



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 01:52 PM EDT

PDB ID : 1Z45  
Title : Crystal structure of the gal10 fusion protein galactose mutarotase/UDP-galactose 4-epimerase from *Saccharomyces cerevisiae* complexed with NAD, UDP-glucose, and galactose  
Authors : Thoden, J.B.; Holden, H.M.  
Deposited on : 2005-03-15  
Resolution : 1.85 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 : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

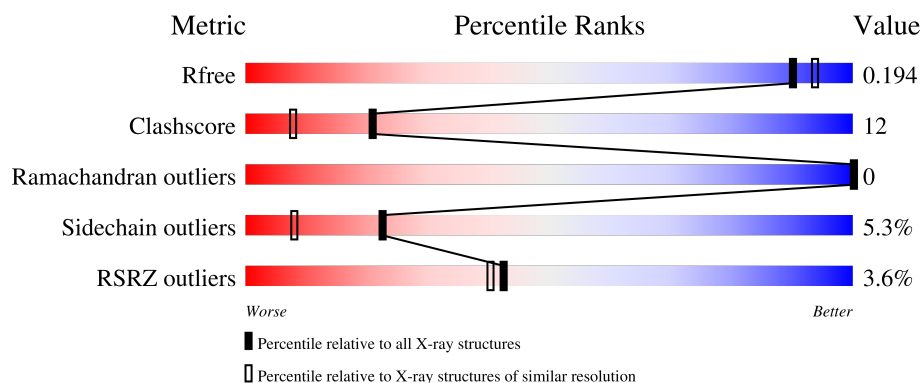
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	699	

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
5	UPG	A	704	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6151 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

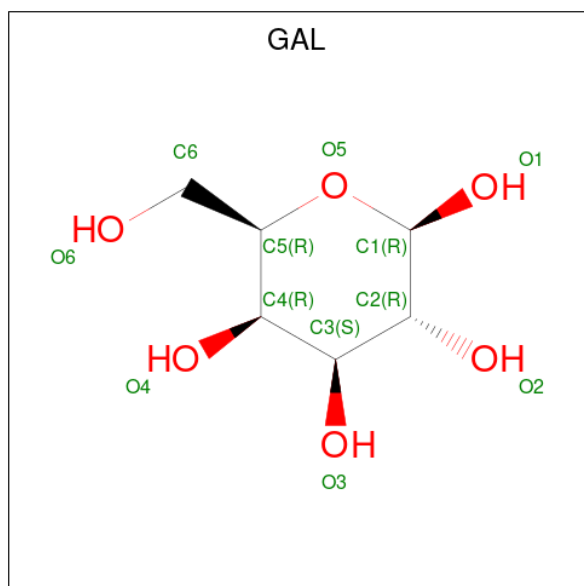
- Molecule 1 is a protein called GAL10 bifunctional protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	674	5335	3400	896	1022	17	0	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	518	ILE	MET	engineered mutation	UNP P04397

- Molecule 2 is beta-D-galactopyranose (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

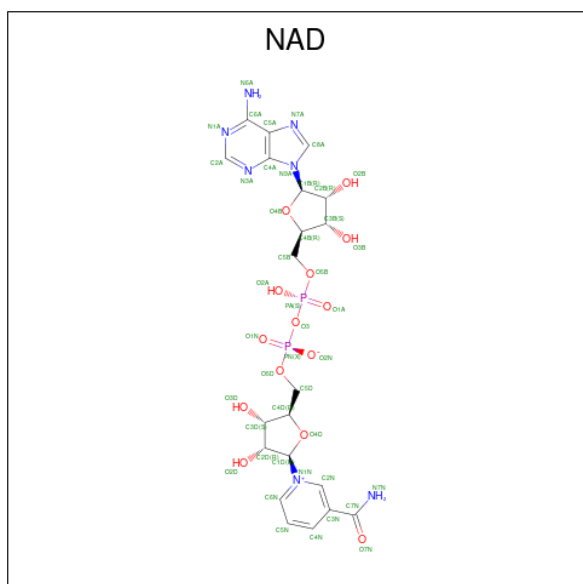


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

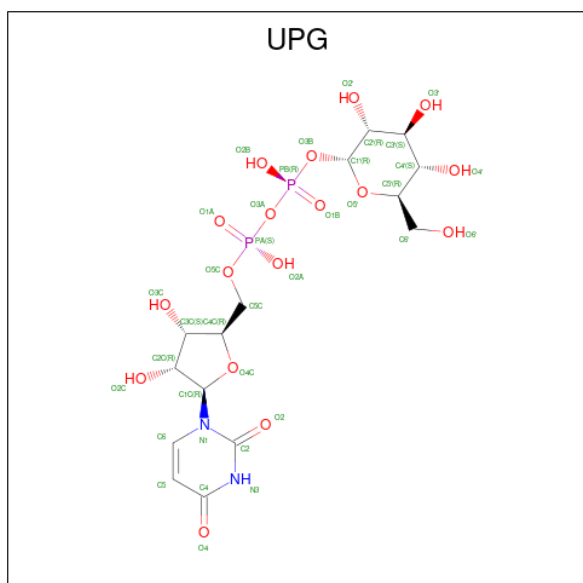
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Na 2 2	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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

- Molecule 5 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula:  $\text{C}_{15}\text{H}_{24}\text{N}_2\text{O}_{17}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

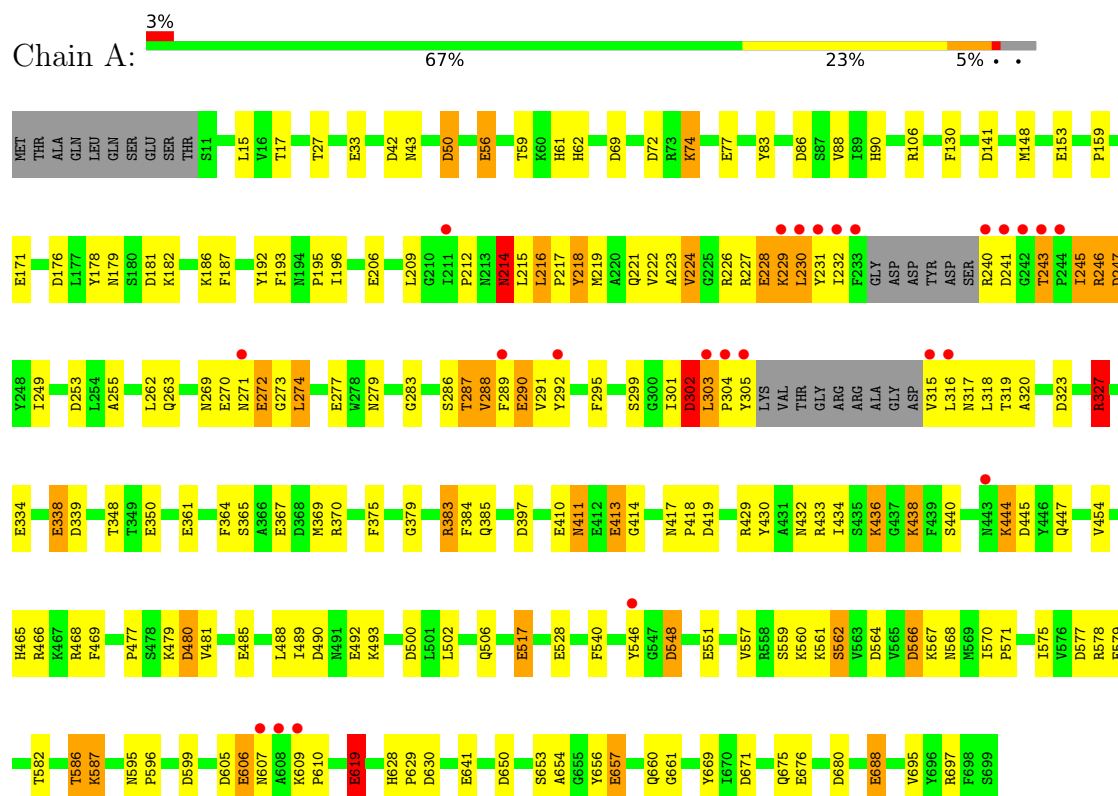
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	722	Total	O	0	0
			722	722		

### 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: GAL10 bifunctional protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.90Å 125.20Å 142.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 28.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-1.85) 97.7 (28.99-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.76 (at 1.85Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.194 , 0.245 0.197 , 0.194	Depositor DCC
$R_{free}$ test set	9080 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 111.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6151	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, NAD, UPG, GAL

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	0.99	30/5468 (0.5%)	1.45	70/7421 (0.9%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	GLU	CD-OE2	7.37	1.33	1.25
1	A	606	GLU	CD-OE2	7.26	1.33	1.25
1	A	619	GLU	CD-OE2	6.83	1.33	1.25
1	A	272	GLU	CD-OE2	6.72	1.33	1.25
1	A	528	GLU	CD-OE2	6.58	1.32	1.25
1	A	338	GLU	CD-OE2	6.50	1.32	1.25
1	A	517[A]	GLU	CD-OE2	6.43	1.32	1.25
1	A	517[B]	GLU	CD-OE2	6.43	1.32	1.25
1	A	77	GLU	CD-OE2	6.42	1.32	1.25
1	A	290	GLU	CD-OE2	6.37	1.32	1.25
1	A	657	GLU	CD-OE2	6.30	1.32	1.25
1	A	413	GLU	CD-OE2	6.25	1.32	1.25
1	A	228	GLU	CD-OE2	6.20	1.32	1.25
1	A	334	GLU	CD-OE2	6.20	1.32	1.25
1	A	579	GLU	CD-OE2	6.15	1.32	1.25
1	A	676	GLU	CD-OE2	6.13	1.32	1.25
1	A	171	GLU	CD-OE2	6.06	1.32	1.25
1	A	56	GLU	CD-OE2	6.05	1.32	1.25
1	A	350	GLU	CD-OE2	5.98	1.32	1.25
1	A	551	GLU	CD-OE2	5.89	1.32	1.25
1	A	492	GLU	CD-OE2	5.85	1.32	1.25
1	A	33	GLU	CD-OE2	5.74	1.31	1.25
1	A	153	GLU	CD-OE2	5.72	1.31	1.25
1	A	410	GLU	CD-OE2	5.58	1.31	1.25
1	A	361	GLU	CD-OE2	5.49	1.31	1.25
1	A	688	GLU	CD-OE2	5.47	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	485	GLU	CD-OE2	5.39	1.31	1.25
1	A	641	GLU	CD-OE2	5.37	1.31	1.25
1	A	206	GLU	CD-OE2	5.18	1.31	1.25
1	A	367	GLU	CD-OE2	5.07	1.31	1.25

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	ASP	CB-CG-OD2	-11.96	107.54	118.30
1	A	327	ARG	NE-CZ-NH1	11.27	125.94	120.30
1	A	241	ASP	CB-CG-OD2	-9.30	109.93	118.30
1	A	680	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	A	176	ASP	CB-CG-OD2	-8.85	110.34	118.30
1	A	697	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	A	327	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	A	323	ASP	CB-CG-OD1	8.41	125.87	118.30
1	A	69	ASP	CB-CG-OD1	8.41	125.87	118.30
1	A	500	ASP	CB-CG-OD1	8.33	125.80	118.30
1	A	69	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	A	176	ASP	CB-CG-OD1	7.76	125.29	118.30
1	A	564	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	A	433	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	83	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	A	566	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	247	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	566	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	A	302	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	A	630	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	A	397	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	562	SER	N-CA-CB	-6.80	100.30	110.50
1	A	650	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	680	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	288	VAL	CA-CB-CG1	-6.51	101.13	110.90
1	A	224	VAL	CA-CB-CG1	6.37	120.46	110.90
1	A	141	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	A	241	ASP	CB-CG-OD1	6.12	123.80	118.30
1	A	323	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	650	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	490	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	214	ASN	CB-CA-C	5.96	122.33	110.40
1	A	339	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	468	ARG	NE-CZ-NH1	5.94	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	397	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	599	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	599	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	433	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	279	ASN	CB-CA-C	-5.77	98.86	110.40
1	A	286	SER	N-CA-CB	5.76	119.14	110.50
1	A	480	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	216	LEU	CA-CB-CG	-5.65	102.31	115.30
1	A	72	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	86	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	480	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	546	TYR	C-N-CA	-5.55	110.64	122.30
1	A	247	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	656	TYR	CA-CB-CG	-5.46	103.03	113.40
1	A	384	PHE	CB-CG-CD1	5.45	124.62	120.80
1	A	106	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	218	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	A	240	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	429	ARG	CB-CA-C	-5.38	99.64	110.40
1	A	445	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	548	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	656	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	72	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	630	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	253	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	263	GLN	CA-CB-CG	-5.28	101.78	113.40
1	A	229	LYS	O-C-N	5.23	131.07	122.70
1	A	42	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	468	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	384	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	A	181	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	50	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	383	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	302	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	218	TYR	CB-CG-CD2	5.09	124.06	121.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5335	0	5225	130	0
2	A	12	0	12	0	0
3	A	2	0	0	0	0
4	A	44	0	26	3	0
5	A	36	0	22	4	0
6	A	722	0	0	12	1
All	All	6151	0	5285	131	1

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 12.

All (131) 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:212:PRO:HB2	1:A:218:TYR:HB2	1.42	1.00
1:A:215:LEU:HB2	5:A:704:UPG:H5C2	1.51	0.93
1:A:229:LYS:HG2	1:A:304:PRO:HG3	1.56	0.85
1:A:222:VAL:HG22	1:A:227:ARG:HB2	1.60	0.84
1:A:246:ARG:HD2	5:A:704:UPG:O1B	1.78	0.82
1:A:230:LEU:HG	1:A:231:TYR:N	1.96	0.80
1:A:212:PRO:HG2	1:A:218:TYR:HA	1.64	0.80
1:A:222:VAL:CG2	1:A:227:ARG:HB2	2.12	0.80
1:A:232:ILE:HG13	1:A:305:TYR:HB2	1.63	0.78
4:A:703:NAD:H4N	5:A:704:UPG:H4'	1.64	0.78
1:A:228:GLU:HG2	1:A:229:LYS:HG3	1.66	0.76
1:A:196:ILE:HG21	1:A:216:LEU:HD13	1.67	0.75
1:A:411[A]:ASN:ND2	1:A:414:GLY:H	1.84	0.73
1:A:411[A]:ASN:ND2	6:A:1073:HOH:O	2.21	0.73
1:A:489:ILE:HD13	1:A:502:LEU:HD12	1.73	0.71
1:A:318:LEU:HD23	5:A:704:UPG:O6'	1.92	0.69
1:A:179:ASN:OD1	1:A:182:LYS:HE3	1.93	0.68
1:A:657:GLU:O	1:A:660:GLN:HG3	1.93	0.68
1:A:610:PRO:HG3	1:A:669:TYR:CZ	2.29	0.68
1:A:245:ILE:O	1:A:246:ARG:NE	2.26	0.68
1:A:548:ASP:C	6:A:1328:HOH:O	2.32	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:H	1:A:304:PRO:HG2	1.61	0.65
1:A:269:ASN:HB2	1:A:272:GLU:OE1	1.96	0.64
1:A:575:ILE:HG21	1:A:606:GLU:HG3	1.81	0.63
1:A:438:LYS:HE3	1:A:447:GLN:OE1	1.99	0.63
1:A:570:ILE:HG23	1:A:571:PRO:HD2	1.81	0.62
1:A:212:PRO:CG	1:A:218:TYR:HA	2.30	0.61
1:A:338:GLU:HG3	6:A:1050:HOH:O	2.00	0.61
1:A:289:PHE:O	1:A:292:TYR:HB3	1.99	0.61
1:A:411[A]:ASN:HD21	1:A:414:GLY:H	1.47	0.61
1:A:586:THR:HG23	6:A:1158:HOH:O	2.00	0.60
1:A:246:ARG:NH2	1:A:315:VAL:O	2.34	0.60
1:A:436:LYS:HA	1:A:454:VAL:O	2.01	0.59
1:A:59:THR:O	1:A:61:HIS:HD2	1.85	0.58
1:A:506:GLN:HB2	6:A:1122:HOH:O	2.03	0.58
1:A:74:LYS:N	1:A:74:LYS:HD3	2.18	0.57
1:A:229:LYS:HA	1:A:304:PRO:HG3	1.85	0.57
1:A:192:TYR:HB2	4:A:703:NAD:H5N	1.87	0.57
1:A:316:LEU:HD12	1:A:316:LEU:C	2.24	0.56
1:A:299:SER:O	1:A:301:ILE:HG13	2.04	0.56
1:A:304:PRO:O	1:A:305:TYR:HB3	2.06	0.56
1:A:619:GLU:HB2	6:A:1255:HOH:O	2.06	0.56
1:A:557:VAL:O	1:A:582:THR:HA	2.05	0.55
1:A:229:LYS:CG	1:A:304:PRO:HG3	2.34	0.55
1:A:292:TYR:OH	1:A:303:LEU:O	2.24	0.55
1:A:218:TYR:HE1	1:A:230:LEU:HA	1.72	0.54
1:A:212:PRO:HB2	1:A:218:TYR:CB	2.27	0.54
1:A:292:TYR:OH	1:A:305:TYR:HD2	1.91	0.54
1:A:196:ILE:CG2	1:A:216:LEU:HD13	2.37	0.53
1:A:222:VAL:HG22	1:A:227:ARG:CB	2.36	0.53
1:A:411[A]:ASN:ND2	1:A:413:GLU:N	2.57	0.53
1:A:477:PRO:HD2	1:A:481:VAL:O	2.08	0.53
1:A:605:ASP:OD1	1:A:607:ASN:HB2	2.10	0.52
1:A:209:LEU:O	1:A:209:LEU:HD23	2.10	0.52
1:A:229:LYS:HA	1:A:304:PRO:CG	2.41	0.51
1:A:327:ARG:HD2	6:A:1368:HOH:O	2.09	0.51
1:A:595:ASN:HB3	1:A:596:PRO:HA	1.91	0.51
1:A:186:LYS:HA	1:A:274:LEU:HD13	1.92	0.51
1:A:245:ILE:HG22	1:A:246:ARG:N	2.25	0.51
1:A:218:TYR:CE1	1:A:230:LEU:HA	2.46	0.51
1:A:610:PRO:HG3	1:A:669:TYR:OH	2.12	0.50
1:A:315:VAL:O	1:A:316:LEU:C	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LYS:HE2	6:A:912:HOH:O	2.11	0.50
1:A:287:THR:HG23	1:A:290:GLU:HB2	1.92	0.49
1:A:489:ILE:HD13	1:A:502:LEU:CD1	2.42	0.49
1:A:440:SER:HA	1:A:444:LYS:O	2.13	0.49
1:A:287:THR:O	1:A:288:VAL:C	2.49	0.49
1:A:222:VAL:HG23	1:A:227:ARG:HB2	1.92	0.48
1:A:561:LYS:HD3	1:A:577:ASP:OD1	2.12	0.48
1:A:214:ASN:O	1:A:217:PRO:HD2	2.13	0.48
1:A:364:PHE:CZ	1:A:369:MET:HA	2.48	0.48
1:A:247:ASP:HB2	1:A:319:THR:HA	1.94	0.48
1:A:193:PHE:O	1:A:195:PRO:HD3	2.13	0.48
1:A:243:THR:CG2	1:A:288:VAL:HB	2.44	0.48
1:A:315:VAL:HG13	6:A:768:HOH:O	2.13	0.47
1:A:56:GLU:OE2	1:A:62:HIS:ND1	2.42	0.47
1:A:316:LEU:HD12	1:A:316:LEU:O	2.14	0.47
1:A:379:GLY:O	1:A:385:GLN:HG2	2.15	0.47
1:A:214:ASN:O	1:A:215:LEU:C	2.53	0.47
1:A:517[A]:GLU:HG2	1:A:695:VAL:HG22	1.98	0.46
1:A:419:ASP:O	1:A:654:ALA:HB2	2.15	0.46
1:A:212:PRO:HB3	1:A:217:PRO:HB2	1.97	0.46
1:A:214:ASN:C	1:A:217:PRO:HD2	2.36	0.46
1:A:465:HIS:CE1	1:A:466:ARG:HG3	2.51	0.46
1:A:223:ALA:HB1	1:A:301:ILE:HD12	1.98	0.45
1:A:229:LYS:HG2	1:A:304:PRO:CG	2.38	0.45
1:A:295:PHE:HD2	1:A:303:LEU:HD11	1.81	0.45
1:A:566:ASP:OD1	1:A:568:ASN:N	2.43	0.45
1:A:301:ILE:HG22	1:A:302:ASP:N	2.31	0.45
1:A:430:TYR:CD2	1:A:434:ILE:HD11	2.51	0.45
1:A:610:PRO:HG3	1:A:669:TYR:CE1	2.52	0.45
1:A:370:ARG:NH1	6:A:1228:HOH:O	2.34	0.45
1:A:214:ASN:HB2	6:A:714:HOH:O	2.16	0.45
1:A:224:VAL:HG21	1:A:348:THR:HG22	1.99	0.45
1:A:283:GLY:HA2	1:A:320:ALA:O	2.17	0.44
1:A:587:LYS:HB3	6:A:1329:HOH:O	2.16	0.44
1:A:130:PHE:HB3	1:A:187:PHE:CD1	2.53	0.44
1:A:195:PRO:HA	1:A:249:ILE:O	2.18	0.44
1:A:243:THR:HG21	1:A:288:VAL:HB	2.00	0.44
1:A:287:THR:OG1	1:A:290:GLU:HG3	2.18	0.44
1:A:562:SER:CB	1:A:578:ARG:HE	2.30	0.44
1:A:27:THR:HA	1:A:255:ALA:HB1	2.00	0.43
1:A:269:ASN:N	1:A:272:GLU:OE1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ILE:CG2	1:A:571:PRO:HD2	2.48	0.43
1:A:606:GLU:O	1:A:606:GLU:HG2	2.18	0.43
1:A:182:LYS:O	1:A:273:GLY:HA3	2.19	0.43
1:A:489:ILE:CD1	1:A:502:LEU:CD1	2.96	0.43
1:A:17:THR:OG1	1:A:90:HIS:HA	2.19	0.43
1:A:540:PHE:O	1:A:661:GLY:HA2	2.19	0.42
1:A:245:ILE:CG2	1:A:246:ARG:N	2.83	0.42
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.81	0.42
1:A:221:GLN:O	1:A:226:ARG:N	2.49	0.42
1:A:479:LYS:O	1:A:480:ASP:HB2	2.19	0.42
1:A:417:ASN:OD1	1:A:418:PRO:HD2	2.20	0.42
1:A:469:PHE:CE2	1:A:488:LEU:HB2	2.55	0.41
1:A:671:ASP:O	1:A:675:GLN:HG2	2.20	0.41
1:A:365:SER:CB	1:A:375:PHE:CE1	3.04	0.41
1:A:212:PRO:CB	1:A:218:TYR:HB2	2.31	0.41
1:A:628:HIS:ND1	1:A:629:PRO:HD2	2.35	0.41
1:A:653:SER:HB2	1:A:654:ALA:H	1.61	0.41
1:A:219:MET:CE	1:A:295:PHE:CB	2.99	0.41
1:A:15:LEU:HB3	1:A:88:VAL:HG22	2.03	0.41
1:A:288:VAL:O	1:A:291:VAL:HB	2.21	0.41
1:A:317:ASN:OD1	1:A:318:LEU:N	2.54	0.41
1:A:178:TYR:CZ	1:A:182:LYS:HG2	2.56	0.40
1:A:318:LEU:HD12	1:A:318:LEU:HA	1.67	0.40
1:A:192:TYR:HB2	4:A:703:NAD:C5N	2.51	0.40
1:A:292:TYR:CZ	1:A:305:TYR:HD2	2.40	0.40
1:A:411[A]:ASN:HD21	1:A:414:GLY:N	2.16	0.40

All (1) 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)
6:A:1156:HOH:O	6:A:1156:HOH:O[2_665]	1.94	0.26

## 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	671/699 (96%)	638 (95%)	33 (5%)	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	583/601 (97%)	551 (94%)	32 (6%)	21	7

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

Mol	Chain	Res	Type
1	A	43	ASN
1	A	50	ASP
1	A	74	LYS
1	A	148	MET
1	A	159	PRO
1	A	214	ASN
1	A	230	LEU
1	A	243	THR
1	A	245	ILE
1	A	246	ARG
1	A	271	ASN
1	A	274	LEU
1	A	277	GLU
1	A	287	THR
1	A	302	ASP
1	A	303	LEU
1	A	327	ARG
1	A	383	ARG
1	A	411[A]	ASN
1	A	411[B]	ASN
1	A	432	ASN

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Mol	Chain	Res	Type
1	A	436	LYS
1	A	438	LYS
1	A	444	LYS
1	A	493	LYS
1	A	559	SER
1	A	567	LYS
1	A	586	THR
1	A	587	LYS
1	A	609	LYS
1	A	619	GLU
1	A	688	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	61	HIS
1	A	506	GLN
1	A	543	ASN
1	A	584	ASN
1	A	612	GLN
1	A	618	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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$
4	NAD	A	703	-	42,48,48	1.33	5 (11%)	50,73,73	1.88	8 (16%)
5	UPG	A	704	-	31,38,38	1.47	4 (12%)	41,58,58	2.11	7 (17%)
2	GAL	A	700	-	12,12,12	0.77	0	17,17,17	1.00	1 (5%)

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
4	NAD	A	703	-	-	7/26/62/62	0/5/5/5
5	UPG	A	704	-	-	12/21/59/59	0/3/3/3
2	GAL	A	700	-	-	2/2/22/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	704	UPG	C4-N3	4.88	1.41	1.33
4	A	703	NAD	C4N-C3N	3.94	1.46	1.39
5	A	704	UPG	C6-C5	-2.99	1.31	1.38
4	A	703	NAD	C3N-C7N	2.92	1.55	1.50
5	A	704	UPG	C6-N1	2.92	1.39	1.35
4	A	703	NAD	C2N-N1N	2.86	1.38	1.35
4	A	703	NAD	C6N-N1N	2.68	1.42	1.35
5	A	704	UPG	PB-O3B	2.57	1.67	1.60
4	A	703	NAD	C2A-N1A	2.43	1.38	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	UPG	O3A-PB-O3B	6.36	115.31	102.48
4	A	703	NAD	C5N-C6N-N1N	-6.34	111.31	120.40
5	A	704	UPG	O4'-C4'-C3'	5.37	122.76	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	NAD	C5N-C4N-C3N	-4.97	114.46	120.34
5	A	704	UPG	C5-C4-N3	-4.86	112.61	123.31
4	A	703	NAD	C3N-C7N-N7N	4.75	123.45	117.75
4	A	703	NAD	C6N-C5N-C4N	4.52	126.01	119.44
5	A	704	UPG	C3'-C4'-C5'	-4.43	102.34	110.24
5	A	704	UPG	C1'-C2'-C3'	4.02	118.38	110.00
4	A	703	NAD	C6N-N1N-C2N	3.86	125.49	121.97
4	A	703	NAD	O7N-C7N-N7N	-3.53	117.57	122.58
5	A	704	UPG	O5C-PA-O1A	3.31	122.00	109.07
5	A	704	UPG	C3C-C2C-C1C	2.76	105.14	100.98
4	A	703	NAD	C5A-C6A-N1A	-2.74	114.14	120.35
4	A	703	NAD	N6A-C6A-N1A	2.25	123.25	118.57
2	A	700	GAL	O5-C5-C6	-2.08	101.25	106.44

There are no chirality outliers.

All (21) torsion outliers are listed below:

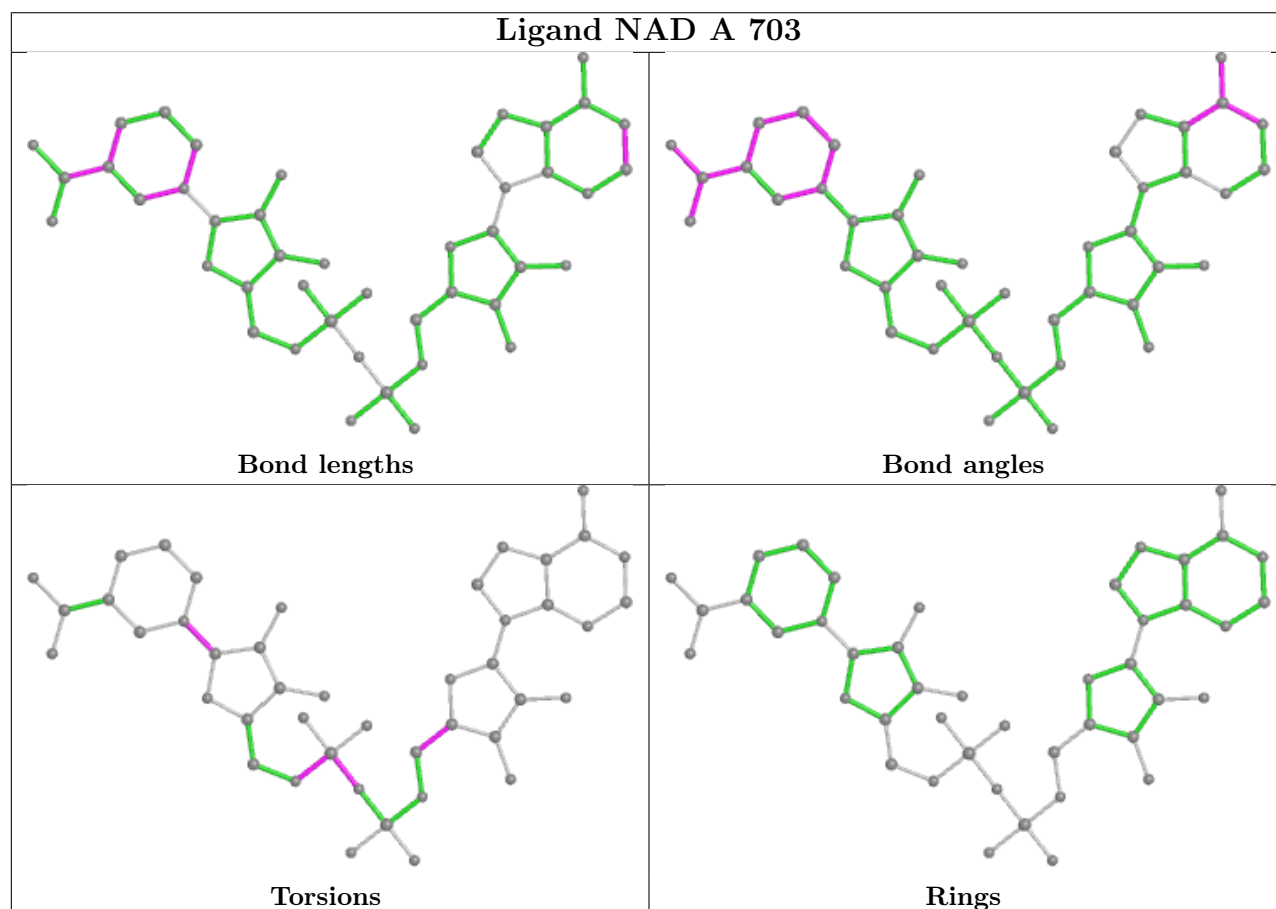
Mol	Chain	Res	Type	Atoms
4	A	703	NAD	C5D-O5D-PN-O2N
4	A	703	NAD	O4D-C1D-N1N-C2N
5	A	704	UPG	C2C-C1C-N1-C6
5	A	704	UPG	O4C-C1C-N1-C6
5	A	704	UPG	C5C-O5C-PA-O2A
2	A	700	GAL	O5-C5-C6-O6
5	A	704	UPG	C3C-C4C-C5C-O5C
5	A	704	UPG	O4C-C4C-C5C-O5C
2	A	700	GAL	C4-C5-C6-O6
5	A	704	UPG	C1'-O3B-PB-O3A
4	A	703	NAD	C5D-O5D-PN-O3
5	A	704	UPG	C5C-O5C-PA-O3A
5	A	704	UPG	O5'-C5'-C6'-O6'
4	A	703	NAD	O4B-C4B-C5B-O5B
5	A	704	UPG	PA-O3A-PB-O2B
4	A	703	NAD	PA-O3-PN-O1N
4	A	703	NAD	PA-O3-PN-O2N
5	A	704	UPG	PA-O3A-PB-O1B
4	A	703	NAD	C5D-O5D-PN-O1N
5	A	704	UPG	C5C-O5C-PA-O1A
5	A	704	UPG	C4'-C5'-C6'-O6'

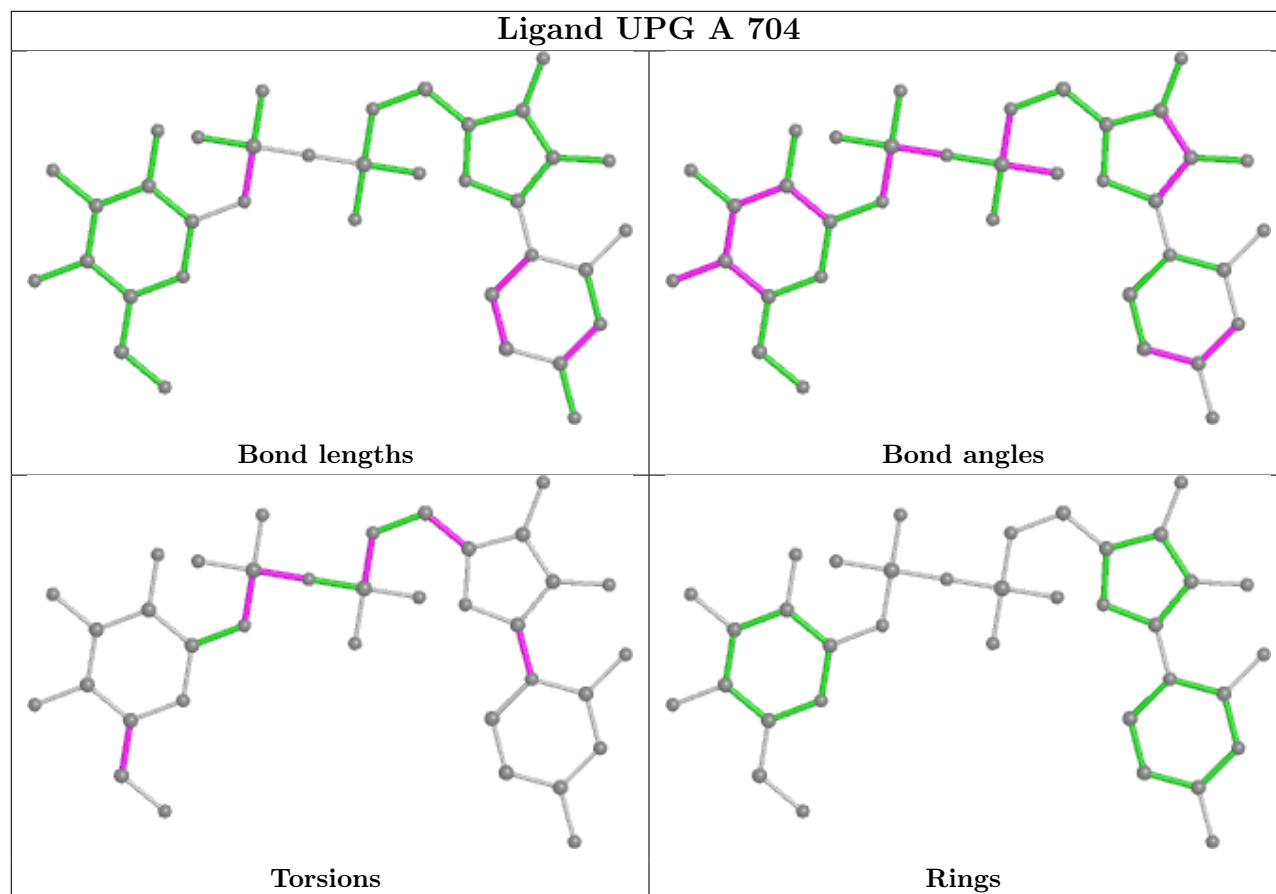
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	NAD	3	0
5	A	704	UPG	4	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	674/699 (96%)	-0.22	24 (3%) 42 40	9, 21, 60, 97	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	PHE	8.7
1	A	304	PRO	6.3
1	A	305	TYR	5.0
1	A	231	TYR	4.7
1	A	230	LEU	4.5
1	A	607	ASN	4.2
1	A	229	LYS	4.2
1	A	289	PHE	3.9
1	A	243	THR	3.8
1	A	211	ILE	3.6
1	A	316	LEU	3.4
1	A	240	ARG	3.3
1	A	443	ASN	3.2
1	A	609	LYS	3.1
1	A	608	ALA	2.9
1	A	232	ILE	2.7
1	A	241	ASP	2.6
1	A	244	PRO	2.6
1	A	315	VAL	2.5
1	A	242	GLY	2.4
1	A	292	TYR	2.4
1	A	271	ASN	2.3
1	A	303	LEU	2.2
1	A	546	TYR	2.1

## 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](#)

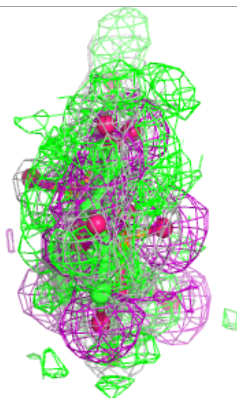
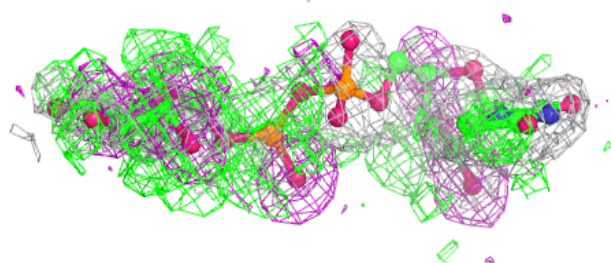
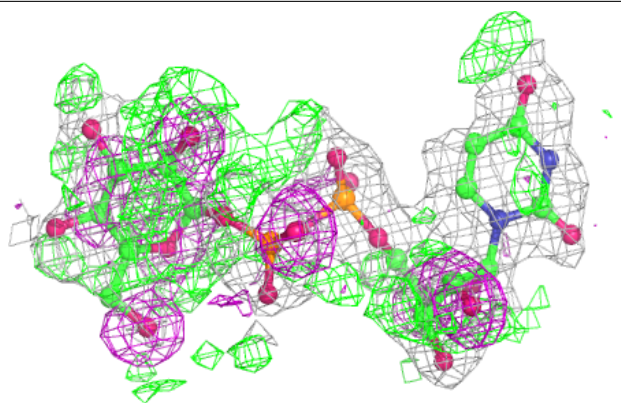
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	UPG	A	704	36/36	0.42	0.40	0,50,88,91	0
3	NA	A	702	1/1	0.78	0.19	51,51,51,51	0
3	NA	A	701	1/1	0.95	0.18	38,38,38,38	0
2	GAL	A	700	12/12	0.97	0.10	15,21,27,29	0
4	NAD	A	703	44/44	0.98	0.09	6,14,19,26	0

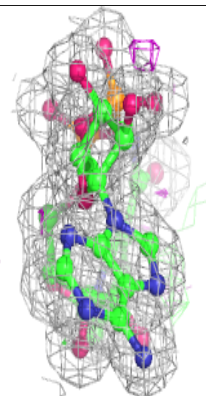
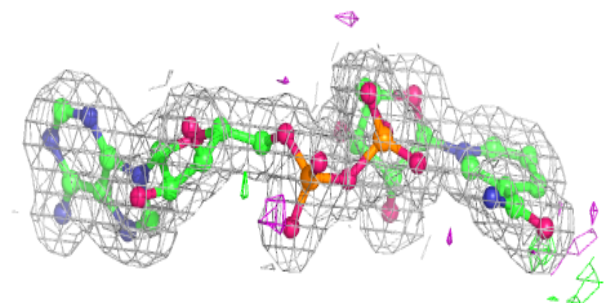
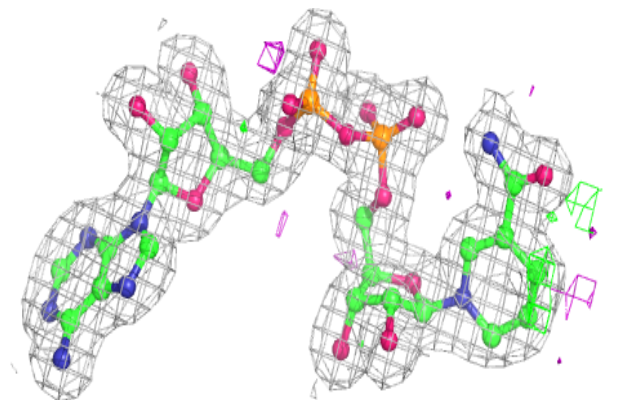
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around UPG A 704:**

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

**Electron density around NAD A 703:**

$2mF_o-DF_c$  (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.