	1:A:107:VAL:HG23	2.17	0.45
1:A:176:ALA:HB1	1:A:190:LYS:HD2	1.99	0.45
1:A:241:GLY:HA3	2:A:601:NAD:C2A	2.46	0.45
2:A:601:NAD:H62A	5:A:605:GOL:C3	2.30	0.45
1:A:42:GLU:HG2	1:A:43:SER:N	2.32	0.45
1:A:106:LEU:HD12	1:A:223:ALA:HB2	1.97	0.44
1:A:296:ASP:OD1	1:A:333:ARG:NH2	2.34	0.44
1:A:53:ASN:N	1:A:60:ILE:HG13	2.32	0.44
1:B:255:PHE:HB3	1:B:279:LEU:HD23	2.00	0.44
1:B:52:CYS:HA	1:B:60:ILE:H	1.81	0.44
1:B:422:PHE:CD2	1:B:428:VAL:HB	2.52	0.44
1:A:276:ARG:N	1:A:276:ARG:CD	2.80	0.44
1:B:253:ILE:HD12	1:B:253:ILE:HA	1.87	0.44
1:B:329:GLU:O	1:B:333:ARG:HG3	2.17	0.44
1:B:369:ILE:HG21	1:B:383:GLY:HA2	2.00	0.44
1:B:425:ILE:O	1:B:428:VAL:HG12	2.18	0.44
1:A:436:ASP:HB3	1:A:482:MET:HE2	1.98	0.44
1:A:499:GLU:OE1	1:B:487:ARG:NH2	2.50	0.44
1:A:364:LYS:HG3	1:A:413:PHE:CZ	2.53	0.44
1:B:429:ILE:HD13	1:B:457:ALA:CB	2.47	0.44
1:A:433:ASN:ND2	1:A:459:GLU:HG3	2.33	0.43
1:B:191:LEU:HD21	1:B:195:LEU:HD12	1.99	0.43
1:B:279:LEU:HD12	1:B:485:ASN:OD1	2.18	0.43
1:A:114:LEU:HD21	1:A:215:TYR:CD1	2.53	0.43
1:A:359:GLN:OE1	1:A:391:LEU:HD21	2.18	0.43
1:B:75:VAL:CG2	1:B:250:ILE:HD11	2.47	0.43
1:A:426:GLU:O	1:A:430:LYS:HG3	2.19	0.43
1:B:276:ARG:CD	1:B:276:ARG:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:R2Q:C22	7:B:704:HOH:O	2.67	0.43
1:B:93:ALA:HB1	1:B:149:ASP:HA	2.01	0.43
1:B:114:LEU:HD21	1:B:215:TYR:CD1	2.52	0.43
1:A:191:LEU:HD23	1:A:191:LEU:C	2.39	0.43
1:A:307:PHE:HD1	1:A:415:PRO:HB3	1.84	0.43
1:A:364:LYS:CD	1:A:413:PHE:HZ	2.31	0.43
1:B:191:LEU:C	1:B:191:LEU:HD23	2.39	0.42
1:B:247:HIS:CE1	1:B:249:GLN:HB2	2.54	0.42
1:B:284:LYS:HZ2	1:B:318:SER:HB3	1.84	0.42
1:B:33:LYS:HB3	1:B:41:HIS:O	2.18	0.42
1:A:370:GLU:HA	1:A:373:LYS:HG2	2.01	0.42
1:B:357:ILE:CG2	1:B:361:GLN:CB	2.97	0.42
1:B:435:THR:HG23	1:B:437:TYR:O	2.18	0.42
1:A:149:ASP:OD1	1:A:150:LYS:HG3	2.18	0.42
1:A:207:GLU:HG2	1:A:236:PHE:CG	2.54	0.42
1:A:425:ILE:O	1:A:429:ILE:HG13	2.19	0.42
1:B:175:GLY:HA2	1:B:202:VAL:O	2.19	0.42
1:B:370:GLU:HA	1:B:373:LYS:HG2	2.01	0.42
1:A:175:GLY:HA2	1:A:202:VAL:O	2.20	0.42
1:A:38:ASN:OD1	1:A:227:PRO:HA	2.19	0.42
1:A:75:VAL:HG11	1:A:247:HIS:CE1	2.55	0.42
1:B:195:LEU:HD23	1:B:195:LEU:HA	1.74	0.42
1:B:71:VAL:CG1	1:B:240:VAL:HG13	2.50	0.42
1:B:412:ILE:HG13	1:B:413:PHE:H	1.84	0.42
2:B:601:NAD:H2D	2:B:601:NAD:H6N	1.59	0.42
2:B:601:NAD:H2B	2:B:601:NAD:H8A	1.98	0.42
1:A:284:LYS:HZ2	1:A:318:SER:HB3	1.84	0.42
1:A:134:LEU:O	1:A:138:ILE:HG13	2.20	0.42
1:B:152:GLN:NE2	7:B:705:HOH:O	2.50	0.42
1:A:345:ASP:OD1	1:A:346:PRO:HD2	2.20	0.41
1:A:123:GLY:O	1:A:355:PRO:HD2	2.19	0.41
1:A:324:GLU:OE1	1:A:423:LYS:HE3	2.20	0.41
2:A:601:NAD:H4D	2:A:601:NAD:O2A	2.20	0.41
1:B:60:ILE:HD11	1:B:120:MET:O	2.20	0.41
1:B:122:THR:HG22	1:B:209:THR:CG2	2.42	0.41
1:A:322:VAL:HG21	1:A:330:PHE:CD2	2.54	0.41
1:A:357:ILE:HG23	1:A:358:ASP:N	2.35	0.41
1:A:42:GLU:HG3	1:A:64:GLU:OE1	2.20	0.41
1:A:68:LYS:HB3	1:A:69:PRO:HD3	2.03	0.41
1:B:207:GLU:HG3	1:B:236:PHE:HA	2.02	0.41
1:B:300:GLU:HG3	1:B:337:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ALA:HB2	1:B:468:TYR:CE1	2.55	0.41
1:A:284:LYS:HE2	1:A:410:GLU:C	2.40	0.41
1:A:375:GLU:OE1	1:A:405:MET:HB3	2.21	0.41
1:A:55:SER:OG	1:A:346:PRO:HG2	2.20	0.41
1:A:33:LYS:HA	1:A:64:GLU:CG	2.51	0.41
1:A:191:LEU:CD2	1:A:195:LEU:HD12	2.50	0.41
1:B:124:LYS:HB2	1:B:124:LYS:HE2	1.85	0.41
1:B:312:GLN:HG2	1:B:413:PHE:O	2.20	0.41
1:A:56:THR:HG22	1:A:58:GLU:CB	2.50	0.41
1:B:306:VAL:HG23	1:B:317:ALA:O	2.21	0.41
1:B:34:ILE:HG12	1:B:234:PRO:HD2	2.03	0.41
1:B:247:HIS:ND1	1:B:248:PRO:HD2	2.36	0.41
1:B:180:TRP:CD2	1:B:357:ILE:HD13	2.55	0.41
1:B:488:GLU:O	1:B:489:LEU:HB2	2.20	0.41
2:A:601:NAD:H2B	2:A:601:NAD:H8A	1.89	0.41
1:B:176:ALA:HB1	1:B:190:LYS:HD2	2.03	0.41
1:A:215:TYR:O	1:A:218:SER:OG	2.25	0.41
1:A:327:TYR:CE1	1:A:421:LYS:HB2	2.56	0.40
1:A:412:ILE:HD13	1:A:416:VAL:CG1	2.45	0.40
1:A:58:GLU:HG2	1:A:59:GLN:N	2.37	0.40
1:A:44:LYS:CD	1:A:69:PRO:CG	2.85	0.40
1:A:110:ASP:N	1:A:110:ASP:OD1	2.53	0.40
1:A:366:LEU:O	1:A:370:GLU:HG3	2.20	0.40
1:B:181:ASN:N	1:B:181:ASN:OD1	2.54	0.40
1:B:455:ALA:HA	1:B:463:VAL:HG11	2.03	0.40

All (3) 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:388:ASP:CB	2:B:601:NAD:O7N[3_544]	2.01	0.19
1:A:388:ASP:C	2:B:601:NAD:O7N[3_544]	2.01	0.19
1:A:92:ASP:OD1	1:A:159:ASP:OD1[2_555]	2.09	0.11

## 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	487/512 (95%)	459 (94%)	28 (6%)	0	100	100
1	B	487/512 (95%)	460 (94%)	26 (5%)	1 (0%)	47	79
All	All	974/1024 (95%)	919 (94%)	54 (6%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	179	PRO

### 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	405/422 (96%)	403 (100%)	2 (0%)	88	95
1	B	405/422 (96%)	403 (100%)	2 (0%)	88	95
All	All	810/844 (96%)	806 (100%)	4 (0%)	88	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	ASP
1	A	196	CYS
1	B	159	ASP
1	B	196	CYS

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	41	HIS
1	A	303	HIS

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Mol	Chain	Res	Type
1	A	304	GLN
1	A	310	GLN
1	B	310	GLN

### 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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	GOL	A	605	-	5,5,5	0.85	0	5,5,5	0.97	0
5	GOL	B	605	-	5,5,5	0.85	0	5,5,5	1.02	1 (20%)
5	GOL	B	603	-	5,5,5	1.13	0	5,5,5	1.25	1 (20%)
5	GOL	A	609	-	5,5,5	0.90	0	5,5,5	1.23	1 (20%)
2	NAD	B	601	1	42,48,48	5.52	17 (40%)	50,73,73	1.97	6 (12%)
3	R2Q	B	602	-	23,26,26	1.92	4 (17%)	28,36,36	1.70	7 (25%)
5	GOL	A	604	-	5,5,5	0.87	0	5,5,5	0.89	0
5	GOL	A	608	-	5,5,5	0.85	0	5,5,5	0.67	0
3	R2Q	A	602	-	23,26,26	1.91	4 (17%)	28,36,36	1.66	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	A	601	-	42,48,48	5.57	17 (40%)	50,73,73	1.71	6 (12%)
5	GOL	A	606	-	5,5,5	0.84	0	5,5,5	1.15	1 (20%)
6	R2K	B	604	1	4,8,8	1.33	0	3,9,9	1.38	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	605	-	-	2/4/4/4	-
5	GOL	B	605	-	-	0/4/4/4	-
5	GOL	B	603	-	-	2/4/4/4	-
5	GOL	A	609	-	-	2/4/4/4	-
2	NAD	B	601	1	-	16/26/62/62	0/5/5/5
3	R2Q	B	602	-	-	0/10/10/10	0/4/4/4
5	GOL	A	604	-	-	0/4/4/4	-
5	GOL	A	608	-	-	4/4/4/4	-
3	R2Q	A	602	-	-	0/10/10/10	0/4/4/4
2	NAD	A	601	-	-	13/26/62/62	0/5/5/5
5	GOL	A	606	-	-	0/4/4/4	-
6	R2K	B	604	1	-	0/4/8/8	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAD	C2D-C1D	-16.72	1.28	1.53
2	A	601	NAD	C2D-C1D	-16.62	1.28	1.53
2	A	601	NAD	C2B-C1B	-16.51	1.28	1.53
2	A	601	NAD	O4D-C1D	16.26	1.63	1.41
2	B	601	NAD	C2B-C1B	-16.05	1.29	1.53
2	B	601	NAD	O4D-C1D	15.84	1.63	1.41
2	B	601	NAD	O4B-C1B	15.04	1.62	1.41
2	A	601	NAD	O4B-C1B	14.90	1.61	1.41
2	A	601	NAD	C7N-N7N	7.25	1.46	1.33
2	B	601	NAD	C7N-N7N	7.22	1.46	1.33
3	B	602	R2Q	C09-N01	7.19	1.40	1.33
3	A	602	R2Q	C09-N01	7.05	1.40	1.33
2	A	601	NAD	O4D-C4D	-5.93	1.31	1.45
2	B	601	NAD	O4D-C4D	-5.91	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAD	O4B-C4B	-5.88	1.31	1.45
2	A	601	NAD	O4B-C4B	-5.84	1.31	1.45
2	A	601	NAD	O3D-C3D	-4.49	1.32	1.43
2	B	601	NAD	O3D-C3D	-4.46	1.32	1.43
2	A	601	NAD	O2B-C2B	4.28	1.53	1.43
2	A	601	NAD	C6A-N6A	4.24	1.49	1.34
2	B	601	NAD	C6A-N6A	4.13	1.49	1.34
2	B	601	NAD	O2B-C2B	4.12	1.52	1.43
2	B	601	NAD	O2D-C2D	3.85	1.52	1.43
2	A	601	NAD	O2D-C2D	3.82	1.52	1.43
3	A	602	R2Q	C18-C22	3.70	1.52	1.44
2	A	601	NAD	C2A-N3A	3.70	1.38	1.32
2	B	601	NAD	C2A-N3A	3.69	1.38	1.32
3	B	602	R2Q	C18-C22	3.48	1.52	1.44
2	B	601	NAD	C5D-C4D	3.29	1.61	1.51
2	A	601	NAD	C5D-C4D	3.16	1.61	1.51
2	B	601	NAD	O3B-C3B	-3.11	1.35	1.43
2	A	601	NAD	O3B-C3B	-3.03	1.35	1.43
3	A	602	R2Q	C08-C09	-2.57	1.37	1.40
3	B	602	R2Q	C08-C09	-2.51	1.37	1.40
2	B	601	NAD	PA-O5B	2.49	1.69	1.59
2	A	601	NAD	PA-O5B	2.43	1.69	1.59
3	A	602	R2Q	C10-C02	2.35	1.52	1.48
2	B	601	NAD	C2N-N1N	2.32	1.37	1.35
3	B	602	R2Q	C05-N04	-2.27	1.33	1.37
2	A	601	NAD	C2N-N1N	2.26	1.37	1.35
2	B	601	NAD	C5A-C4A	-2.05	1.35	1.40
2	A	601	NAD	C4N-C3N	-2.00	1.35	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAD	C5A-C6A-N6A	8.86	133.81	120.35
2	A	601	NAD	C5A-C6A-N6A	7.32	131.47	120.35
2	B	601	NAD	N6A-C6A-N1A	-6.26	105.58	118.57
3	A	602	R2Q	C02-C03-N04	5.80	113.80	107.89
3	B	602	R2Q	C02-C03-N04	5.57	113.56	107.89
2	B	601	NAD	N3A-C2A-N1A	-5.33	120.34	128.68
2	A	601	NAD	N3A-C2A-N1A	-5.09	120.72	128.68
2	A	601	NAD	N6A-C6A-N1A	-4.73	108.75	118.57
3	A	602	R2Q	C07-C06-C16	-3.06	116.05	121.36
2	A	601	NAD	C6N-N1N-C2N	-2.74	119.48	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	R2Q	C15-C10-C02	-2.70	117.02	121.28
3	B	602	R2Q	C15-C10-C02	-2.69	117.03	121.28
2	A	601	NAD	PN-O3-PA	-2.68	123.64	132.83
3	B	602	R2Q	C17-C16-C06	-2.53	116.67	120.86
5	A	609	GOL	C3-C2-C1	-2.53	101.85	111.70
2	B	601	NAD	PN-O3-PA	-2.48	124.31	132.83
2	B	601	NAD	C5B-C4B-C3B	-2.38	106.26	115.18
3	A	602	R2Q	C07-C08-C09	-2.21	117.08	119.76
3	B	602	R2Q	C07-C08-C09	-2.18	117.12	119.76
3	B	602	R2Q	C17-C18-C22	-2.17	116.65	119.54
5	B	603	GOL	C3-C2-C1	-2.16	103.30	111.70
3	B	602	R2Q	C07-C06-C16	-2.13	117.67	121.36
2	B	601	NAD	C4A-C5A-N7A	-2.12	107.19	109.40
6	B	604	R2K	O01-C02-C03	-2.12	118.52	124.24
3	B	602	R2Q	C21-C16-C17	2.11	121.15	118.16
2	A	601	NAD	C3N-C7N-N7N	2.07	120.24	117.75
5	B	605	GOL	C3-C2-C1	-2.01	103.89	111.70
5	A	606	GOL	C3-C2-C1	-2.00	103.91	111.70

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	603	GOL	O1-C1-C2-C3
2	B	601	NAD	O4B-C4B-C5B-O5B
2	B	601	NAD	C3B-C4B-C5B-O5B
2	B	601	NAD	C5D-O5D-PN-O1N
2	B	601	NAD	C5D-O5D-PN-O2N
2	B	601	NAD	O4D-C4D-C5D-O5D
2	B	601	NAD	C3D-C4D-C5D-O5D
2	B	601	NAD	O4D-C1D-N1N-C2N
2	B	601	NAD	O4D-C1D-N1N-C6N
2	B	601	NAD	C2D-C1D-N1N-C2N
2	B	601	NAD	C2D-C1D-N1N-C6N
5	A	608	GOL	C1-C2-C3-O3
2	A	601	NAD	O4B-C4B-C5B-O5B
2	A	601	NAD	C3B-C4B-C5B-O5B
2	A	601	NAD	C5D-O5D-PN-O3
2	A	601	NAD	C5D-O5D-PN-O2N
2	A	601	NAD	C2D-C1D-N1N-C2N
2	A	601	NAD	C2N-C3N-C7N-O7N
2	A	601	NAD	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
2	A	601	NAD	C4N-C3N-C7N-N7N
2	A	601	NAD	C4N-C3N-C7N-O7N
5	A	609	GOL	C1-C2-C3-O3
5	A	608	GOL	O1-C1-C2-C3
5	A	609	GOL	O2-C2-C3-O3
5	A	608	GOL	O1-C1-C2-O2
5	B	603	GOL	O1-C1-C2-O2
2	B	601	NAD	C4D-C5D-O5D-PN
5	A	605	GOL	O2-C2-C3-O3
5	A	608	GOL	O2-C2-C3-O3
2	A	601	NAD	C5D-O5D-PN-O1N
2	B	601	NAD	C4N-C3N-C7N-N7N
2	B	601	NAD	PN-O3-PA-O2A
2	A	601	NAD	PN-O3-PA-O1A
2	B	601	NAD	C4N-C3N-C7N-O7N
2	B	601	NAD	C5D-O5D-PN-O3
2	A	601	NAD	C2D-C1D-N1N-C6N
2	B	601	NAD	PN-O3-PA-O1A
5	A	605	GOL	C1-C2-C3-O3
2	A	601	NAD	O4D-C4D-C5D-O5D

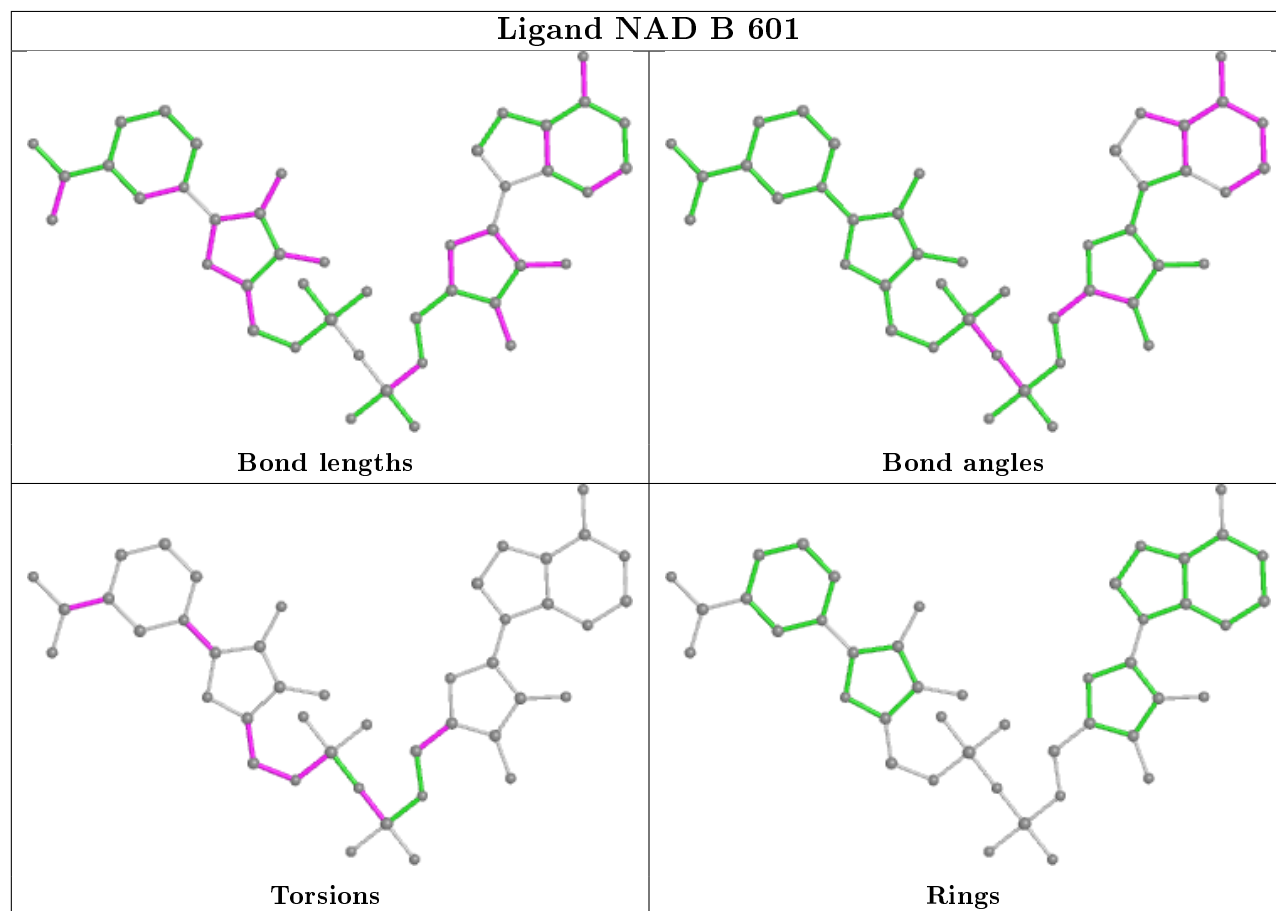
There are no ring outliers.

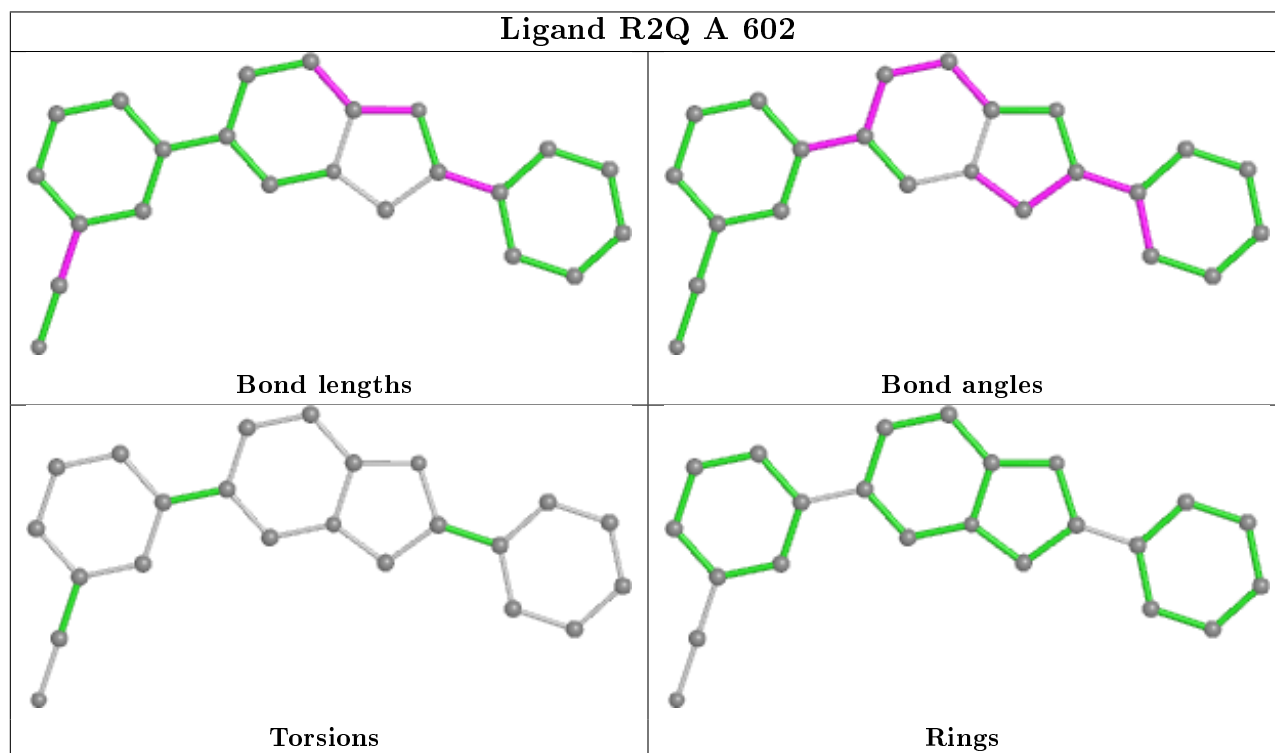
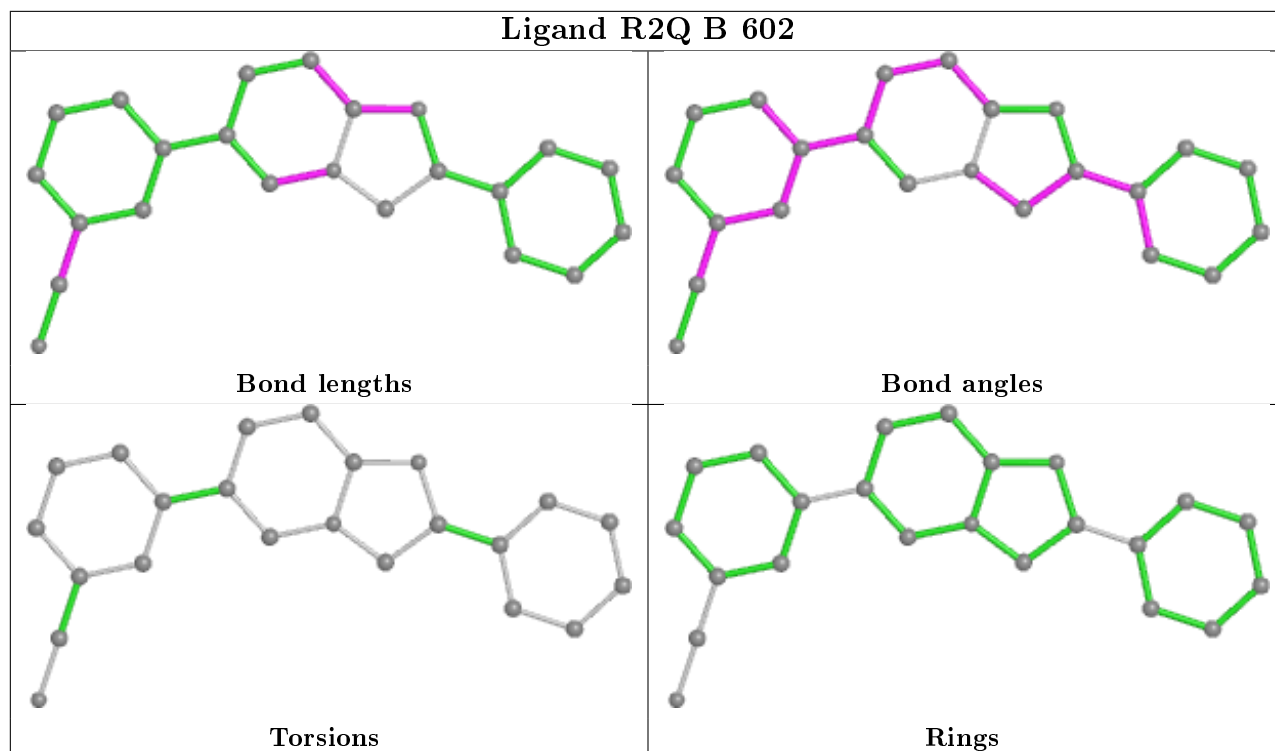
9 monomers are involved in 20 short contacts:

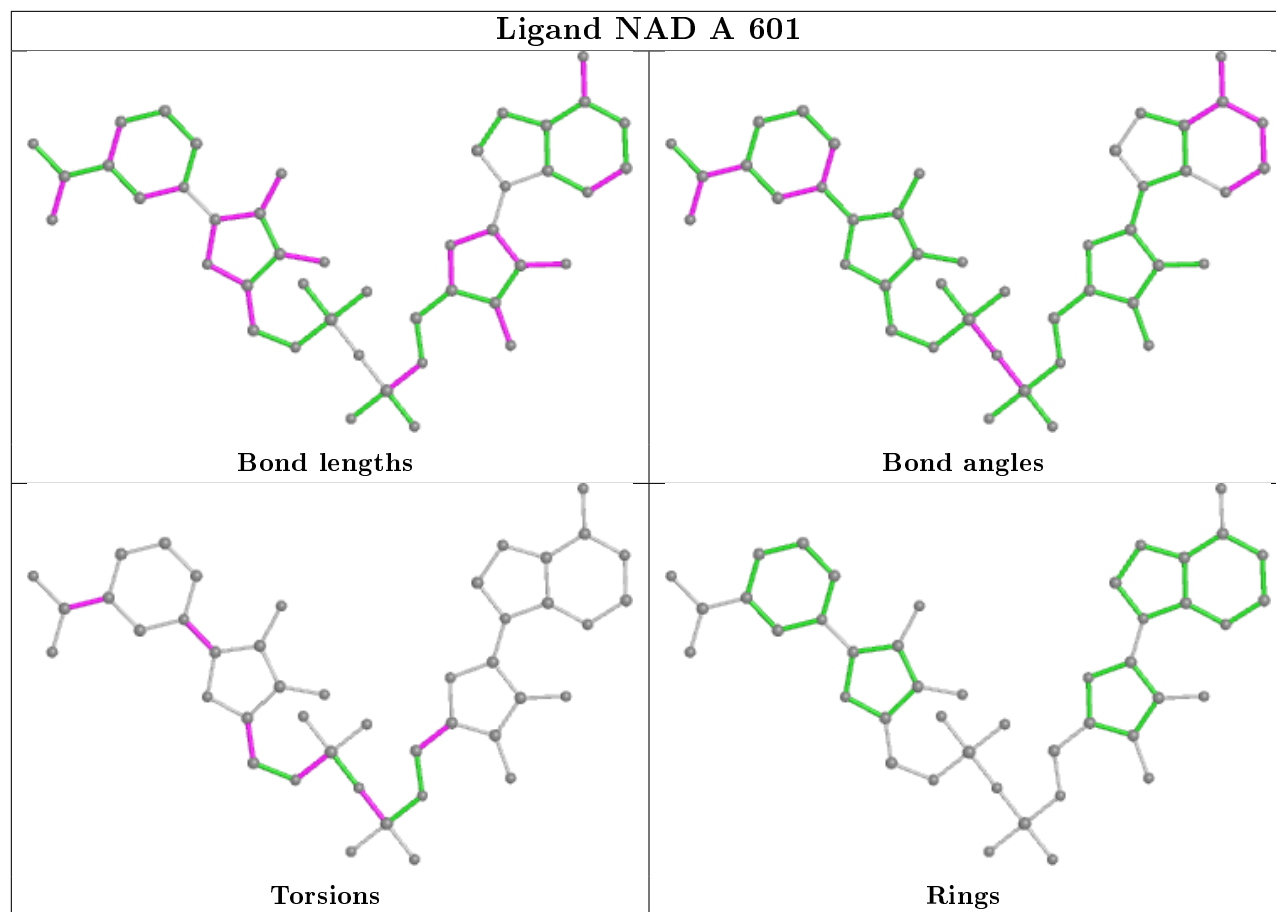
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	GOL	2	0
5	B	603	GOL	1	0
5	A	609	GOL	1	0
2	B	601	NAD	3	2
3	B	602	R2Q	1	0
5	A	608	GOL	1	0
3	A	602	R2Q	1	0
2	A	601	NAD	10	0
6	B	604	R2K	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	489/512 (95%)	1.00	69 (14%) <b>2</b> <b>1</b>	42, 67, 141, 172	0
1	B	489/512 (95%)	1.05	86 (17%) <b>1</b> <b>1</b>	41, 68, 124, 157	0
All	All	978/1024 (95%)	1.02	155 (15%) <b>2</b> <b>1</b>	41, 67, 133, 172	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	ALA	17.0
1	B	19	ALA	12.1
1	B	20	LEU	10.4
1	A	346	PRO	8.6
1	A	342	PRO	8.5
1	B	23	PRO	8.5
1	A	350	LYS	8.4
1	A	349	VAL	8.3
1	B	381	CYS	8.1
1	B	21	PRO	7.6
1	A	22	ARG	7.5
1	A	23	PRO	7.2
1	A	353	GLN	7.1
1	A	21	PRO	6.9
1	A	392	PHE	6.9
1	B	22	ARG	6.8
1	B	386	MET	6.7
1	B	348	ASP	6.7
1	A	390	GLY	6.7
1	A	404	ASN	6.5
1	B	372	GLY	6.3
1	A	24	ILE	6.3
1	B	343	VAL	6.2
1	A	20	LEU	6.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	382	GLY	6.0
1	A	351	THR	5.7
1	B	390	GLY	5.7
1	A	347	PHE	5.7
1	B	377	ALA	5.6
1	B	351	THR	5.5
1	B	406	ARG	5.3
1	A	386	MET	5.3
1	A	348	ASP	5.2
1	B	369	ILE	5.1
1	B	383	GLY	4.9
1	B	349	VAL	4.9
1	B	338	ALA	4.9
1	B	384	SER	4.7
1	B	389	LYS	4.6
1	A	372	GLY	4.6
1	A	344	GLY	4.6
1	A	352	GLU	4.5
1	A	381	CYS	4.5
1	B	395	PRO	4.4
1	B	374	LYS	4.3
1	B	337	TYR	4.3
1	B	336	GLU	4.2
1	B	398	PHE	4.1
1	B	397	VAL	4.1
1	B	388	ASP	3.9
1	B	346	PRO	3.9
1	B	371	SER	3.9
1	B	402	THR	3.9
1	A	374	LYS	3.9
1	B	403	ASP	3.9
1	B	407	ILE	3.9
1	B	373	LYS	3.8
1	A	377	ALA	3.8
1	B	307	PHE	3.8
1	B	405	MET	3.8
1	B	335	VAL	3.7
1	A	25	ARG	3.7
1	A	389	LYS	3.7
1	A	44	LYS	3.6
1	A	338	ALA	3.6
1	B	352	GLU	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	387	GLU	3.6
1	B	355	PRO	3.6
1	B	24	ILE	3.6
1	A	345	ASP	3.6
1	B	342	PRO	3.5
1	B	376	GLY	3.5
1	A	127	LEU	3.5
1	A	370	GLU	3.5
1	A	341	ARG	3.5
1	A	391	LEU	3.5
1	B	366	LEU	3.5
1	B	25	ARG	3.5
1	B	26	ASN	3.4
1	B	392	PHE	3.4
1	B	375	GLU	3.4
1	A	383	GLY	3.4
1	A	337	TYR	3.3
1	B	391	LEU	3.3
1	B	334	SER	3.2
1	B	416	VAL	3.2
1	A	340	LYS	3.2
1	B	396	THR	3.1
1	B	340	LYS	3.1
1	B	332	ARG	3.0
1	B	380	GLU	3.0
1	A	402	THR	3.0
1	A	69	PRO	3.0
1	A	400	GLU	3.0
1	A	403	ASP	3.0
1	B	27	LEU	3.0
1	B	344	GLY	3.0
1	A	376	GLY	3.0
1	B	419	ILE	3.0
1	B	379	LEU	2.9
1	B	401	VAL	2.9
1	B	370	GLU	2.9
1	A	343	VAL	2.9
1	B	329	GLU	2.8
1	B	418	PRO	2.8
1	B	417	GLN	2.8
1	B	350	LYS	2.7
1	B	347	PHE	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	314	CYS	2.7
1	A	388	ASP	2.7
1	A	303	HIS	2.7
1	A	307	PHE	2.7
1	A	359	GLN	2.7
1	A	373	LYS	2.7
1	B	394	LYS	2.7
1	B	303	HIS	2.7
1	A	358	ASP	2.6
1	B	28	GLU	2.6
1	A	361	GLN	2.6
1	B	356	GLN	2.6
1	B	420	LEU	2.6
1	B	404	ASN	2.6
1	A	304	GLN	2.6
1	A	215	TYR	2.5
1	A	74	ALA	2.5
1	A	382	GLY	2.5
1	A	398	PHE	2.4
1	B	339	LYS	2.4
1	A	314	CYS	2.4
1	A	61	CYS	2.4
1	A	76	GLU	2.4
1	A	339	LYS	2.4
1	B	412	ILE	2.4
1	A	401	VAL	2.3
1	B	345	ASP	2.3
1	A	380	GLU	2.3
1	A	384	SER	2.2
1	B	421	LYS	2.2
1	B	333	ARG	2.2
1	A	112	ALA	2.2
1	A	409	LYS	2.2
1	B	364	LYS	2.2
1	A	336	GLU	2.2
1	A	369	ILE	2.2
1	B	358	ASP	2.1
1	A	27	LEU	2.1
1	A	407	ILE	2.1
1	B	327	TYR	2.1
1	A	81	ALA	2.1
1	B	309	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	73	LYS	2.1
1	B	318	SER	2.1
1	B	284	LYS	2.0
1	B	409	LYS	2.0
1	B	38	ASN	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.

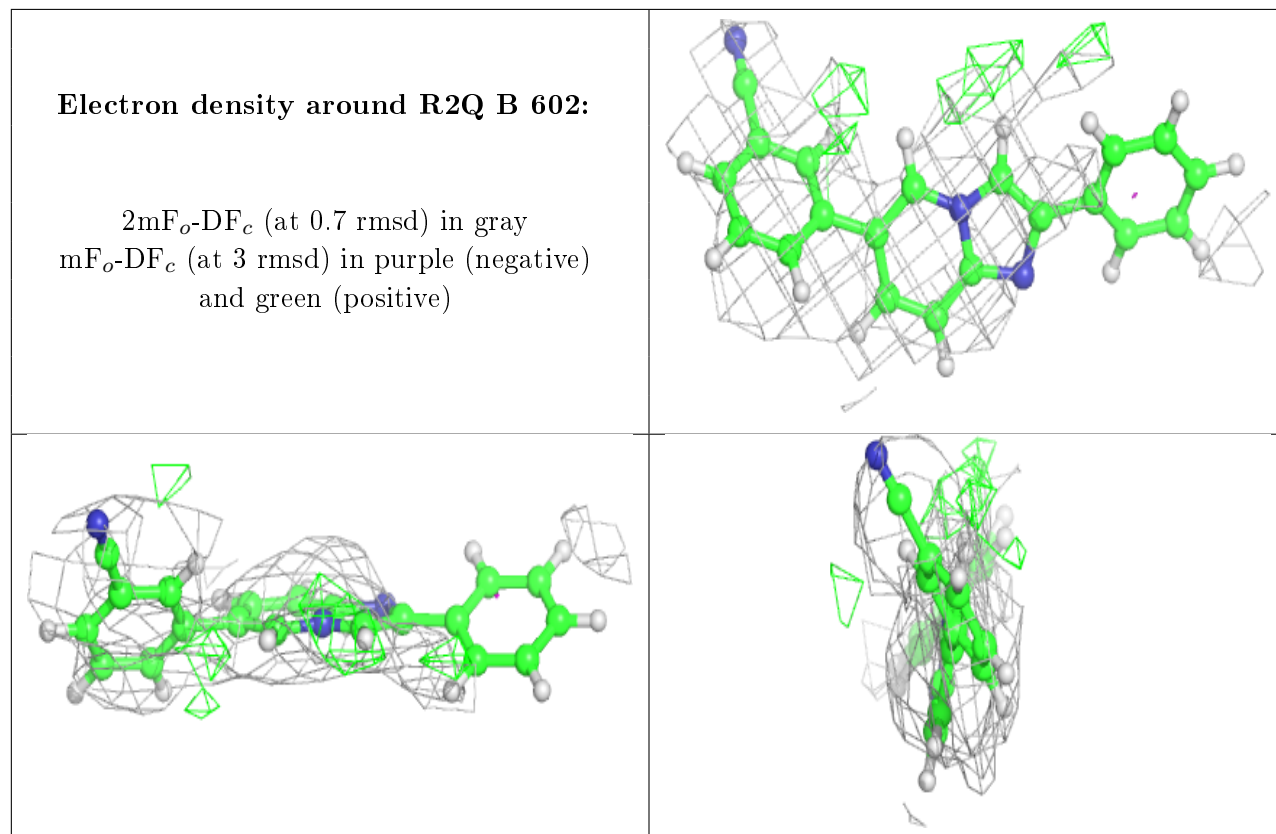
## 6.4 Ligands [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NA	A	603	1/1	0.48	0.49	97,97,97,97	0
6	R2K	B	604	9/9	0.58	0.42	88,108,116,126	0
3	R2Q	B	602	23/23	0.60	0.39	68,126,158,168	0
5	GOL	B	605	6/6	0.65	0.34	71,90,108,108	0
3	R2Q	A	602	23/23	0.65	0.34	75,121,153,157	0
5	GOL	A	605	6/6	0.75	0.32	70,88,97,111	0
5	GOL	A	609	6/6	0.75	0.32	70,85,102,102	0
4	NA	B	607	1/1	0.78	0.45	83,83,83,83	0
5	GOL	B	603	6/6	0.81	0.29	65,83,100,114	0
5	GOL	A	608	6/6	0.85	0.31	59,72,89,89	0
5	GOL	A	604	6/6	0.89	0.30	57,78,94,101	0
2	NAD	B	601	44/44	0.91	0.26	46,75,171,178	0
2	NAD	A	601	44/44	0.91	0.21	51,78,136,141	0
5	GOL	A	606	6/6	0.92	0.24	61,80,97,98	0
4	NA	B	606	1/1	0.93	1.00	66,66,66,66	0
4	NA	A	607	1/1	0.94	0.55	56,56,56,56	0

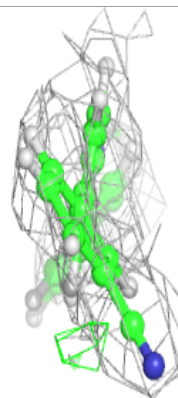
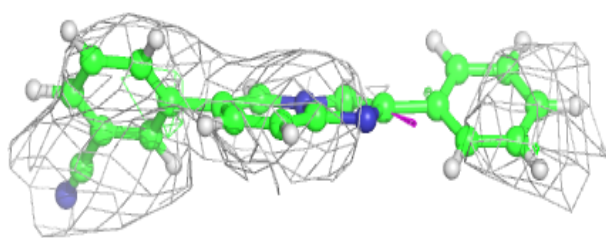
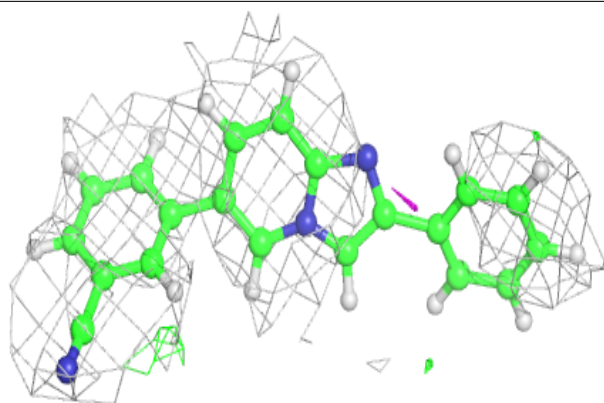
The following is a graphical depiction of the model fit to experimental electron density of all

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.



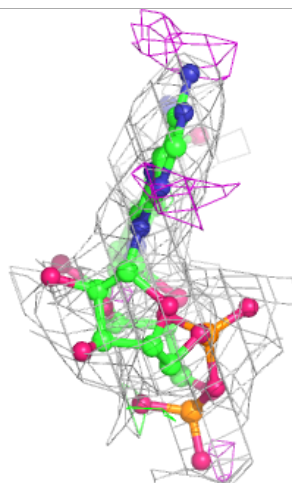
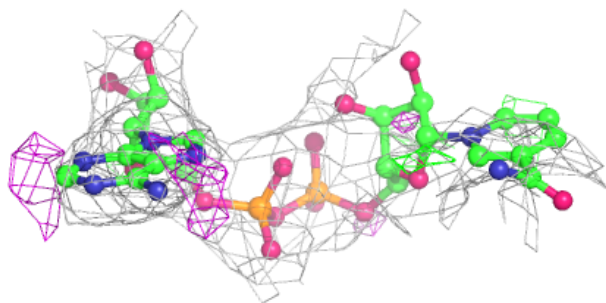
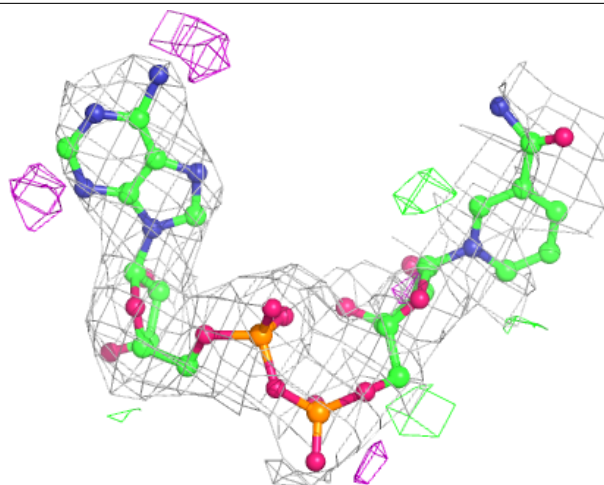
**Electron density around R2Q A 602:**

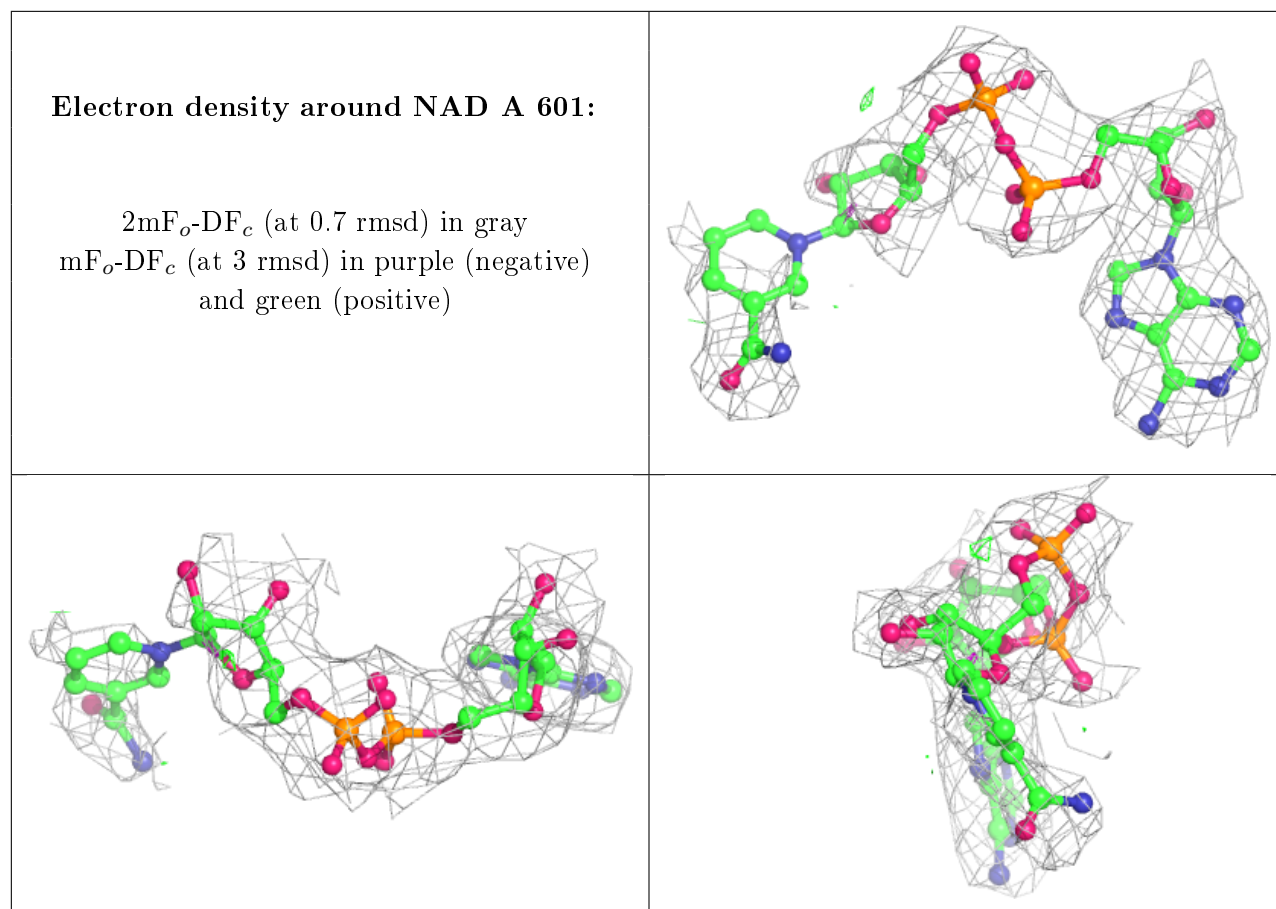
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around NAD B 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.