



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:55 PM UTC

PDB ID : 1Z45 / pdb_00001z45
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

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

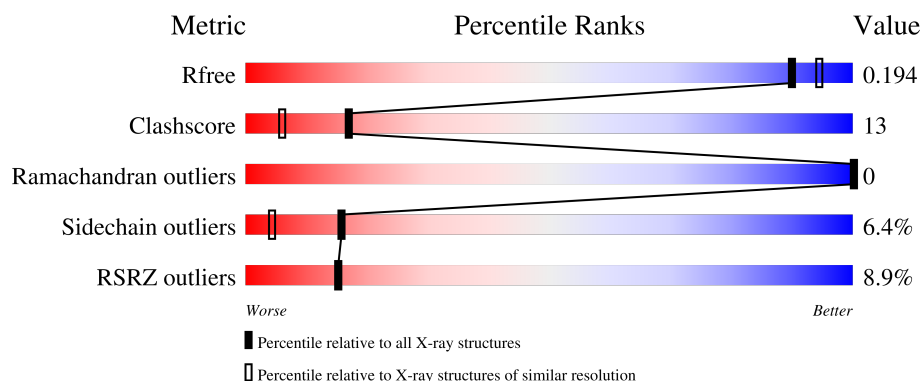
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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 ≥ 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	9% 68% 23% 5%

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.

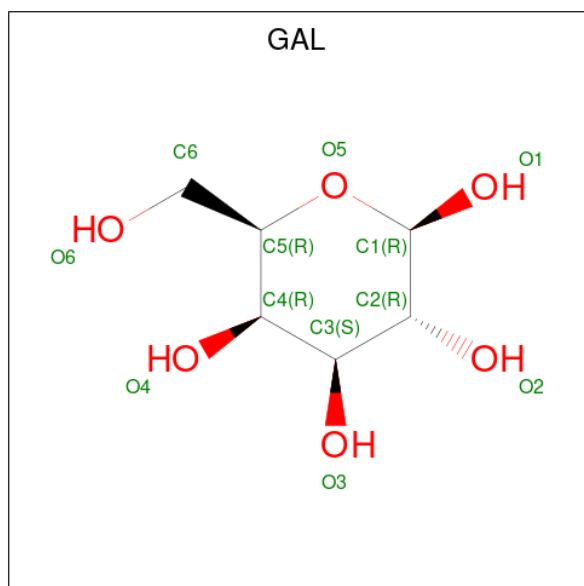
- Molecule 1 is a protein called GAL10 bifunctional protein.

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 (CCD ID: GAL) (formula: C₆H₁₂O₆).

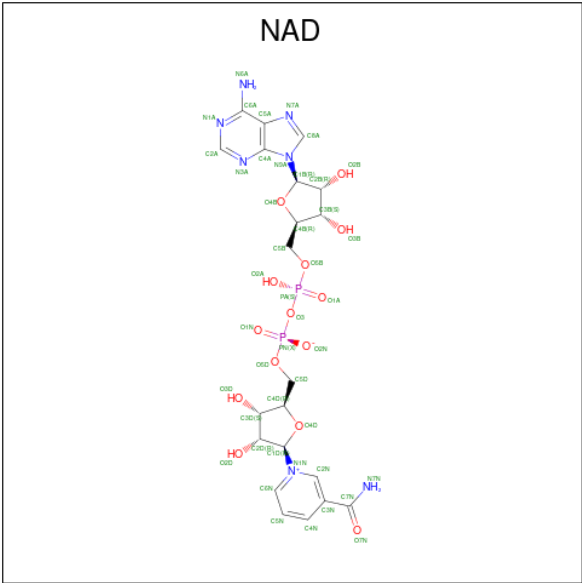


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

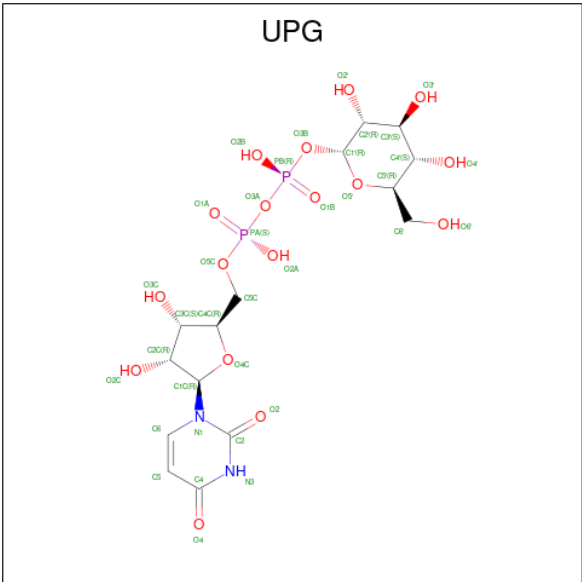
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 5 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: C₁₅H₂₄N₂O₁₇P₂).



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

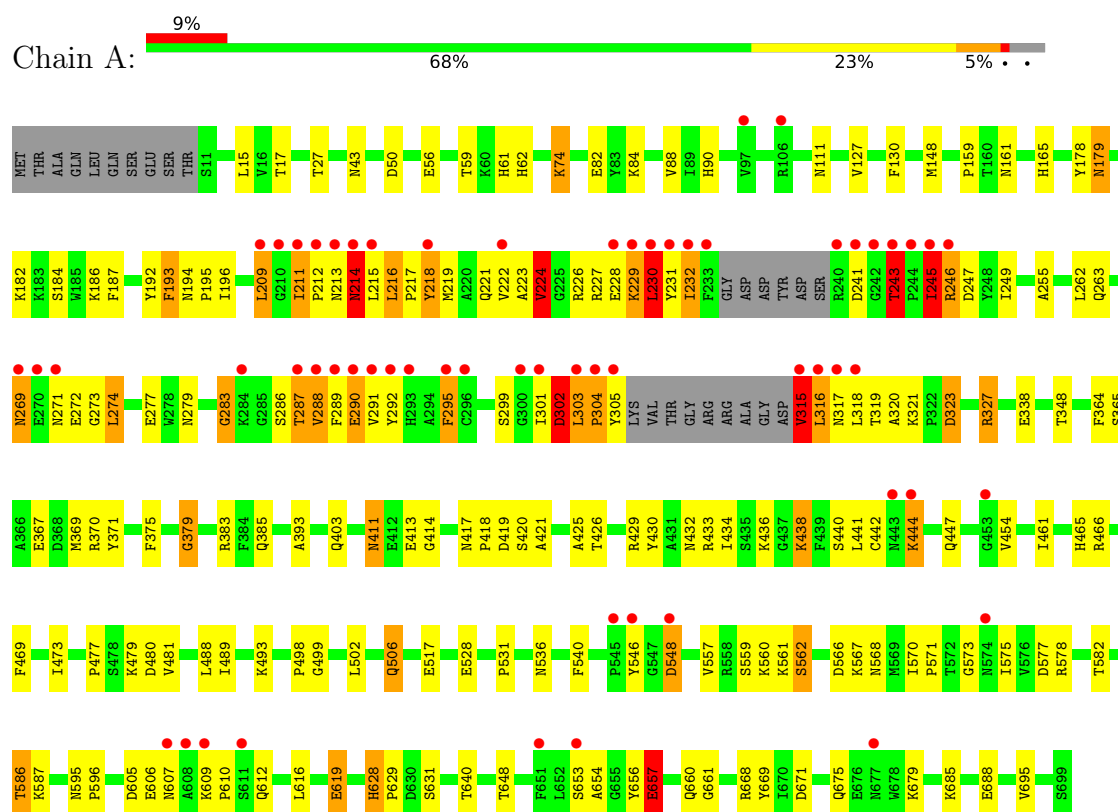
- Molecule 6 is water.

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, α , β , γ	120.90Å 125.20Å 142.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 30.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-1.85) 97.7 (30.00-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	17.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 109.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.12	0/5468	1.65	79/7421 (1.1%)

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ASN	CA-CB-CG	-9.34	103.26	112.60
1	A	243	THR	N-CA-C	9.09	121.10	109.65
1	A	612	GLN	N-CA-C	8.83	124.12	109.46
1	A	214	ASN	CB-CA-C	7.76	122.33	109.53
1	A	216	LEU	N-CA-C	7.67	122.91	112.55
1	A	165	HIS	CA-CB-CG	-7.57	106.23	113.80
1	A	211	ILE	N-CA-CB	7.23	121.33	111.21
1	A	321	LYS	N-CA-C	-7.23	98.05	109.04
1	A	245	ILE	N-CA-C	7.13	120.02	108.97
1	A	628	HIS	CA-CB-CG	-7.02	106.78	113.80
1	A	425	ALA	N-CA-C	6.96	119.95	110.55
1	A	229	LYS	O-C-N	6.86	131.07	123.25
1	A	214	ASN	N-CA-C	6.80	121.38	109.96
1	A	631	SER	N-CA-C	-6.77	105.31	113.97
1	A	536	ASN	CA-CB-CG	-6.75	105.84	112.60
1	A	179	ASN	CA-CB-CG	-6.74	105.86	112.60
1	A	433	ARG	N-CA-C	6.70	121.21	109.96
1	A	562	SER	N-CA-CB	-6.55	100.30	111.69
1	A	379	GLY	N-CA-C	-6.42	105.19	115.08
1	A	315	VAL	CA-C-N	-6.41	109.29	121.54
1	A	315	VAL	C-N-CA	-6.41	109.29	121.54
1	A	159	PRO	N-CA-CB	6.37	108.89	103.35
1	A	279	ASN	CB-CA-C	-6.31	98.86	109.53
1	A	213	ASN	N-CA-C	-6.23	105.51	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	ASP	CA-CB-CG	-6.19	106.41	112.60
1	A	263	GLN	CA-CB-CG	-6.16	101.78	114.10
1	A	241	ASP	N-CA-C	-6.14	105.69	113.43
1	A	656	TYR	CA-CB-CG	-6.04	103.03	113.90
1	A	371	TYR	N-CA-C	5.96	119.81	112.54
1	A	573	GLY	N-CA-C	-5.94	106.89	114.37
1	A	224	VAL	CA-CB-CG1	5.92	120.46	110.40
1	A	302	ASP	CB-CA-C	-5.90	101.83	111.68
1	A	528	GLU	CB-CG-CD	-5.89	102.58	112.60
1	A	82	GLU	CA-CB-CG	-5.77	102.55	114.10
1	A	426	THR	N-CA-C	-5.77	100.58	109.76
1	A	111	ASN	N-CA-C	5.75	117.35	111.14
1	A	127	VAL	CA-C-O	-5.68	114.49	120.57
1	A	193	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	403	GLN	N-CA-CB	-5.63	101.71	110.55
1	A	304	PRO	CB-CA-C	-5.62	101.62	110.96
1	A	161	ASN	CA-CB-CG	-5.58	107.02	112.60
1	A	230	LEU	N-CA-CB	5.52	119.58	110.69
1	A	420	SER	N-CA-C	5.51	118.02	110.24
1	A	429	ARG	CB-CA-C	-5.51	99.64	110.10
1	A	546	TYR	CA-C-N	-5.50	110.64	121.41
1	A	546	TYR	C-N-CA	-5.50	110.64	121.41
1	A	224	VAL	N-CA-CB	-5.45	105.07	112.16
1	A	288	VAL	CA-CB-CG1	-5.45	101.13	110.40
1	A	679	LYS	N-CA-C	5.42	118.69	111.75
1	A	499	GLY	N-CA-C	5.38	119.45	112.68
1	A	616	LEU	CA-C-N	-5.37	113.67	122.54
1	A	616	LEU	C-N-CA	-5.37	113.67	122.54
1	A	302	ASP	CA-C-N	-5.32	112.96	121.57
1	A	302	ASP	C-N-CA	-5.32	112.96	121.57
1	A	290	GLU	CA-C-N	5.31	127.19	120.72
1	A	290	GLU	C-N-CA	5.31	127.19	120.72
1	A	648	THR	N-CA-C	5.29	119.44	113.15
1	A	295	PHE	CA-CB-CG	-5.29	108.51	113.80
1	A	283	GLY	N-CA-C	-5.26	108.05	115.32
1	A	194	ASN	CA-CB-CG	-5.26	107.34	112.60
1	A	323	ASP	N-CA-C	5.26	117.02	111.28
1	A	640	THR	N-CA-C	-5.26	106.64	113.16
1	A	304	PRO	N-CA-C	-5.24	101.97	110.40
1	A	184	SER	CB-CA-C	-5.22	101.90	110.72
1	A	209	LEU	N-CA-CB	-5.21	101.69	110.49
1	A	498	PRO	CB-CA-C	-5.21	103.18	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	SER	CA-C-O	5.19	125.96	120.36
1	A	657	GLU	CB-CG-CD	-5.19	103.78	112.60
1	A	393	ALA	N-CA-C	-5.18	104.50	111.54
1	A	461	ILE	N-CA-C	5.14	117.48	111.05
1	A	218	TYR	CB-CA-C	5.13	119.00	110.90
1	A	531	PRO	N-CA-C	-5.12	102.56	111.32
1	A	473	ILE	N-CA-C	-5.11	100.52	107.99
1	A	668	ARG	N-CA-C	5.10	118.34	107.67
1	A	224	VAL	CB-CA-C	5.09	117.86	111.65
1	A	506	GLN	CA-CB-CG	-5.07	103.96	114.10
1	A	421	ALA	N-CA-C	-5.06	106.36	112.88
1	A	286	SER	N-CA-CB	5.04	119.14	110.68
1	A	127	VAL	N-CA-C	-5.01	101.20	108.36

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	5335	0	5225	135	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	5	0
6	A	722	0	0	12	1
All	All	6151	0	5285	136	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 13.

All (136) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:548:ASP:C	6:A:1328:HOH:O	2.32	0.71
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: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:316:LEU:HD12	1:A:316:LEU:C	2.24	0.62
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:315:VAL:O	1:A:316:LEU:C	2.46	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:287:THR:O	1:A:288:VAL:C	2.49	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:214:ASN:O	1:A:215:LEU:C	2.53	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:214:ASN:C	1:A:217:PRO:HD2	2.36	0.50
1:A:610:PRO:HG3	1:A:669:TYR:OH	2.12	0.50
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:441:LEU:O	1:A:442:CYS:C	2.63	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:318:LEU:HD23	5:A:704:UPG:HO6'	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:245:ILE:C	1:A:246:ARG:HE	2.29	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
1:A:657:GLU:HG2	1:A:660:GLN:CD	2.47	0.40
1:A:277:GLU:CD	1:A:277:GLU:N	2.80	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 [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	583/601 (97%)	545 (94%)	38 (6%)	15 4

All (38) 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	84	LYS
1	A	148	MET
1	A	211	ILE
1	A	214	ASN
1	A	224	VAL
1	A	230	LEU
1	A	232	ILE
1	A	243	THR
1	A	245	ILE
1	A	246	ARG
1	A	271	ASN
1	A	274	LEU
1	A	287	THR
1	A	302	ASP
1	A	303	LEU
1	A	315	VAL
1	A	316	LEU
1	A	323	ASP
1	A	327	ARG
1	A	367	GLU
1	A	383	ARG
1	A	411[A]	ASN
1	A	411[B]	ASN
1	A	432	ASN
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	609	LYS
1	A	619	GLU
1	A	657	GLU

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Mol	Chain	Res	Type
1	A	685	LYS
1	A	688	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	61	HIS
1	A	390	ASN
1	A	491	ASN
1	A	506	GLN
1	A	543	ASN
1	A	612	GLN
1	A	618	ASN
1	A	686	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	GAL	A	700	-	12,12,12	0.76	0	17,17,17	1.00	1 (5%)
5	UPG	A	704	-	37,38,38	1.39	3 (8%)	55,58,58	1.61	7 (12%)
4	NAD	A	703	-	46,48,48	1.40	7 (15%)	64,73,73	1.73	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	A	700	-	-	2/2/22/22	0/1/1/1
5	UPG	A	704	-	-	11/23/59/59	0/3/3/3
4	NAD	A	703	-	-	7/30/62/62	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	704	UPG	PA-O3A	5.66	1.65	1.59
4	A	703	NAD	C4N-C3N	4.38	1.46	1.39
4	A	703	NAD	C2N-N1N	3.14	1.38	1.35
4	A	703	NAD	C3N-C7N	2.93	1.55	1.50
4	A	703	NAD	C6N-N1N	2.91	1.42	1.35
5	A	704	UPG	PB-O3A	-2.82	1.56	1.59
5	A	704	UPG	PB-O3B	2.63	1.67	1.59
4	A	703	NAD	C2A-N1A	2.53	1.38	1.33
4	A	703	NAD	C5N-C4N	2.22	1.42	1.38
4	A	703	NAD	C7N-N7N	2.05	1.36	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	NAD	C5N-C6N-N1N	-6.65	111.31	120.38
4	A	703	NAD	C5N-C4N-C3N	-6.01	114.46	120.36
5	A	704	UPG	O4'-C4'-C3'	5.25	122.76	110.38
4	A	703	NAD	C3N-C7N-N7N	4.64	123.45	117.74
4	A	703	NAD	C6N-C5N-C4N	4.55	126.01	119.45
5	A	704	UPG	C3'-C4'-C5'	-4.35	102.34	110.23
4	A	703	NAD	C6N-N1N-C2N	4.25	125.49	121.88
5	A	704	UPG	C1'-C2'-C3'	3.98	118.38	110.01
4	A	703	NAD	O7N-C7N-N7N	-3.49	117.57	122.62
5	A	704	UPG	O5C-PA-O1A	3.30	122.00	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	UPG	O4C-C1C-N1	2.75	114.60	108.36
5	A	704	UPG	O3A-PB-O1B	-2.37	103.57	110.70
5	A	704	UPG	O4-C4-N3	2.27	122.56	119.27
4	A	703	NAD	N6A-C6A-N1A	2.19	123.25	118.38
2	A	700	GAL	O5-C5-C6	-2.09	101.25	106.44

There are no chirality outliers.

All (20) 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	C5C-O5C-PA-O2A
5	A	704	UPG	C3C-C4C-C5C-O5C
5	A	704	UPG	O4C-C4C-C5C-O5C
2	A	700	GAL	O5-C5-C6-O6
2	A	700	GAL	C4-C5-C6-O6
4	A	703	NAD	C5D-O5D-PN-O3
5	A	704	UPG	C1'-O3B-PB-O3A
5	A	704	UPG	O5'-C5'-C6'-O6'
5	A	704	UPG	C2C-C1C-N1-C6
5	A	704	UPG	O4C-C1C-N1-C6
4	A	703	NAD	O4D-C1D-N1N-C6N
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	O4B-C4B-C5B-O5B
5	A	704	UPG	O4C-C1C-N1-C2
5	A	704	UPG	C4'-C5'-C6'-O6'

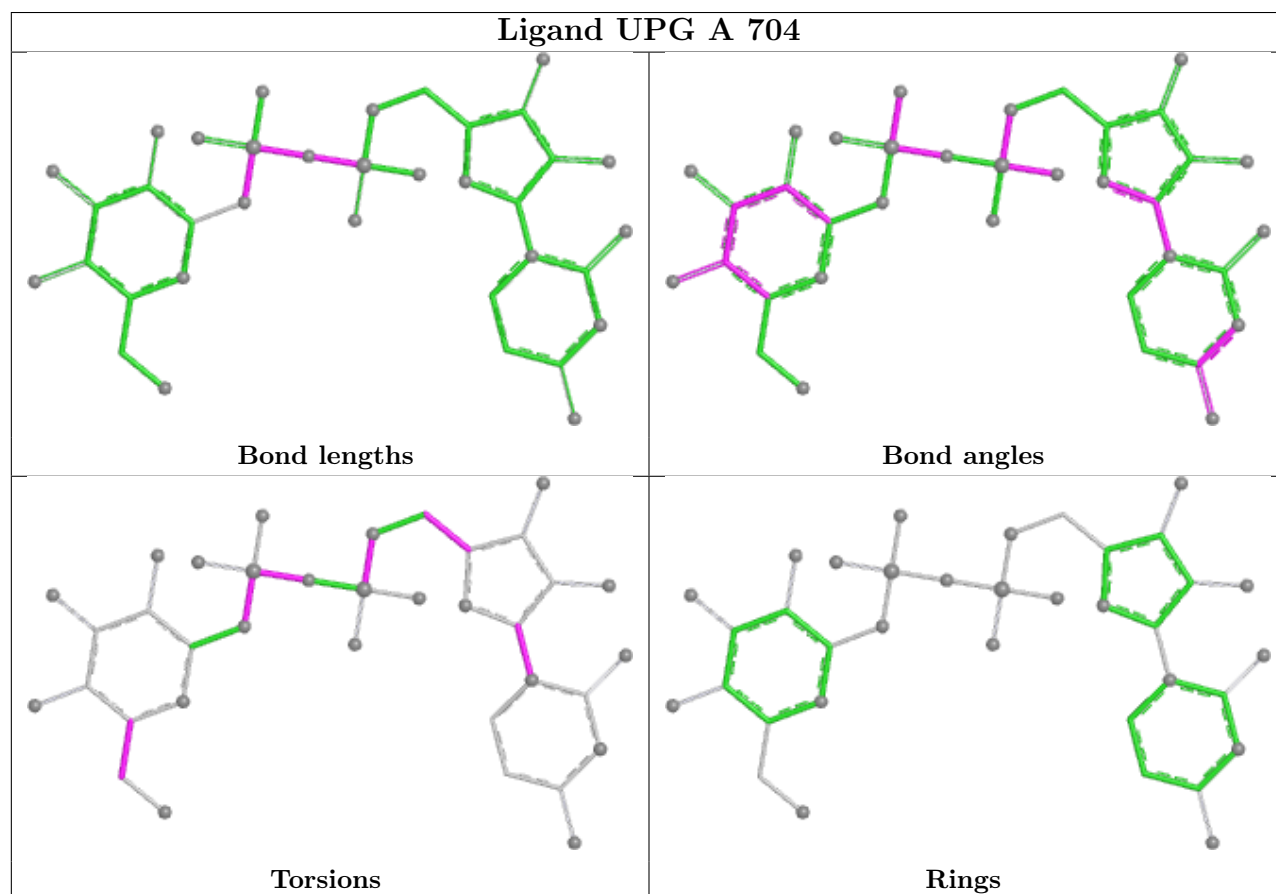
There are no ring outliers.

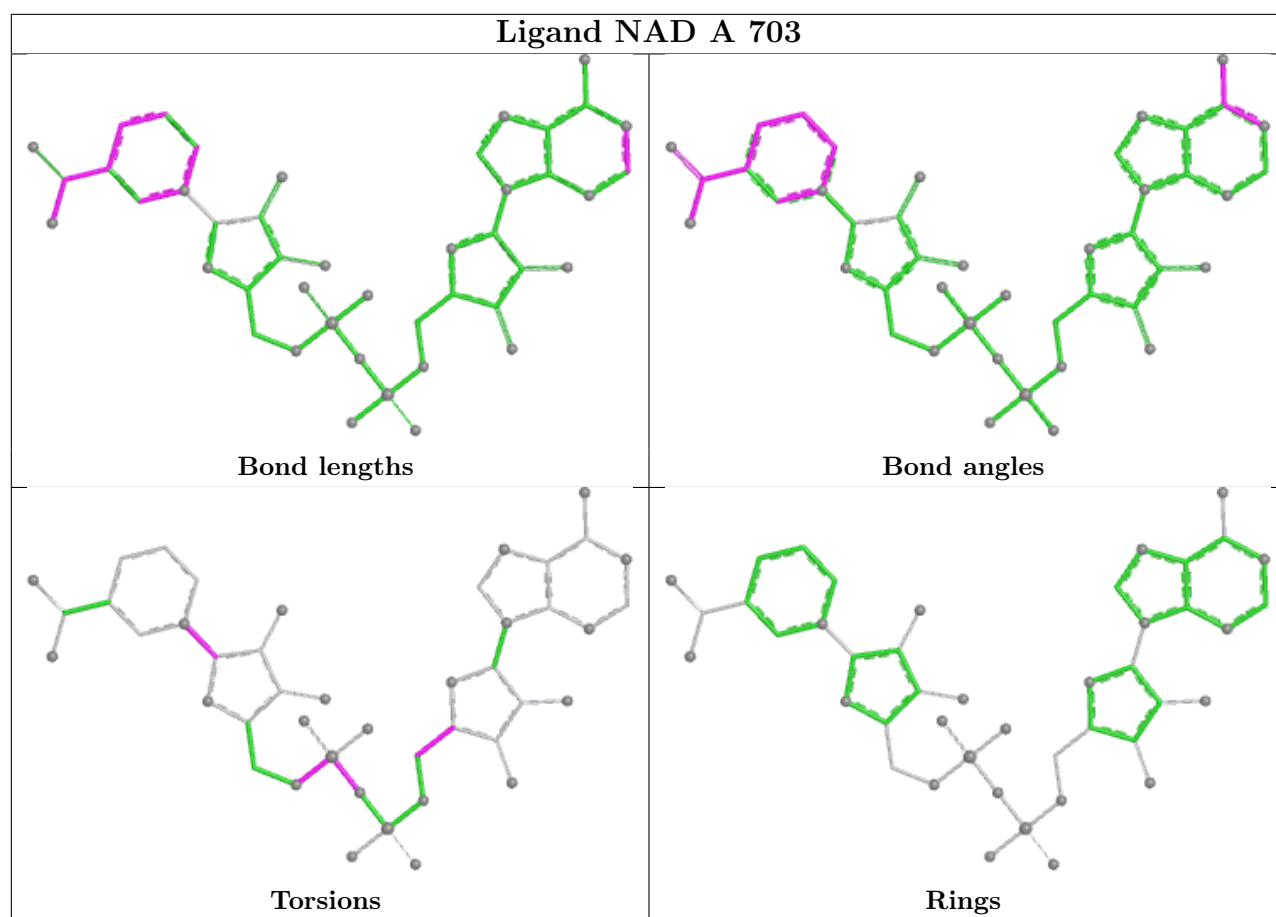
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	UPG	5	0
4	A	703	NAD	3	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	674/699 (96%)	0.08	60 (8%) 15 15	9, 21, 60, 97	3 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	PHE	11.2
1	A	230	LEU	8.2
1	A	305	TYR	8.1
1	A	231	TYR	7.9
1	A	304	PRO	7.8
1	A	243	THR	7.1
1	A	232	ILE	6.9
1	A	211	ILE	6.8
1	A	316	LEU	6.6
1	A	546	TYR	6.5
1	A	289	PHE	6.3
1	A	209	LEU	6.3
1	A	244	PRO	6.3
1	A	210	GLY	6.1
1	A	218	TYR	5.7
1	A	242	GLY	5.6
1	A	229	LYS	5.3
1	A	240	ARG	5.3
1	A	292	TYR	5.0
1	A	287	THR	4.9
1	A	241	ASP	4.8
1	A	212	PRO	4.6
1	A	215	LEU	4.5
1	A	293	HIS	4.3
1	A	222	VAL	4.1
1	A	315	VAL	4.1
1	A	213	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	608	ALA	4.0
1	A	245	ILE	3.9
1	A	607	ASN	3.8
1	A	303	LEU	3.8
1	A	271	ASN	3.7
1	A	284	LYS	3.5
1	A	548	ASP	3.3
1	A	609	LYS	3.1
1	A	291	VAL	3.0
1	A	288	VAL	3.0
1	A	290	GLU	3.0
1	A	318	LEU	2.9
1	A	317	ASN	2.9
1	A	653	SER	2.7
1	A	443	ASN	2.7
1	A	545	PRO	2.7
1	A	301	ILE	2.6
1	A	270	GLU	2.5
1	A	300	GLY	2.5
1	A	611	SER	2.4
1	A	444	LYS	2.4
1	A	228	GLU	2.4
1	A	269	ASN	2.3
1	A	97	VAL	2.2
1	A	453	GLY	2.2
1	A	574	ASN	2.1
1	A	677	ASN	2.1
1	A	295	PHE	2.1
1	A	246	ARG	2.1
1	A	296	CYS	2.1
1	A	651	PHE	2.0
1	A	106	ARG	2.0
1	A	214	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](#)

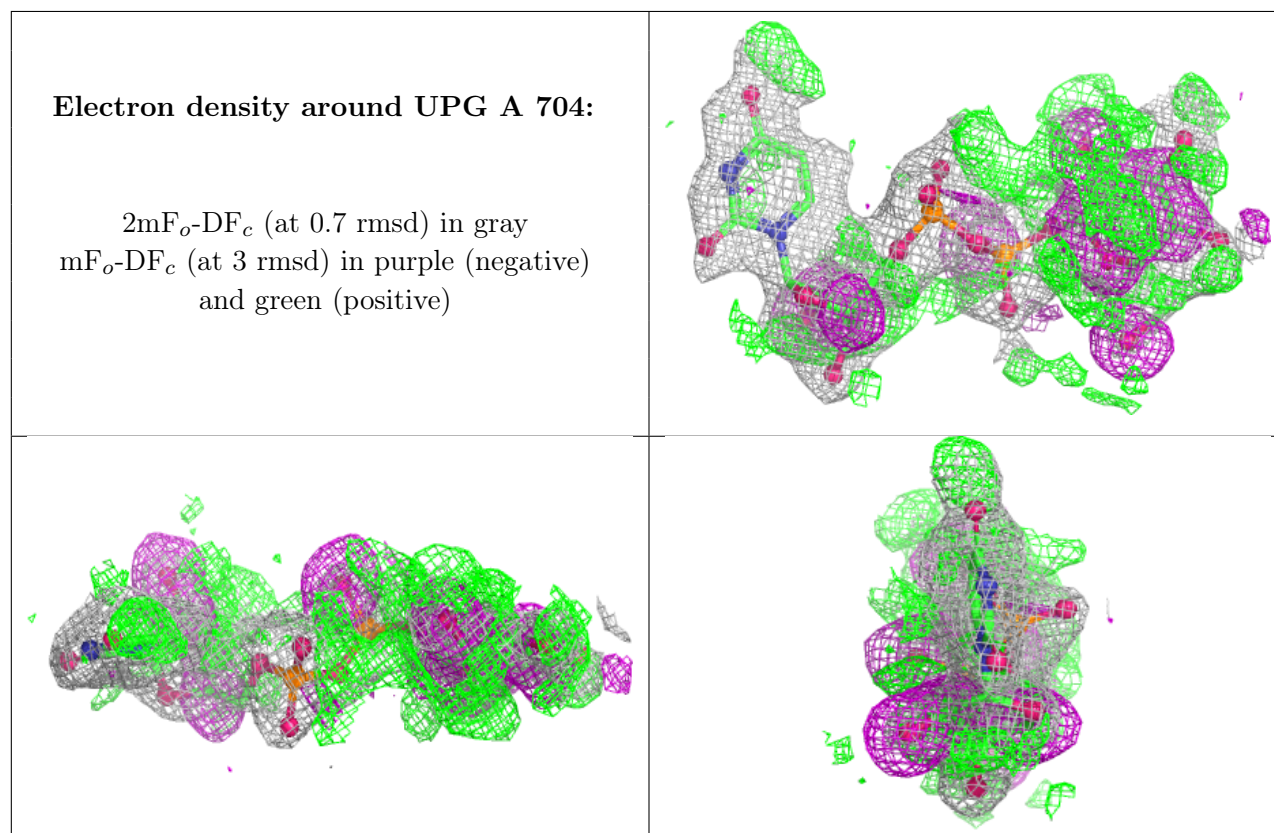
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

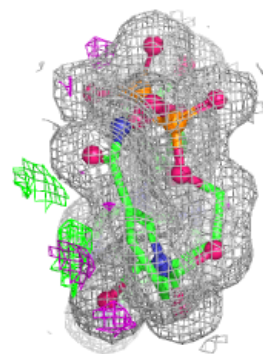
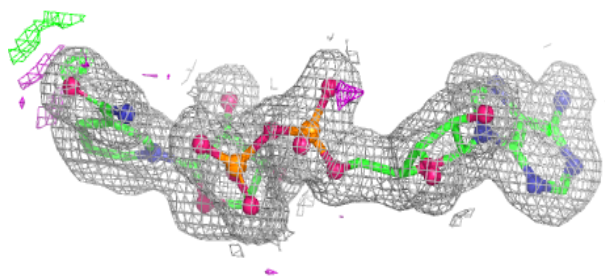
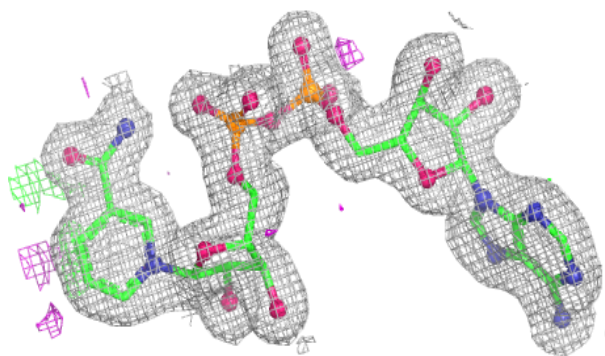
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	UPG	A	704	36/36	0.56	0.34	0,50,88,91	0
3	NA	A	702	1/1	0.86	0.17	51,51,51,51	0
3	NA	A	701	1/1	0.95	0.11	38,38,38,38	0
2	GAL	A	700	12/12	0.97	0.05	15,21,27,29	0
4	NAD	A	703	44/44	0.99	0.04	6,14,19,26	0

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 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 [i](#)

There are no such residues in this entry.