



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 11:29 PM UTC

PDB ID : 9M37 / pdb_00009m37
Title : Crystal structure of the DgpA2 protein from P581a bound to homoorientin
Authors : Ma, W.
Deposited on : 2025-03-01
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

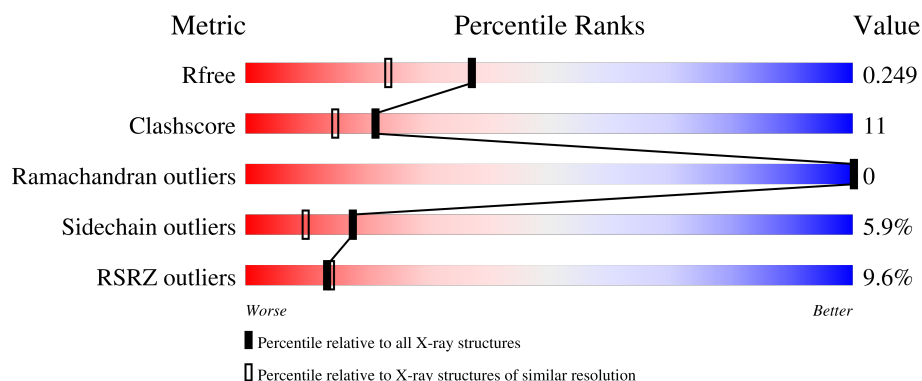
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	361	 3% 78% 11% • 9%
1	B	361	 14% 65% 22% • 9%

2 Entry composition [i](#)

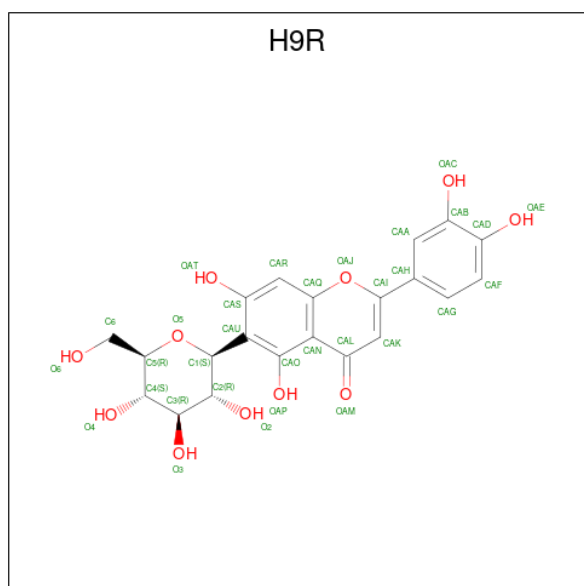
There are 4 unique types of molecules in this entry. The entry contains 5502 atoms, of which 52 are hydrogens and 0 are deuteriums.

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 P581a DgpA2 and isoorientin complex structure.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2584	1659	434	476	15			
1	B	329	Total	C	N	O	S	0	0	0
			2595	1664	434	482	15			

- Molecule 2 is 2-[3,4-bis(oxidanyl)phenyl]-6-[(2S,3R,4R,5S,6R)-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]-5,7-bis(oxidanyl)chromen-4-one (CCD ID: H9R) (formula: $C_{21}H_{20}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			32	21	11		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
3	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

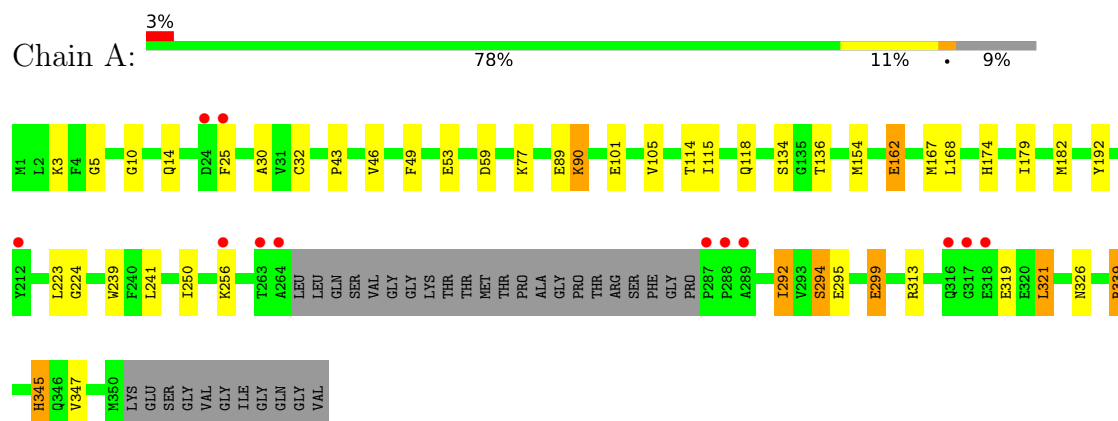
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	57	Total	O	0	0
			57	57		

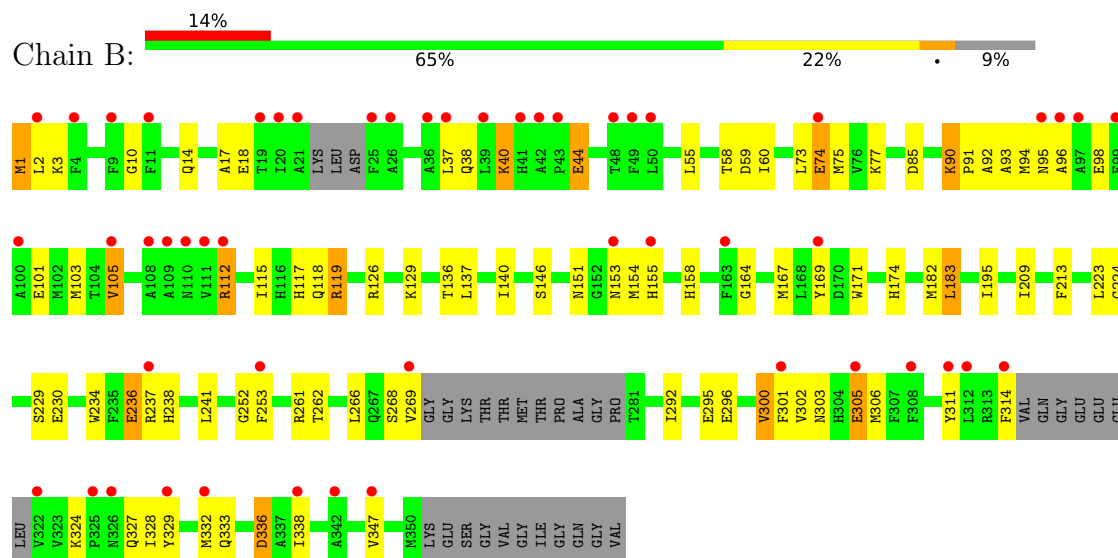
3 Residue-property plots [i](#)

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: P581a DgpA2 and isoorientin complex structure



- Molecule 1: P581a DgpA2 and isoorientin complex structure



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.66Å 45.64Å 104.80Å 90.00° 103.13° 90.00°	Depositor
Resolution (Å)	36.74 – 1.90 36.74 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (36.74-1.90) 99.6 (36.74-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.212 , 0.248 0.213 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5502	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H9R, 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	0.38	0/2645	0.54	1/3587 (0.0%)
1	B	0.37	0/2655	0.57	0/3602
All	All	0.37	0/5300	0.56	1/7189 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	PHE	N-CA-CB	-5.32	102.78	110.70

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	2584	0	2494	37	0
1	B	2595	0	2499	79	0
2	A	32	0	0	1	0
3	A	44	26	26	2	0
3	B	44	26	26	1	0
4	A	94	0	0	2	0
4	B	57	0	0	3	0
All	All	5450	52	5045	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (113) 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:118:GLN:HE22	3:A:402:NAD:H72N	1.30	0.77
1:B:183:LEU:HD12	1:B:213:PHE:CG	2.19	0.77
1:B:137:LEU:HB2	1:B:140:ILE:HD11	1.69	0.75
1:A:43:PRO:HG2	1:A:46:VAL:HG21	1.72	0.72
1:A:313:ARG:HB3	1:A:319:GLU:HB2	1.74	0.70
1:A:134:SER:OG	1:A:136:THR:HG23	1.92	0.70
1:B:55:LEU:O	1:B:58:THR:HG22	1.91	0.70
1:B:119:ARG:HB2	4:B:525:HOH:O	1.92	0.69
1:A:294:SER:HB2	1:B:230:GLU:OE2	1.95	0.66
1:B:302:VAL:HA	1:B:306:MET:HE3	1.78	0.65
1:B:73:LEU:HD22	1:B:98:GLU:HG2	1.78	0.65
1:B:324:LYS:HE2	1:B:327:GLN:NE2	2.13	0.63
1:B:229:SER:HB3	1:B:234:TRP:CD2	2.34	0.63
1:A:154:MET:HE3	1:A:167:MET:HE2	1.80	0.63
1:B:74:GLU:HG3	1:B:75:MET:N	2.12	0.62
1:B:303:ASN:OD1	1:B:306:MET:HG3	1.99	0.62
1:A:90:LYS:HE2	2:A:401:H9R:O3	2.00	0.61
1:A:239:TRP:HB2	1:A:250:ILE:HB	1.82	0.61
1:B:37:LEU:HD12	1:B:37:LEU:H	1.64	0.60
1:B:209:ILE:HD13	1:B:338:ILE:HD13	1.84	0.60
1:B:73:LEU:HD22	1:B:98:GLU:CG	2.32	0.60
1:B:303:ASN:ND2	1:B:305:GLU:HG3	2.17	0.59
1:B:92:ALA:HB2	1:B:115:ILE:HD12	1.85	0.59
1:B:146:SER:OG	1:B:238:HIS:HB2	2.03	0.58
1:B:183:LEU:HD12	1:B:213:PHE:CD2	2.39	0.58
1:B:236:GLU:HG2	1:B:253:PHE:CD2	2.39	0.58
1:A:223:LEU:C	1:A:223:LEU:HD23	2.29	0.57
1:A:115:ILE:N	1:A:115:ILE:HD12	2.19	0.57
1:A:345:HIS:O	1:B:347:VAL:HG11	2.04	0.57
1:B:223:LEU:HD23	1:B:224:GLY:N	2.19	0.57
1:B:103:MET:HE3	1:B:103:MET:HA	1.87	0.56
1:A:256:LYS:HD3	1:A:256:LYS:C	2.30	0.56
1:B:90:LYS:HD3	1:B:174:HIS:CE1	2.41	0.56
1:B:223:LEU:HD23	1:B:223:LEU:C	2.31	0.56
1:B:14:GLN:O	1:B:17:ALA:HB3	2.07	0.55
1:B:167:MET:CE	1:B:171:TRP:HB2	2.36	0.55
1:A:313:ARG:HD2	1:A:319:GLU:OE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:HG23	1:B:60:ILE:HG23	1.88	0.54
1:A:43:PRO:HG2	1:A:46:VAL:CG2	2.37	0.54
1:A:3:LYS:NZ	1:A:59:ASP:OD2	2.37	0.54
1:B:154:MET:HE3	1:B:158:HIS:HB3	1.89	0.53
1:B:10:GLY:O	1:B:14:GLN:HG3	2.09	0.53
1:B:112:ARG:HG3	1:B:314:PHE:CE2	2.45	0.52
1:B:311:TYR:O	1:B:314:PHE:HB3	2.09	0.52
1:A:3:LYS:HZ1	1:A:59:ASP:CG	2.17	0.52
1:A:3:LYS:HE2	1:A:59:ASP:O	2.10	0.52
1:B:85:ASP:CG	1:B:112:ARG:HB2	2.34	0.51
1:B:112:ARG:HG3	1:B:314:PHE:HE2	1.76	0.51
1:A:90:LYS:HD2	1:A:90:LYS:C	2.36	0.50
1:A:101:GLU:O	1:A:105:VAL:HG13	2.10	0.50
1:B:236:GLU:HG2	1:B:253:PHE:H	1.76	0.50
1:B:262:THR:HG22	1:B:292:ILE:HD13	1.92	0.50
1:B:103:MET:HE3	1:B:103:MET:CA	2.41	0.50
1:B:151:ASN:HB3	4:B:535:HOH:O	2.12	0.50
1:B:118:GLN:HE22	3:B:401:NAD:H72N	1.59	0.49
1:B:136:THR:HB	1:B:261:ARG:HH22	1.78	0.49
1:B:38:GLN:NE2	1:B:38:GLN:HA	2.28	0.48
1:A:192:TYR:HB2	1:A:347:VAL:HG22	1.95	0.48
1:B:55:LEU:C	1:B:55:LEU:HD23	2.37	0.48
1:B:328:ILE:O	1:B:332:MET:HG2	2.12	0.48
1:B:171:TRP:HZ3	1:B:237:ARG:NH1	2.12	0.48
1:B:96:ALA:HB1	1:B:329:TYR:CE1	2.48	0.48
1:A:241:LEU:HD12	1:A:241:LEU:N	2.28	0.48
1:A:321:LEU:CD2	4:A:554:HOH:O	2.61	0.47
1:B:93:ALA:HB1	1:B:98:GLU:HB3	1.95	0.47
1:B:302:VAL:HA	1:B:306:MET:CE	2.44	0.47
1:B:229:SER:HB3	1:B:234:TRP:CG	2.50	0.47
1:B:1:MET:HG2	1:B:2:LEU:N	2.27	0.46
1:B:119:ARG:NH1	1:B:171:TRP:CH2	2.83	0.46
1:A:162:GLU:H	1:A:162:GLU:CD	2.24	0.46
1:B:91:PRO:HD3	1:B:169:TYR:O	2.15	0.46
1:B:236:GLU:HB3	1:B:252:GLY:HA2	1.98	0.46
1:A:3:LYS:NZ	1:A:59:ASP:CG	2.73	0.46
1:B:77:LYS:NZ	1:B:101:GLU:HG2	2.30	0.45
1:A:299:GLU:O	4:A:501:HOH:O	2.21	0.45
1:B:38:GLN:HA	1:B:38:GLN:HE21	1.82	0.45
1:A:90:LYS:HE2	1:A:174:HIS:NE2	2.32	0.45
1:B:151:ASN:ND2	1:B:153:ASN:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:HD13	1:A:182:MET:CE	2.47	0.45
1:B:129:LYS:HA	1:B:182:MET:HE2	2.00	0.44
1:A:5:GLY:HA2	1:A:30:ALA:O	2.17	0.44
1:B:301:PHE:O	1:B:302:VAL:HG13	2.17	0.44
1:A:89:GLU:OE1	3:A:402:NAD:H2N	2.18	0.44
1:B:126:ARG:HB3	1:B:300:VAL:HG21	1.99	0.44
1:A:294:SER:HB2	1:B:230:GLU:CD	2.43	0.44
1:B:119:ARG:HA	1:B:119:ARG:HD2	1.65	0.44
1:B:129:LYS:NZ	4:B:508:HOH:O	2.50	0.43
1:B:324:LYS:HE3	1:B:324:LYS:HB2	1.78	0.43
1:B:115:ILE:HG13	1:B:328:ILE:HG13	2.01	0.43
1:A:10:GLY:O	1:A:14:GLN:HG3	2.18	0.43
1:A:77:LYS:CE	1:A:101:GLU:OE2	2.67	0.43
1:A:168:LEU:HD23	1:A:339:ARG:HH11	1.83	0.43
1:B:333:GLN:HA	1:B:336:ASP:OD2	2.19	0.43
1:B:44:GLU:H	1:B:44:GLU:HG2	1.63	0.43
1:B:266:LEU:C	1:B:266:LEU:HD23	2.43	0.43
1:B:94:MET:HE1	1:B:164:GLY:N	2.34	0.42
1:B:119:ARG:HG2	1:B:174:HIS:CG	2.54	0.42
1:B:241:LEU:HD12	1:B:241:LEU:N	2.34	0.42
1:B:167:MET:HE2	1:B:223:LEU:HD11	2.01	0.42
1:A:114:THR:C	1:A:115:ILE:HD12	2.45	0.42
1:B:1:MET:HE2	1:B:1:MET:HB3	1.68	0.42
1:A:223:LEU:HD23	1:A:224:GLY:N	2.35	0.42
1:B:324:LYS:CE	1:B:327:GLN:NE2	2.81	0.41
1:B:73:LEU:HB2	1:B:98:GLU:HG2	2.02	0.41
1:A:292:ILE:HD12	1:A:292:ILE:HA	1.94	0.41
1:B:236:GLU:HG2	1:B:253:PHE:HD2	1.84	0.41
1:B:117:HIS:ND1	1:B:328:ILE:HD12	2.35	0.41
1:B:171:TRP:HZ3	1:B:237:ARG:HH11	1.68	0.41
1:A:32:CYS:HA	1:A:49:PHE:O	2.21	0.40
1:B:195:ILE:HD11	1:B:338:ILE:HG22	2.03	0.40
1:B:59:ASP:O	1:B:59:ASP:CG	2.63	0.40
1:B:40:LYS:H	1:B:40:LYS:HG2	1.48	0.40
1:B:101:GLU:O	1:B:105:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

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	324/361 (90%)	317 (98%)	7 (2%)	0	100	100
1	B	321/361 (89%)	311 (97%)	10 (3%)	0	100	100
All	All	645/722 (89%)	628 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	269/303 (89%)	258 (96%)	11 (4%)	27	19
1	B	273/303 (90%)	252 (92%)	21 (8%)	12	5
All	All	542/606 (89%)	510 (94%)	32 (6%)	18	10

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	90	LYS
1	A	162	GLU
1	A	292	ILE
1	A	294	SER
1	A	295	GLU
1	A	299	GLU
1	A	321	LEU

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Mol	Chain	Res	Type
1	A	326	ASN
1	A	339	ARG
1	A	345	HIS
1	B	1	MET
1	B	3	LYS
1	B	18	GLU
1	B	40	LYS
1	B	44	GLU
1	B	74	GLU
1	B	90	LYS
1	B	95	ASN
1	B	105	VAL
1	B	112	ARG
1	B	119	ARG
1	B	155	HIS
1	B	183	LEU
1	B	236	GLU
1	B	268	SER
1	B	269	VAL
1	B	295	GLU
1	B	296	GLU
1	B	300	VAL
1	B	305	GLU
1	B	336	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	ASN
1	B	38	GLN
1	B	145	ASN
1	B	151	ASN
1	B	208	ASN
1	B	210	GLN
1	B	220	GLN
1	B	267	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	NAD	A	402	-	46,48,48	1.19	2 (4%)	64,73,73	1.29	7 (10%)
2	H9R	A	401	-	35,35,35	2.97	22 (62%)	51,53,53	1.35	6 (11%)
3	NAD	B	401	-	46,48,48	1.36	2 (4%)	64,73,73	1.19	5 (7%)

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	NAD	A	402	-	-	2/30/62/62	0/5/5/5
2	H9R	A	401	-	-	0/10/30/30	0/4/4/4
3	NAD	B	401	-	-	8/30/62/62	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	H9R	OAM-CAL	7.10	1.39	1.24
3	B	401	NAD	PA-O3	6.89	1.66	1.59
2	A	401	H9R	OAJ-CAI	-5.22	1.29	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	H9R	OAT-CAS	5.11	1.46	1.36
3	A	402	NAD	PA-O3	4.90	1.64	1.59
2	A	401	H9R	OAP-CAO	4.77	1.47	1.36
3	A	402	NAD	PN-O3	4.64	1.64	1.59
2	A	401	H9R	O3-C3	3.96	1.52	1.43
2	A	401	H9R	CAR-CAQ	3.86	1.45	1.38
2	A	401	H9R	CAH-CAI	3.85	1.56	1.48
2	A	401	H9R	OAC-CAB	3.34	1.43	1.36
3	B	401	NAD	PN-O3	3.33	1.63	1.59
2	A	401	H9R	CAA-CAB	3.29	1.43	1.38
2	A	401	H9R	CAU-C1	3.28	1.56	1.51
2	A	401	H9R	OAE-CAD	3.15	1.42	1.36
2	A	401	H9R	C2-C3	-3.13	1.44	1.52
2	A	401	H9R	CAG-CAF	3.11	1.43	1.38
2	A	401	H9R	O5-C5	2.95	1.51	1.44
2	A	401	H9R	O5-C1	2.72	1.47	1.43
2	A	401	H9R	CAS-CAU	2.60	1.43	1.40
2	A	401	H9R	C4-C5	2.42	1.58	1.53
2	A	401	H9R	O2-C2	2.35	1.48	1.43
2	A	401	H9R	CAN-CAO	2.35	1.46	1.41
2	A	401	H9R	C6-C5	-2.35	1.43	1.51
2	A	401	H9R	OAJ-CAQ	-2.20	1.35	1.38
2	A	401	H9R	CAR-CAS	2.02	1.41	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	H9R	OAJ-CAI-CAH	4.07	117.56	111.89
3	A	402	NAD	C4D-O4D-C1D	-3.81	106.44	109.92
3	A	402	NAD	O7N-C7N-N7N	3.62	127.85	122.62
2	A	401	H9R	CAI-CAK-CAL	-3.34	118.70	122.14
2	A	401	H9R	CAQ-OAJ-CAI	3.25	123.62	119.67
3	B	401	NAD	C4D-O4D-C1D	-3.17	107.03	109.92
2	A	401	H9R	CAS-CAU-CAO	3.09	119.99	117.08
2	A	401	H9R	CAQ-CAN-CAO	3.05	120.88	117.54
3	A	402	NAD	O3-PA-O1A	-2.84	102.15	110.70
3	A	402	NAD	O2A-PA-O1A	2.49	124.03	112.44
3	B	401	NAD	C2B-C1B-N9A	2.42	119.32	113.30
3	A	402	NAD	C2B-C3B-C4B	2.30	107.05	102.61
3	A	402	NAD	O7N-C7N-C3N	-2.29	116.79	119.60
3	B	401	NAD	O4B-C4B-C5B	2.14	116.19	109.33
3	B	401	NAD	O2N-PN-O3	2.14	113.06	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	H9R	O6-C6-C5	-2.13	104.07	111.33
3	B	401	NAD	O7N-C7N-C3N	-2.03	117.11	119.60
3	A	402	NAD	C6N-N1N-C1D	-2.02	115.75	119.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

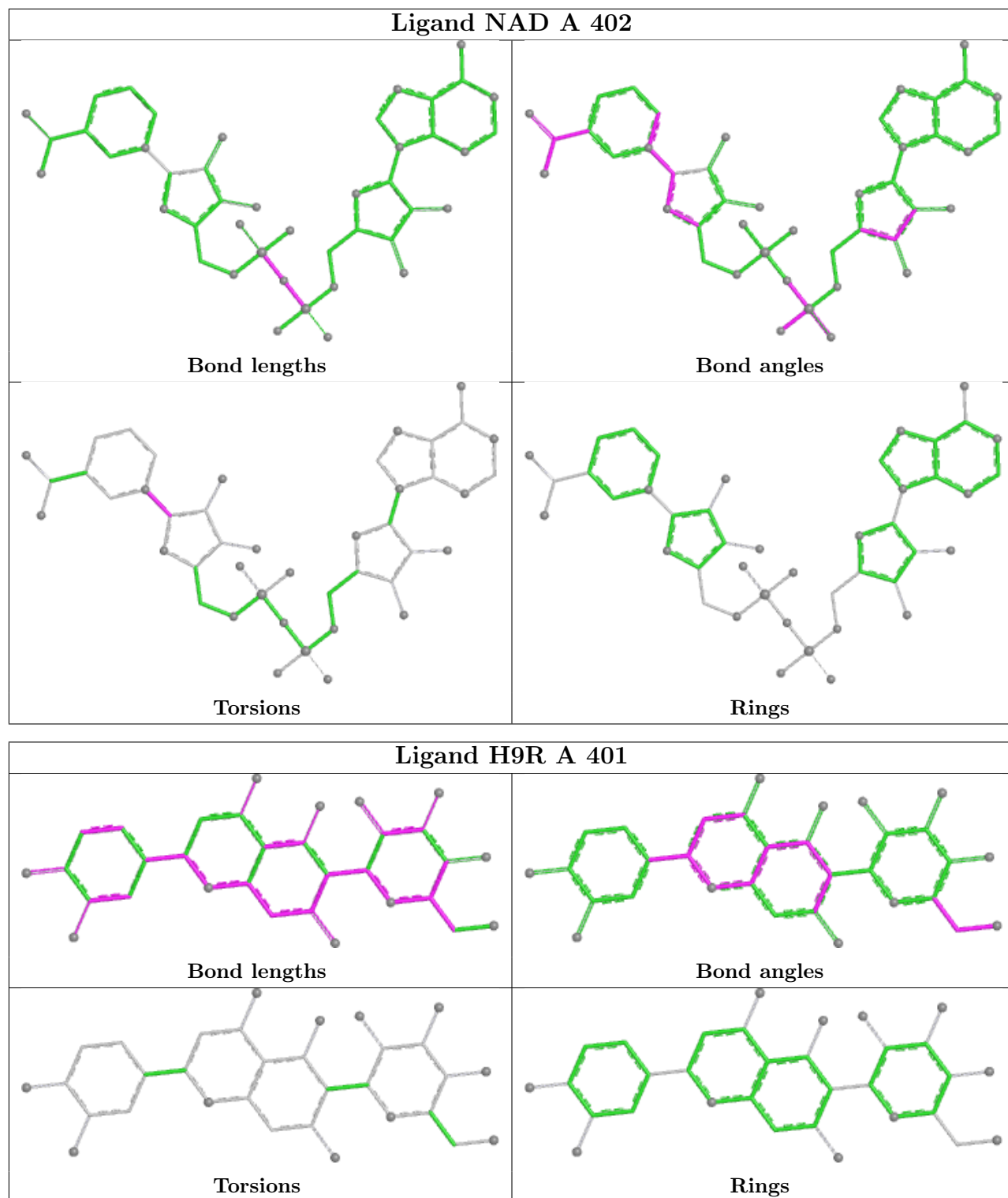
Mol	Chain	Res	Type	Atoms
3	A	402	NAD	O4D-C1D-N1N-C6N
3	B	401	NAD	O4D-C1D-N1N-C6N
3	B	401	NAD	O4D-C4D-C5D-O5D
3	B	401	NAD	O4B-C4B-C5B-O5B
3	B	401	NAD	C3B-C4B-C5B-O5B
3	A	402	NAD	O4D-C1D-N1N-C2N
3	B	401	NAD	O4D-C1D-N1N-C2N
3	B	401	NAD	PA-O3-PN-O1N
3	B	401	NAD	C3D-C4D-C5D-O5D
3	B	401	NAD	PN-O3-PA-O2A

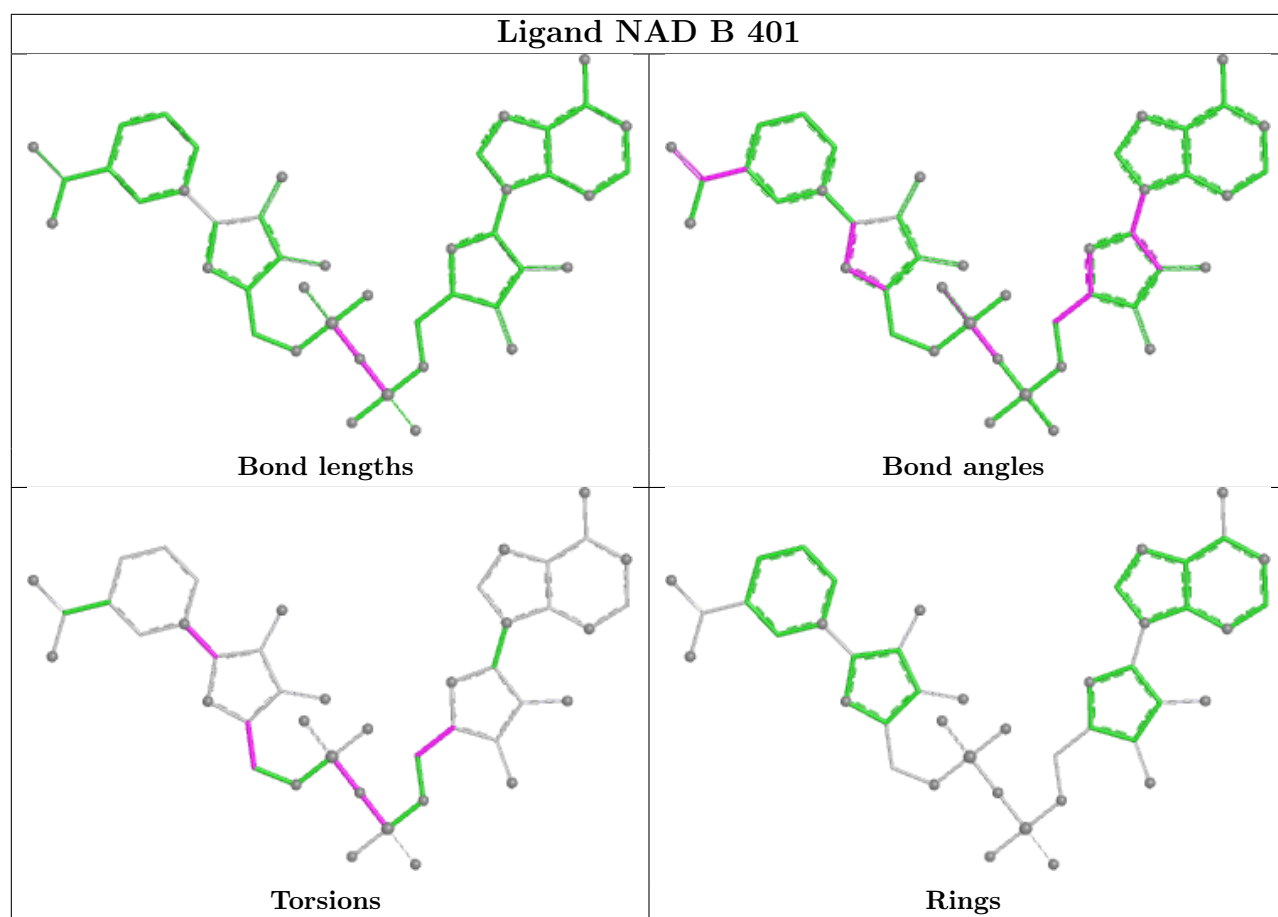
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	NAD	2	0
2	A	401	H9R	1	0
3	B	401	NAD	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, 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	328/361 (90%)	0.44	12 (3%) 45 48	23, 31, 49, 72	0
1	B	329/361 (91%)	1.03	51 (15%) 5 5	26, 42, 75, 98	0
All	All	657/722 (90%)	0.74	63 (9%) 13 14	23, 37, 70, 98	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	GLY	5.3
1	A	289	ALA	4.9
1	B	269	VAL	4.7
1	B	25	PHE	4.7
1	B	301	PHE	4.5
1	B	314	PHE	4.0
1	B	312	LEU	3.8
1	B	322	VAL	3.7
1	B	108	ALA	3.6
1	B	2	LEU	3.5
1	B	42	ALA	3.5
1	B	21	ALA	3.4
1	B	325	PRO	3.4
1	A	316	GLN	3.3
1	B	96	ALA	3.2
1	B	169	TYR	3.2
1	A	287	PRO	3.1
1	B	155	HIS	2.8
1	A	318	GLU	2.8
1	A	25	PHE	2.8
1	B	99	PHE	2.8
1	B	74	GLU	2.7
1	B	20	ILE	2.7
1	B	97	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	100	ALA	2.6
1	B	237	ARG	2.6
1	B	342	ALA	2.6
1	B	39	LEU	2.6
1	B	111	VAL	2.6
1	B	43	PRO	2.5
1	B	37	LEU	2.5
1	B	36	ALA	2.5
1	A	256	LYS	2.5
1	B	41	HIS	2.4
1	B	329	TYR	2.4
1	B	95	ASN	2.4
1	B	253	PHE	2.3
1	A	264	ALA	2.3
1	A	263	THR	2.3
1	B	109	ALA	2.3
1	B	26	ALA	2.3
1	B	50	LEU	2.3
1	A	288	PRO	2.2
1	B	305	GLU	2.2
1	B	19	THR	2.2
1	B	163	PHE	2.2
1	B	110	ASN	2.2
1	B	48	THR	2.2
1	B	11	PHE	2.1
1	B	332	MET	2.1
1	B	49	PHE	2.1
1	B	105	VAL	2.1
1	B	326	ASN	2.1
1	B	4	PHE	2.1
1	B	9	PHE	2.1
1	B	308	PHE	2.1
1	A	24	ASP	2.1
1	B	311	TYR	2.1
1	B	112	ARG	2.1
1	A	212	TYR	2.0
1	B	338	ILE	2.0
1	B	153	ASN	2.0
1	B	347	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

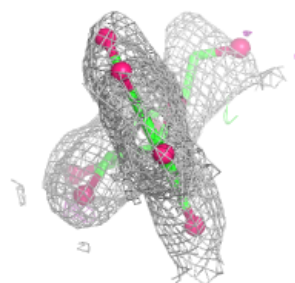
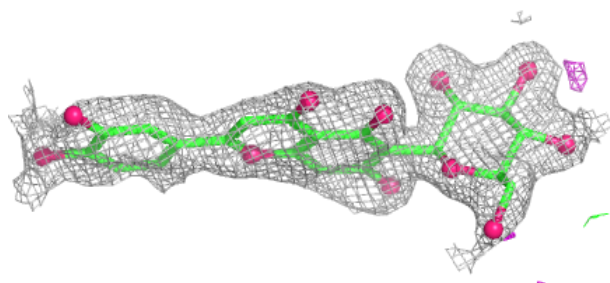
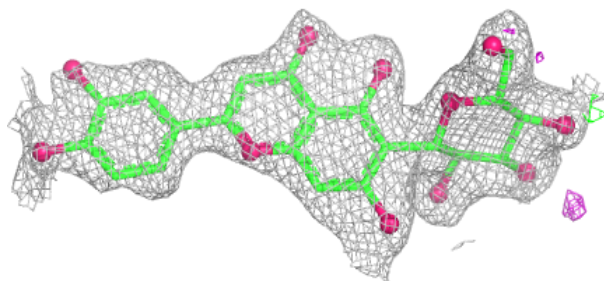
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	H9R	A	401	32/32	0.86	0.10	30,41,52,59	0
3	NAD	B	401	44/44	0.90	0.09	36,50,61,65	0
3	NAD	A	402	44/44	0.96	0.06	22,30,38,43	0

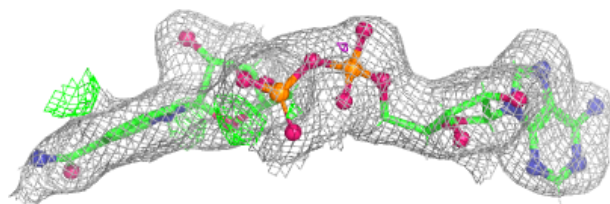
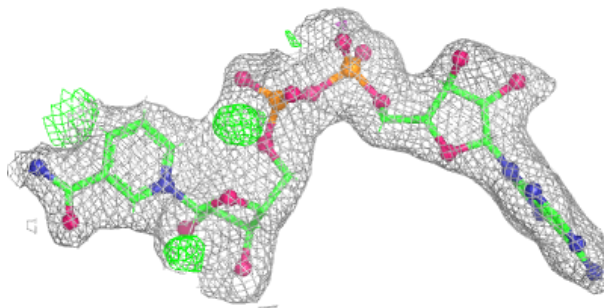
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

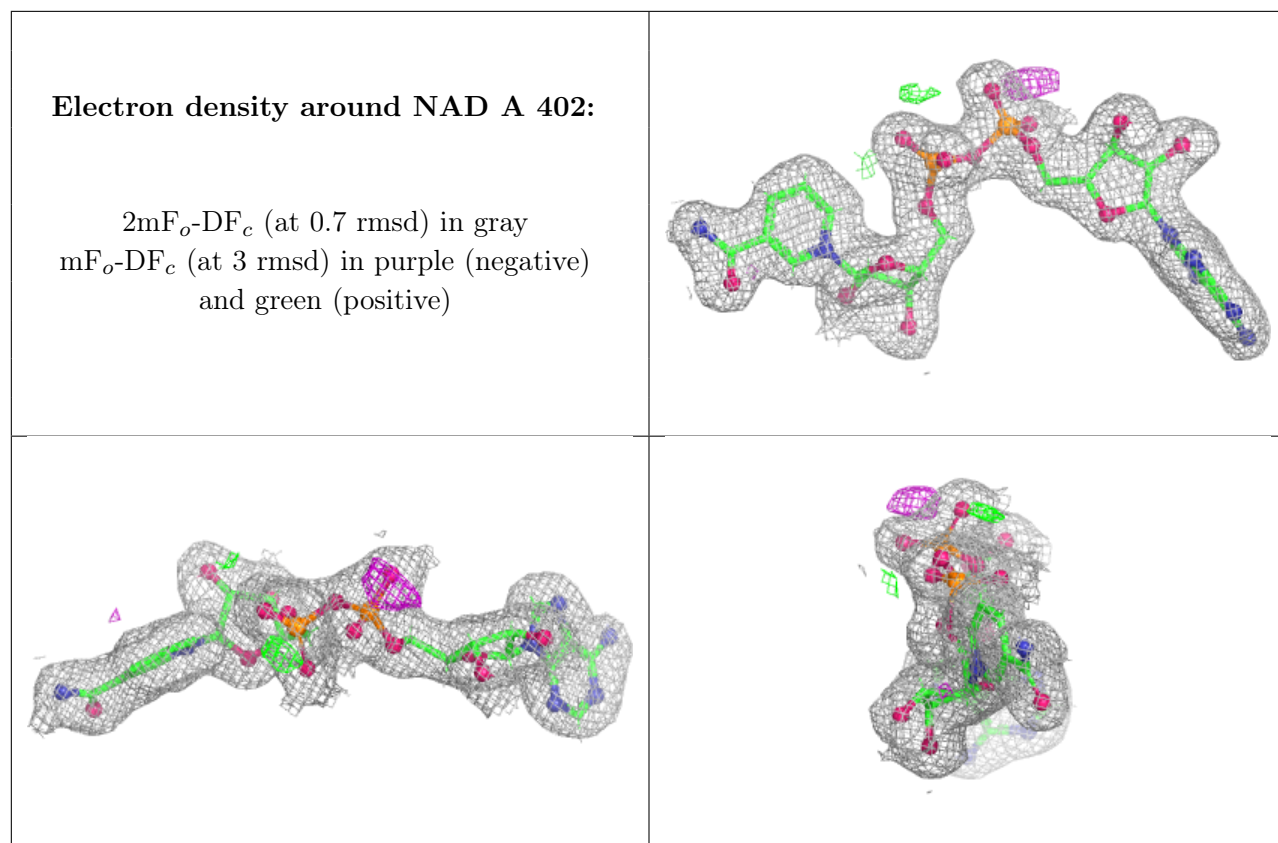
Electron density around H9R A 401:

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

**Electron density around NAD B 401:**

$2mF_o-DF_c$ (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.