



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 8YVR / pdb_00008yvr
Title : Crystal structure of GH65 alpha-1,2-glucosidase from *Flavobacterium johnsoniae* in complex with 1-deoxynojirimycin
Authors : Nakamura, S.; Miyazaki, T.
Deposited on : 2024-03-29
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

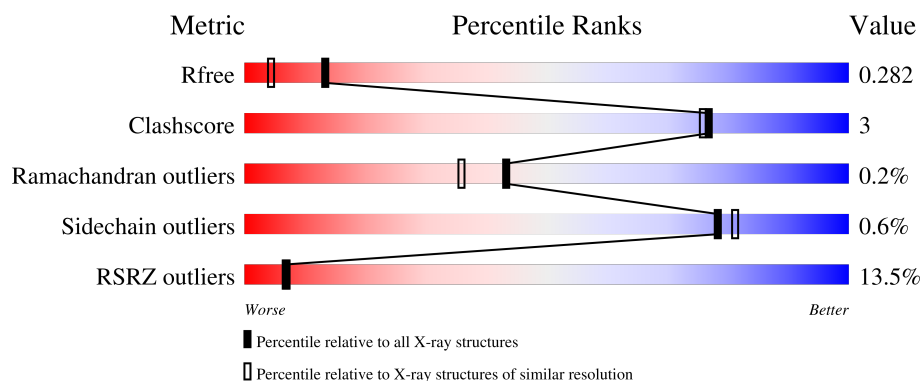
1 Overall quality at a glance

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	678	
1	B	678	
1	C	678	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32187 atoms, of which 15519 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 Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	659	Total	C	H	N	O	S	154	0	0
			10403	3346	5156	882	998	21			
1	B	659	Total	C	H	N	O	S	154	0	0
			10403	3346	5156	882	998	21			
1	C	659	Total	C	H	N	O	S	154	0	0
			10403	3346	5156	882	998	21			

There are 60 discrepancies between the modelled and reference sequences:

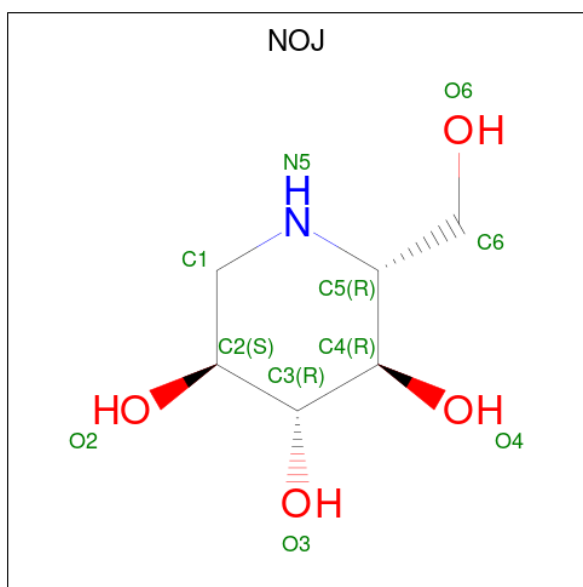
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP A5FBJ5
A	5	GLY	-	expression tag	UNP A5FBJ5
A	6	SER	-	expression tag	UNP A5FBJ5
A	7	SER	-	expression tag	UNP A5FBJ5
A	8	HIS	-	expression tag	UNP A5FBJ5
A	9	HIS	-	expression tag	UNP A5FBJ5
A	10	HIS	-	expression tag	UNP A5FBJ5
A	11	HIS	-	expression tag	UNP A5FBJ5
A	12	HIS	-	expression tag	UNP A5FBJ5
A	13	HIS	-	expression tag	UNP A5FBJ5
A	14	SER	-	expression tag	UNP A5FBJ5
A	15	SER	-	expression tag	UNP A5FBJ5
A	16	GLY	-	expression tag	UNP A5FBJ5
A	17	LEU	-	expression tag	UNP A5FBJ5
A	18	VAL	-	expression tag	UNP A5FBJ5
A	19	PRO	-	expression tag	UNP A5FBJ5
A	20	ARG	-	expression tag	UNP A5FBJ5
A	21	GLY	-	expression tag	UNP A5FBJ5
A	22	SER	-	expression tag	UNP A5FBJ5
A	23	HIS	-	expression tag	UNP A5FBJ5
B	4	MET	-	initiating methionine	UNP A5FBJ5
B	5	GLY	-	expression tag	UNP A5FBJ5

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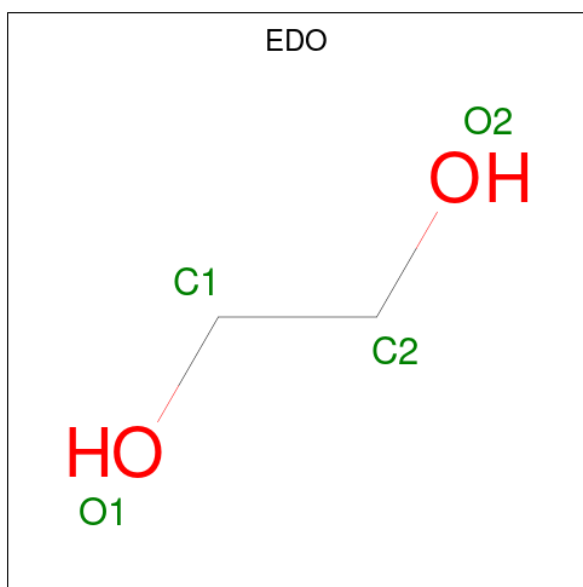
Chain	Residue	Modelled	Actual	Comment	Reference
B	6	SER	-	expression tag	UNP A5FBJ5
B	7	SER	-	expression tag	UNP A5FBJ5
B	8	HIS	-	expression tag	UNP A5FBJ5
B	9	HIS	-	expression tag	UNP A5FBJ5
B	10	HIS	-	expression tag	UNP A5FBJ5
B	11	HIS	-	expression tag	UNP A5FBJ5
B	12	HIS	-	expression tag	UNP A5FBJ5
B	13	HIS	-	expression tag	UNP A5FBJ5
B	14	SER	-	expression tag	UNP A5FBJ5
B	15	SER	-	expression tag	UNP A5FBJ5
B	16	GLY	-	expression tag	UNP A5FBJ5
B	17	LEU	-	expression tag	UNP A5FBJ5
B	18	VAL	-	expression tag	UNP A5FBJ5
B	19	PRO	-	expression tag	UNP A5FBJ5
B	20	ARG	-	expression tag	UNP A5FBJ5
B	21	GLY	-	expression tag	UNP A5FBJ5
B	22	SER	-	expression tag	UNP A5FBJ5
B	23	HIS	-	expression tag	UNP A5FBJ5
C	4	MET	-	initiating methionine	UNP A5FBJ5
C	5	GLY	-	expression tag	UNP A5FBJ5
C	6	SER	-	expression tag	UNP A5FBJ5
C	7	SER	-	expression tag	UNP A5FBJ5
C	8	HIS	-	expression tag	UNP A5FBJ5
C	9	HIS	-	expression tag	UNP A5FBJ5
C	10	HIS	-	expression tag	UNP A5FBJ5
C	11	HIS	-	expression tag	UNP A5FBJ5
C	12	HIS	-	expression tag	UNP A5FBJ5
C	13	HIS	-	expression tag	UNP A5FBJ5
C	14	SER	-	expression tag	UNP A5FBJ5
C	15	SER	-	expression tag	UNP A5FBJ5
C	16	GLY	-	expression tag	UNP A5FBJ5
C	17	LEU	-	expression tag	UNP A5FBJ5
C	18	VAL	-	expression tag	UNP A5FBJ5
C	19	PRO	-	expression tag	UNP A5FBJ5
C	20	ARG	-	expression tag	UNP A5FBJ5
C	21	GLY	-	expression tag	UNP A5FBJ5
C	22	SER	-	expression tag	UNP A5FBJ5
C	23	HIS	-	expression tag	UNP A5FBJ5

- Molecule 2 is 1-DEOXYNOJIRIMYCIN (CCD ID: NOJ) (formula: C₆H₁₃NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	5	0
			24	6	13	1	4		
2	B	1	Total	C	H	N	O	5	0
			24	6	13	1	4		
2	C	1	Total	C	H	N	O	5	0
			24	6	13	1	4		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	2	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	2	0
			10	2	6	2		

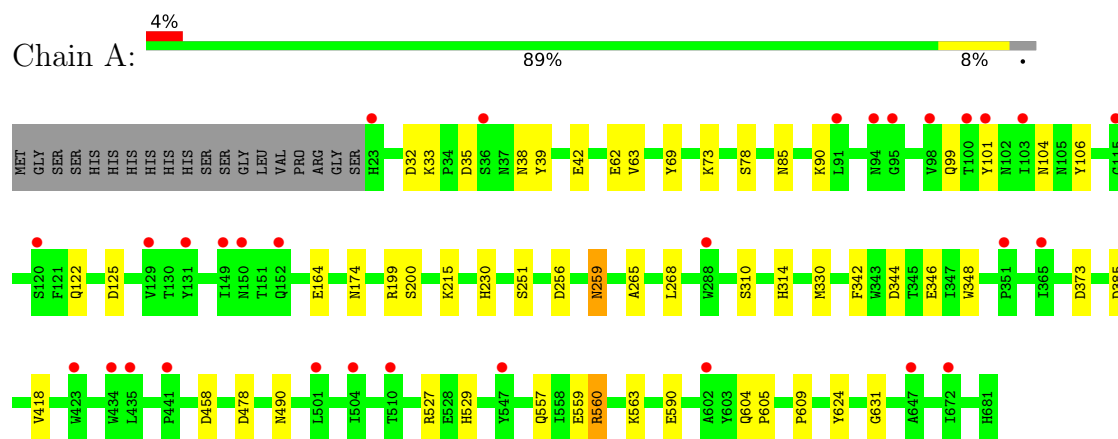
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	329	Total	O	0	0
			329	329		
4	B	207	Total	O	0	0
			207	207		
4	C	350	Total	O	0	0
			350	350		

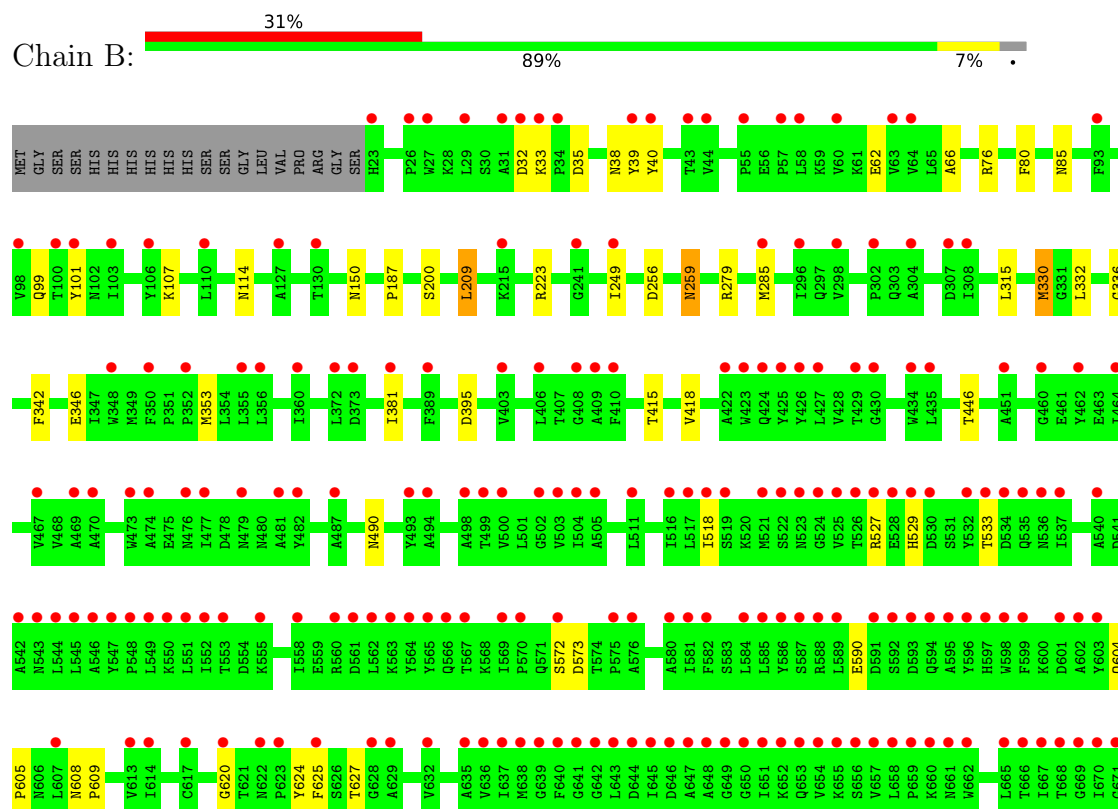
3 Residue-property plots [i](#)

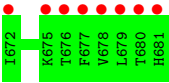
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65

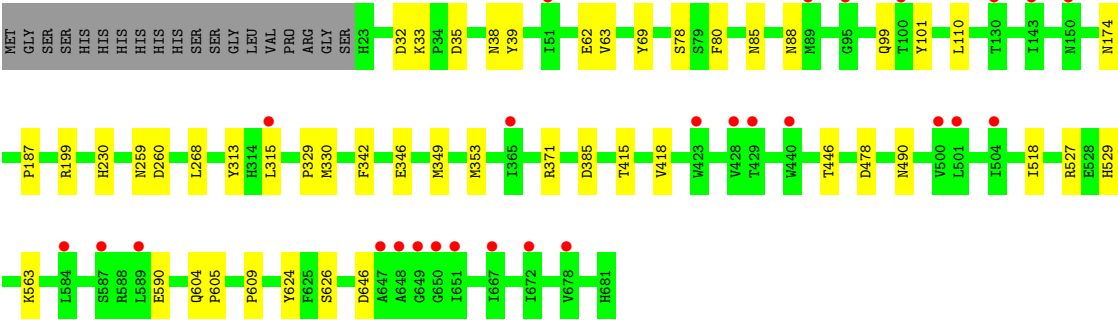
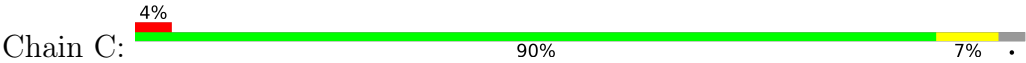


- Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65





● Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.84Å 194.37Å 112.13Å 90.00° 116.54° 90.00°	Depositor
Resolution (Å)	48.64 – 1.90 48.64 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.64-1.90) 99.5 (48.64-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.254 , 0.276 0.262 , 0.282	Depositor DCC
R_{free} test set	9198 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.0	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	0.93	EDS
Total number of atoms	32187	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: NOJ, EDO

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	0.64	0/5376	1.02	3/7296 (0.0%)
1	B	0.58	0/5376	0.99	4/7296 (0.1%)
1	C	0.62	0/5376	1.00	7/7296 (0.1%)
All	All	0.61	0/16128	1.00	14/21888 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	342	PHE	CA-CB-CG	6.58	120.38	113.80
1	C	260	ASP	CA-CB-CG	6.57	119.17	112.60
1	B	187	PRO	N-CD-CG	-6.33	93.70	103.20
1	B	342	PHE	CA-CB-CG	6.28	120.08	113.80
1	C	646	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	342	PHE	CA-CB-CG	5.96	119.76	113.80
1	C	385	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	330	MET	CG-SD-CE	5.63	113.28	100.90
1	C	80	PHE	CA-CB-CG	5.62	119.42	113.80
1	C	478	ASP	CA-CB-CG	5.44	118.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	PHE	CA-CB-CG	5.22	119.02	113.80
1	A	385	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	478	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	187	PRO	N-CD-CG	-5.10	95.56	103.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	560	ARG	Sidechain
1	B	279	ARG	Sidechain
1	B	76	ARG	Sidechain
1	C	371	ARG	Sidechain

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	5247	5156	5139	35	0
1	B	5247	5156	5139	31	0
1	C	5247	5156	5139	24	0
2	A	11	13	13	0	0
2	B	11	13	13	0	0
2	C	11	13	13	0	0
3	A	4	6	6	0	0
3	C	4	6	6	0	0
4	A	329	0	0	10	0
4	B	207	0	0	6	0
4	C	350	0	0	7	0
All	All	16668	15519	15468	89	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 3.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:MET:HG3	1:B:336:GLY:HA3	1.35	1.04
1:A:251:SER:HB3	4:A:1102:HOH:O	1.70	0.91
1:A:42:GLU:OE1	1:A:314:HIS:HE1	1.65	0.80
1:B:32:ASP:OD1	1:B:107:LYS:HD2	1.85	0.76
1:B:330:MET:HG3	1:B:336:GLY:CA	2.16	0.73
1:C:329:PRO:HA	4:C:898:HOH:O	1.98	0.63
1:A:73:LYS:HD2	4:A:1000:HOH:O	2.00	0.62
1:A:268:LEU:CD1	4:A:1102:HOH:O	2.50	0.59
1:A:310:SER:O	1:A:314:HIS:HD2	1.85	0.59
1:C:349:MET:SD	4:C:898:HOH:O	2.57	0.59
1:A:104:ASN:O	1:A:106:TYR:N	2.37	0.58
1:B:395:ASP:CB	4:B:900:HOH:O	2.52	0.58
1:A:164:GLU:CD	4:A:868:HOH:O	2.47	0.57
1:A:42:GLU:OE1	1:A:314:HIS:CE1	2.54	0.56
1:C:349:MET:CE	4:C:898:HOH:O	2.54	0.56
1:A:490:ASN:HD22	1:A:490:ASN:C	2.17	0.53
1:C:490:ASN:C	1:C:490:ASN:HD22	2.16	0.53
1:A:268:LEU:HD12	4:A:1102:HOH:O	2.07	0.53
1:B:490:ASN:C	1:B:490:ASN:HD22	2.17	0.52
1:B:200:SER:OG	1:B:256:ASP:OD2	2.29	0.51
1:A:69:TYR:HB3	1:A:78:SER:HB2	1.94	0.49
1:B:330:MET:HA	1:B:624:TYR:O	2.12	0.49
1:C:604:GLN:N	1:C:605:PRO:CD	2.77	0.48
1:B:395:ASP:HB3	4:B:900:HOH:O	2.12	0.48
1:C:346:GLU:HG2	1:C:418:VAL:HA	1.96	0.47
1:C:69:TYR:HB3	1:C:78:SER:HB2	1.94	0.47
1:A:604:GLN:N	1:A:605:PRO:CD	2.77	0.47
1:C:199:ARG:NH2	4:C:811:HOH:O	2.41	0.47
1:A:200:SER:OG	1:A:256:ASP:OD2	2.29	0.47
1:C:62:GLU:HA	1:C:85:ASN:HD21	1.79	0.47
1:A:557:GLN:HA	1:A:560:ARG:HG2	1.97	0.47
1:B:223:ARG:HD2	4:B:840:HOH:O	2.14	0.47
1:A:310:SER:O	1:A:314:HIS:CD2	2.68	0.46
1:B:604:GLN:N	1:B:605:PRO:CD	2.78	0.46
1:A:346:GLU:HG2	1:A:418:VAL:HA	1.98	0.46
1:A:330:MET:HA	1:A:624:TYR:O	2.16	0.46
1:B:346:GLU:HG2	1:B:418:VAL:HA	1.98	0.46
1:C:330:MET:HA	1:C:624:TYR:O	2.14	0.46
1:B:62:GLU:HA	1:B:85:ASN:HD21	1.80	0.45
1:A:35:ASP:O	1:A:39:TYR:HB2	2.16	0.45
1:B:35:ASP:O	1:B:39:TYR:HB2	2.16	0.45
1:B:150:ASN:ND2	4:B:801:HOH:O	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:GLY:HA3	4:B:920:HOH:O	2.17	0.45
1:B:66:ALA:HB2	1:B:332:LEU:HD21	1.99	0.45
1:A:259:ASN:HD22	1:A:259:ASN:H	1.64	0.44
1:A:122:GLN:HE21	1:A:125:ASP:HA	1.83	0.44
1:B:99:GLN:HG3	1:B:101:TYR:CE2	2.52	0.44
1:C:38:ASN:HD21	1:C:609:PRO:HG3	1.83	0.44
1:B:40:TYR:CD2	1:B:608:ASN:HB3	2.52	0.44
1:C:174:ASN:HB3	1:C:230:HIS:CG	2.53	0.44
1:A:38:ASN:HD21	1:A:609:PRO:HG3	1.82	0.44
1:B:259:ASN:ND2	1:B:259:ASN:H	2.14	0.44
1:C:88:ASN:ND2	4:C:830:HOH:O	2.50	0.44
1:C:259:ASN:ND2	4:C:804:HOH:O	2.37	0.43
1:C:626:SER:HB3	4:C:898:HOH:O	2.17	0.43
1:B:38:ASN:HD21	1:B:609:PRO:HG3	1.84	0.43
1:B:209:LEU:HD22	1:B:249:ILE:CD1	2.49	0.43
1:B:259:ASN:H	1:B:259:ASN:HD22	1.66	0.43
1:B:381:ILE:HG22	1:C:268:LEU:HD21	2.01	0.43
1:C:315:LEU:HD23	1:C:353:MET:HE3	2.00	0.43
1:A:62:GLU:HA	1:A:85:ASN:HD21	1.83	0.43
1:A:259:ASN:H	1:A:259:ASN:ND2	2.17	0.42
1:A:63:VAL:HG23	1:A:85:ASN:HD22	1.84	0.42
1:A:268:LEU:HB2	4:A:1102:HOH:O	2.18	0.42
1:A:265:ALA:HA	4:A:1102:HOH:O	2.18	0.42
1:B:85:ASN:ND2	4:B:825:HOH:O	2.52	0.42
1:C:63:VAL:HG23	1:C:85:ASN:HD22	1.84	0.42
1:A:199:ARG:NH1	4:A:842:HOH:O	2.52	0.42
1:A:373:ASP:HB3	4:A:1054:HOH:O	2.20	0.42
1:C:32:ASP:O	1:C:33:LYS:C	2.63	0.42
1:A:174:ASN:HB3	1:A:230:HIS:CG	2.55	0.42
1:C:99:GLN:HG3	1:C:101:TYR:CE2	2.55	0.42
1:B:415:THR:HG23	1:B:446:THR:HG22	2.02	0.41
1:B:625:PHE:CZ	1:B:627:THR:HB	2.55	0.41
1:A:99:GLN:HG3	1:A:101:TYR:CE2	2.54	0.41
1:A:527:ARG:HG2	1:A:529:HIS:O	2.21	0.41
1:B:114:ASN:HB3	1:B:285:MET:SD	2.60	0.41
1:A:344:ASP:O	1:A:348:TRP:HB2	2.21	0.41
1:A:559:GLU:HG2	1:A:563:LYS:HE2	2.02	0.41
1:B:32:ASP:O	1:B:33:LYS:C	2.63	0.41
1:B:572:SER:HB3	1:B:573:ASP:OD1	2.20	0.41
1:C:35:ASP:O	1:C:39:TYR:HB2	2.20	0.41
1:C:110:LEU:HD21	1:C:313:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:THR:HG23	1:C:446:THR:HG22	2.03	0.41
1:A:32:ASP:O	1:A:33:LYS:C	2.64	0.41
1:A:631:GLY:HA3	4:A:982:HOH:O	2.21	0.41
1:B:315:LEU:HD23	1:B:353:MET:HE3	2.02	0.40
1:C:527:ARG:HG2	1:C:529:HIS:O	2.21	0.40
1:B:527:ARG:HG2	1:B:529:HIS:O	2.22	0.40

There are no symmetry-related clashes.

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	657/678 (97%)	631 (96%)	25 (4%)	1 (0%)	43	36
1	B	657/678 (97%)	633 (96%)	23 (4%)	1 (0%)	43	36
1	C	657/678 (97%)	635 (97%)	21 (3%)	1 (0%)	43	36
All	All	1971/2034 (97%)	1899 (96%)	69 (4%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	590	GLU
1	A	590	GLU
1	C	590	GLU

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	565/581 (97%)	561 (99%)	4 (1%)	76	78
1	B	565/581 (97%)	561 (99%)	4 (1%)	76	78
1	C	565/581 (97%)	563 (100%)	2 (0%)	84	87
All	All	1695/1743 (97%)	1685 (99%)	10 (1%)	78	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LYS
1	A	215	LYS
1	A	259	ASN
1	A	458	ASP
1	B	209	LEU
1	B	259	ASN
1	B	518	ILE
1	B	533	THR
1	C	518	ILE
1	C	563	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	85	ASN
1	A	108	GLN
1	A	122	GLN
1	A	150	ASN
1	A	171	ASN
1	A	259	ASN
1	A	286	GLN
1	A	314	HIS
1	A	571	GLN
1	A	608	ASN
1	B	38	ASN
1	B	85	ASN
1	B	108	GLN
1	B	171	ASN
1	B	178	ASN
1	B	185	ASN

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Mol	Chain	Res	Type
1	B	206	ASN
1	B	259	ASN
1	B	286	GLN
1	B	608	ASN
1	C	23	HIS
1	C	38	ASN
1	C	85	ASN
1	C	108	GLN
1	C	171	ASN
1	C	206	ASN
1	C	286	GLN
1	C	293	GLN
1	C	404	ASN
1	C	476	ASN
1	C	566	GLN
1	C	571	GLN
1	C	608	ASN
1	C	681	HIS

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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	C	702	-	3,3,3	0.20	0	2,2,2	0.06	0
3	EDO	A	702	-	3,3,3	0.36	0	2,2,2	0.26	0
2	NOJ	B	701	-	11,11,11	0.34	0	13,15,15	1.21	1 (7%)
2	NOJ	C	701	-	11,11,11	0.75	0	13,15,15	1.26	2 (15%)
2	NOJ	A	701	-	11,11,11	0.67	0	13,15,15	1.41	3 (23%)

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	EDO	C	702	-	-	0/1/1/1	-
3	EDO	A	702	-	-	0/1/1/1	-
2	NOJ	B	701	-	-	0/2/19/19	0/1/1/1
2	NOJ	C	701	-	-	0/2/19/19	0/1/1/1
2	NOJ	A	701	-	-	0/2/19/19	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	NOJ	C1-N5-C5	2.74	115.72	109.71
2	A	701	NOJ	C4-C5-N5	2.44	114.03	109.12
2	A	701	NOJ	C1-N5-C5	2.39	114.96	109.71
2	B	701	NOJ	C3-C4-C5	2.37	114.49	111.02
2	C	701	NOJ	O4-C4-C5	-2.31	104.61	109.40
2	A	701	NOJ	O2-C2-C1	2.06	113.64	109.65

There are no chirality outliers.

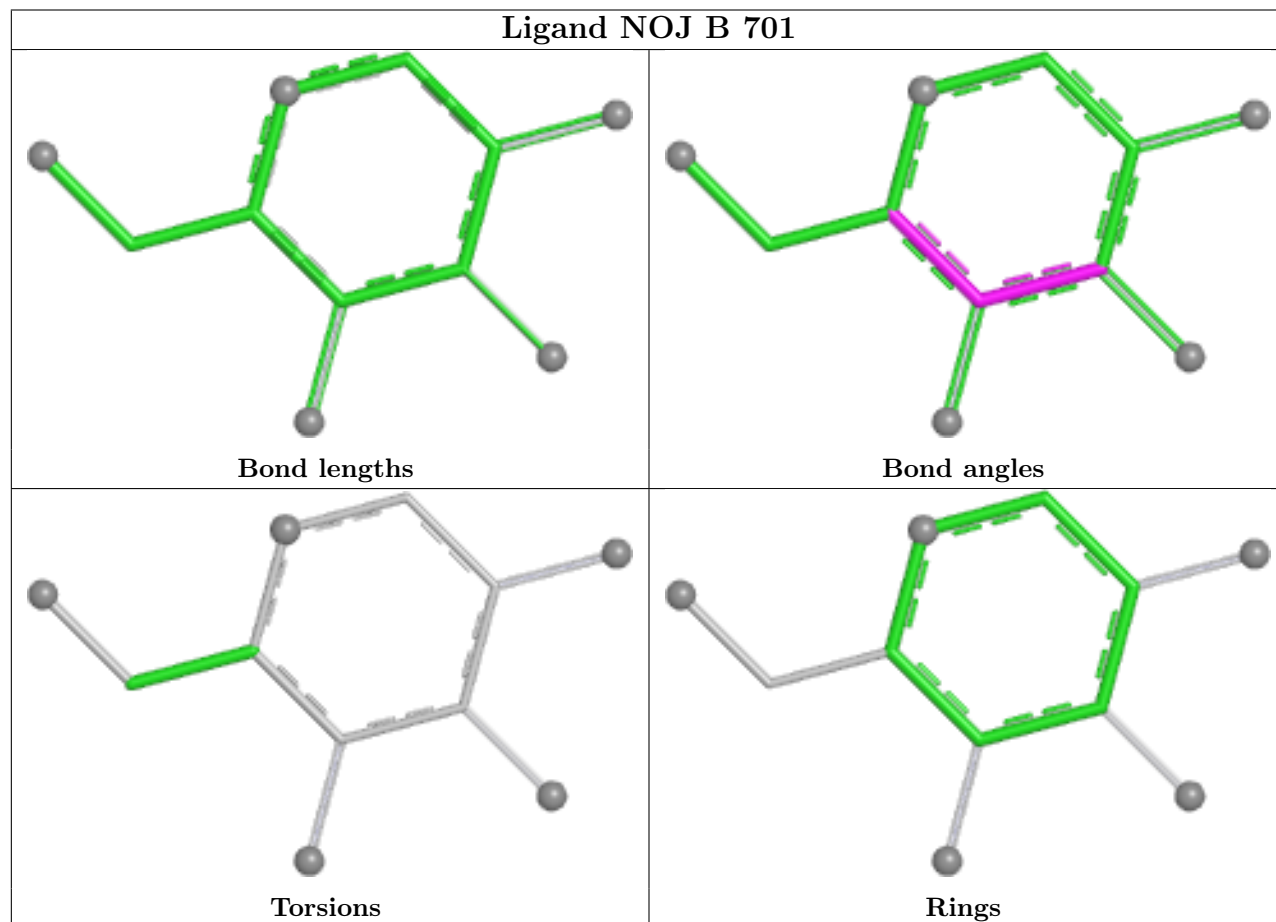
There are no torsion outliers.

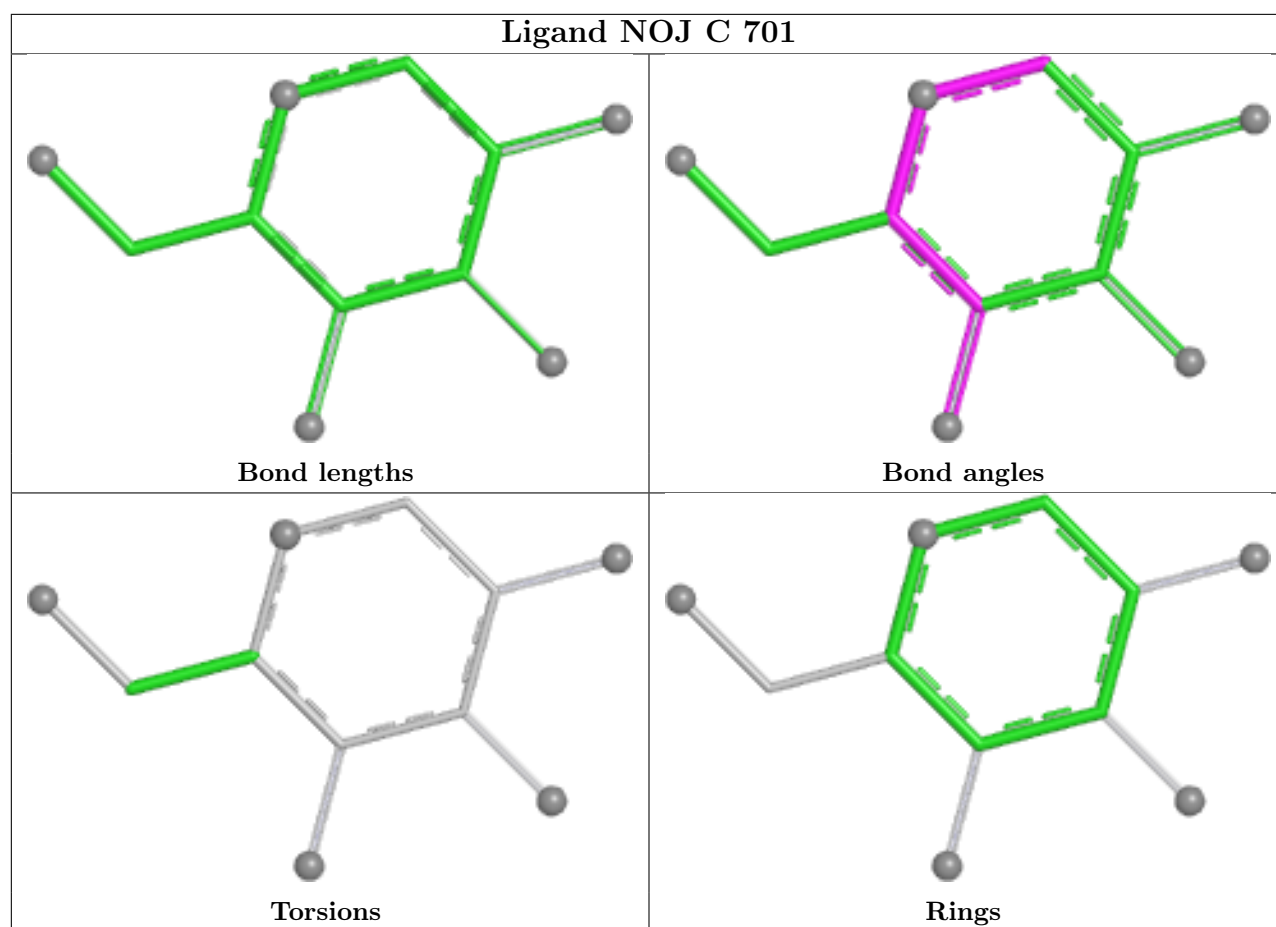
There are no ring outliers.

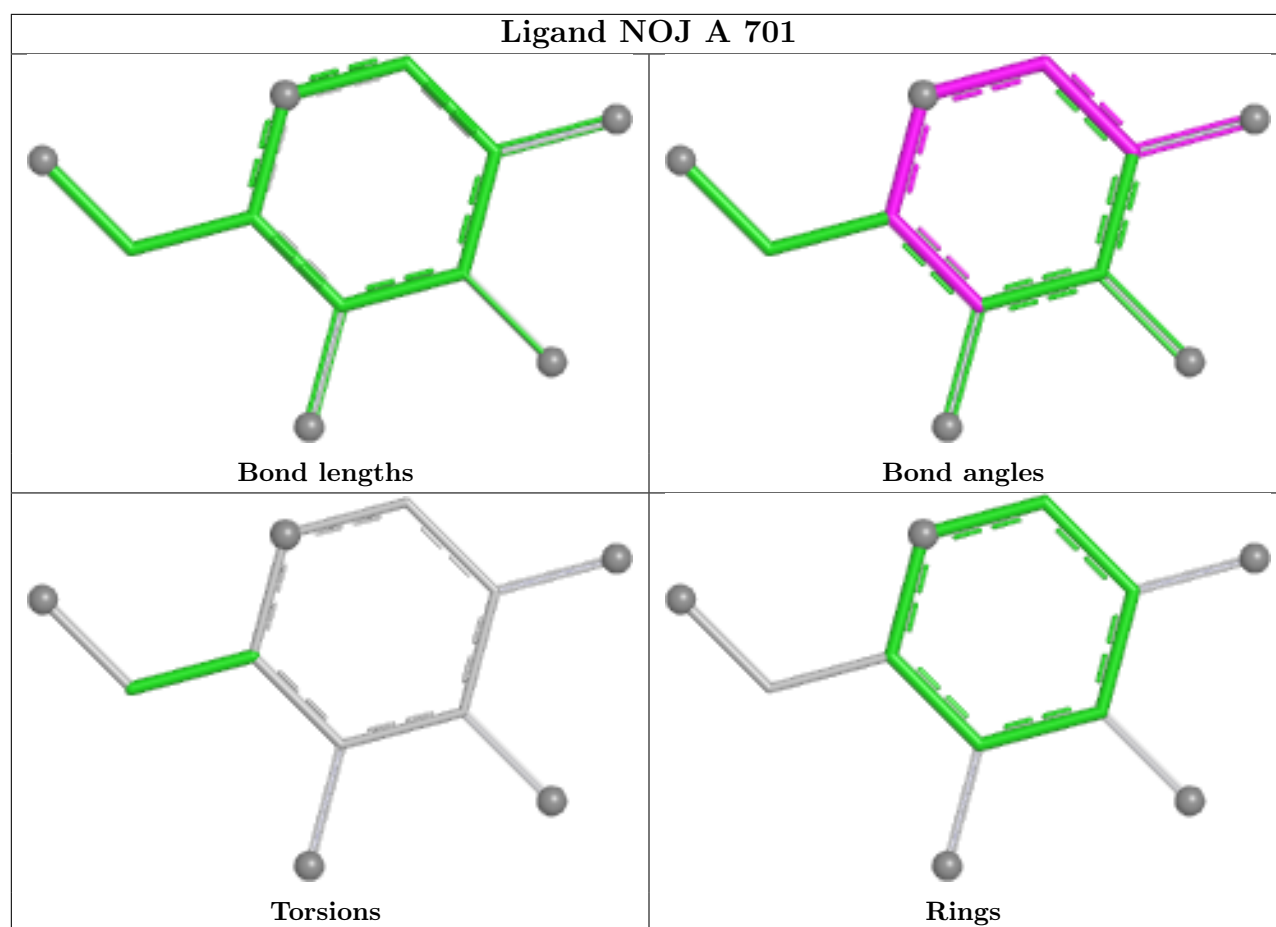
No monomer is involved in short contacts.

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	659/678 (97%)	0.72	30 (4%) 37 40	22, 34, 53, 73	0
1	B	659/678 (97%)	1.62	210 (31%) 1 1	21, 43, 81, 100	0
1	C	659/678 (97%)	0.74	27 (4%) 41 44	22, 34, 50, 68	0
All	All	1977/2034 (97%)	1.03	267 (13%) 7 7	21, 36, 67, 100	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	ALA	7.0
1	B	565	TYR	6.0
1	B	562	LEU	5.9
1	B	532	TYR	5.8
1	B	632	VAL	5.6
1	B	546	ALA	5.6
1	B	677	PHE	5.6
1	B	552	ILE	5.5
1	B	298	VAL	5.4
1	B	564	TYR	5.2
1	B	533	THR	5.1
1	B	540	ALA	4.9
1	B	558	ILE	4.8
1	B	658	LEU	4.8
1	B	537	ILE	4.7
1	B	584	LEU	4.6
1	B	296	ILE	4.6
1	B	643	LEU	4.6
1	B	589	LEU	4.5
1	B	678	VAL	4.5
1	B	636	VAL	4.4
1	B	467	VAL	4.4
1	B	654	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	672	ILE	4.4
1	B	525	VAL	4.4
1	B	563	LYS	4.3
1	B	599	PHE	4.3
1	B	569	ILE	4.2
1	B	679	LEU	4.2
1	B	647	ALA	4.1
1	B	524	GLY	4.1
1	B	670	ILE	4.1
1	B	586	TYR	4.0
1	B	523	ASN	4.0
1	B	477	ILE	3.9
1	C	504	ILE	3.8
1	B	473	TRP	3.8
1	B	542	ALA	3.8
1	B	582	PHE	3.8
1	A	672	ILE	3.7
1	B	517	LEU	3.7
1	B	522	SER	3.7
1	B	521	MET	3.7
1	B	662	TRP	3.7
1	B	519	SER	3.6
1	A	98	VAL	3.6
1	B	355	LEU	3.6
1	B	518	ILE	3.6
1	B	640	PHE	3.6
1	B	543	ASN	3.6
1	B	657	VAL	3.6
1	B	635	ALA	3.5
1	B	553	THR	3.5
1	B	430	GLY	3.5
1	B	660	LYS	3.5
1	A	101	TYR	3.5
1	B	598	TRP	3.5
1	B	665	LEU	3.4
1	B	581	ILE	3.4
1	B	637	ILE	3.4
1	B	592	SER	3.4
1	B	648	ALA	3.4
1	B	551	LEU	3.4
1	B	668	THR	3.4
1	B	667	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	639	GLY	3.3
1	B	516	ILE	3.3
1	B	34	PRO	3.3
1	B	527	ARG	3.3
1	B	545	LEU	3.2
1	B	567	THR	3.2
1	B	106	TYR	3.2
1	B	464	ILE	3.2
1	B	470	ALA	3.2
1	B	487	ALA	3.2
1	B	651	ILE	3.2
1	B	64	VAL	3.2
1	B	348	TRP	3.1
1	B	504	ILE	3.1
1	B	482	TYR	3.1
1	B	58	LEU	3.1
1	A	115	GLY	3.1
1	B	40	TYR	3.1
1	B	547	TYR	3.1
1	B	544	LEU	3.1
1	B	596	TYR	3.1
1	B	500	VAL	3.0
1	B	529	HIS	3.0
1	B	650	GLY	3.0
1	B	474	ALA	3.0
1	B	534	ASP	3.0
1	B	659	PRO	3.0
1	A	100	THR	3.0
1	B	27	TRP	3.0
1	B	652	LYS	3.0
1	B	406	LEU	2.9
1	C	584	LEU	2.9
1	B	603	TYR	2.9
1	A	152	GLN	2.9
1	B	566	GLN	2.9
1	B	661	ASN	2.9
1	B	356	LEU	2.9
1	B	555	LYS	2.9
1	B	585	LEU	2.9
1	B	669	GLY	2.9
1	B	597	HIS	2.9
1	C	648	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	381	ILE	2.9
1	B	645	ILE	2.9
1	C	589	LEU	2.9
1	B	649	GLY	2.8
1	B	561	ASP	2.8
1	B	646	ASP	2.8
1	B	469	ALA	2.8
1	C	89	MET	2.8
1	B	591	ASP	2.8
1	B	23	HIS	2.8
1	A	435	LEU	2.8
1	B	526	THR	2.8
1	C	672	ILE	2.8
1	B	505	ALA	2.7
1	B	580	ALA	2.7
1	B	426	TYR	2.7
1	B	629	ALA	2.7
1	B	410	PHE	2.7
1	B	680	THR	2.7
1	C	501	LEU	2.7
1	B	570	PRO	2.7
1	B	602	ALA	2.7
1	A	91	LEU	2.7
1	B	435	LEU	2.7
1	B	511	LEU	2.7
1	A	501	LEU	2.6
1	B	587	SER	2.6
1	B	549	LEU	2.6
1	A	149	ILE	2.6
1	A	504	ILE	2.6
1	A	129	VAL	2.6
1	B	498	ALA	2.6
1	B	666	THR	2.6
1	B	26	PRO	2.6
1	B	427	LEU	2.6
1	B	33	LYS	2.6
1	B	304	ALA	2.6
1	B	613	VAL	2.6
1	B	302	PRO	2.5
1	B	653	GLN	2.5
1	B	249	ILE	2.5
1	B	620	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	536	ASN	2.5
1	B	372	LEU	2.5
1	A	95	GLY	2.5
1	B	434	TRP	2.5
1	C	651	ILE	2.5
1	B	31	ALA	2.5
1	B	576	ALA	2.5
1	B	43	THR	2.5
1	B	593	ASP	2.5
1	B	548	PRO	2.5
1	B	479	ASN	2.4
1	B	535	GLN	2.4
1	C	647	ALA	2.4
1	B	601	ASP	2.4
1	B	57	PRO	2.4
1	B	617	CYS	2.4
1	C	150	ASN	2.4
1	B	681	HIS	2.4
1	B	389	PHE	2.4
1	B	560	ARG	2.4
1	B	676	THR	2.4
1	C	365	ILE	2.4
1	B	307	ASP	2.3
1	B	29	LEU	2.3
1	B	425	TYR	2.3
1	B	625	PHE	2.3
1	B	424	GLN	2.3
1	B	308	ILE	2.3
1	B	451	ALA	2.3
1	B	494	ALA	2.3
1	C	650	GLY	2.3
1	C	500	VAL	2.3
1	C	587	SER	2.3
1	C	423	TRP	2.3
1	B	39	TYR	2.3
1	B	93	PHE	2.3
1	B	101	TYR	2.3
1	B	422	ALA	2.3
1	A	351	PRO	2.3
1	B	641	GLY	2.3
1	B	528	GLU	2.3
1	B	638	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	360	ILE	2.3
1	B	656	SER	2.3
1	B	594	GLN	2.3
1	B	285	MET	2.3
1	C	440	TRP	2.2
1	B	530	ASP	2.2
1	B	614	ILE	2.2
1	B	60	VAL	2.2
1	B	100	THR	2.2
1	B	460	GLY	2.2
1	C	95	GLY	2.2
1	A	602	ALA	2.2
1	A	131	TYR	2.2
1	A	150	ASN	2.2
1	B	675	LYS	2.2
1	B	429	THR	2.2
1	C	315	LEU	2.2
1	A	120	SER	2.2
1	B	408	GLY	2.2
1	B	572	SER	2.2
1	B	127	ALA	2.2
1	A	94	ASN	2.2
1	B	44	VAL	2.2
1	B	32	ASP	2.2
1	B	110	LEU	2.2
1	C	649	GLY	2.2
1	B	595	ALA	2.2
1	B	476	ASN	2.1
1	B	622	ASN	2.1
1	A	365	ILE	2.1
1	C	143	ILE	2.1
1	C	667	ILE	2.1
1	A	423	TRP	2.1
1	B	423	TRP	2.1
1	A	510	THR	2.1
1	B	373	ASP	2.1
1	B	98	VAL	2.1
1	C	100	THR	2.1
1	B	215	LYS	2.1
1	B	623	PRO	2.1
1	A	647	ALA	2.1
1	B	481	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	51	ILE	2.1
1	A	36	SER	2.1
1	C	130	THR	2.1
1	C	429	THR	2.1
1	B	550	LYS	2.1
1	B	352	PRO	2.1
1	B	575	PRO	2.1
1	B	607	LEU	2.1
1	B	350	PHE	2.1
1	B	103	ILE	2.1
1	B	655	LYS	2.1
1	B	241	GLY	2.1
1	B	671	GLY	2.1
1	B	503	VAL	2.1
1	B	644	ASP	2.1
1	B	462	TYR	2.0
1	B	499	THR	2.0
1	B	628	GLY	2.0
1	A	441	PRO	2.0
1	B	55	PRO	2.0
1	C	678	VAL	2.0
1	A	288	TRP	2.0
1	A	434	TRP	2.0
1	A	23	HIS	2.0
1	A	103	ILE	2.0
1	B	130	THR	2.0
1	B	502	GLY	2.0
1	B	642	GLY	2.0
1	A	547	TYR	2.0
1	B	493	TYR	2.0
1	B	63	VAL	2.0
1	B	403	VAL	2.0
1	B	588	ARG	2.0
1	C	428	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

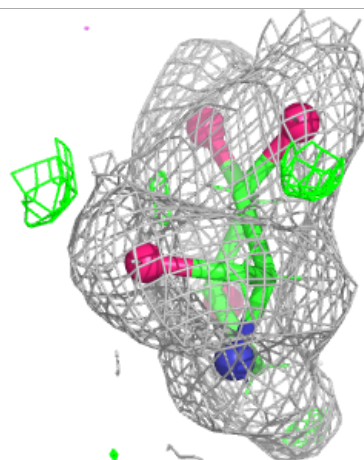
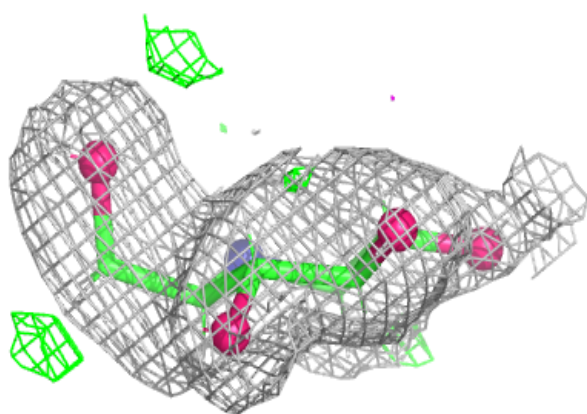
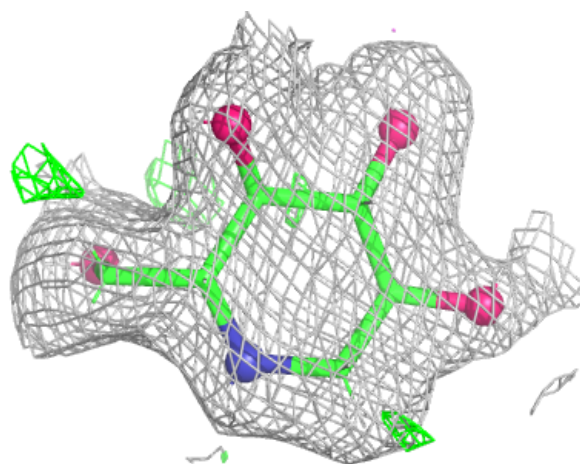
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NOJ	B	701	11/11	0.85	0.13	30,38,41,42	5
2	NOJ	C	701	11/11	0.91	0.09	24,26,30,30	5
3	EDO	C	702	4/4	0.92	0.09	28,30,31,32	2
2	NOJ	A	701	11/11	0.93	0.08	24,25,30,30	5
3	EDO	A	702	4/4	0.96	0.06	28,29,30,30	2

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.

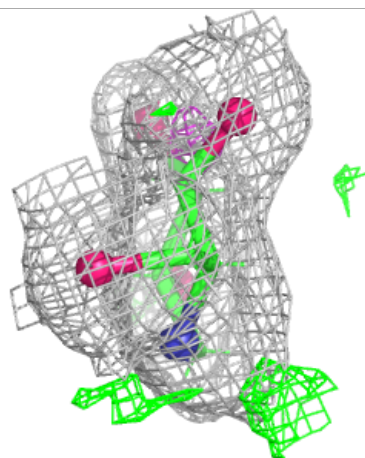
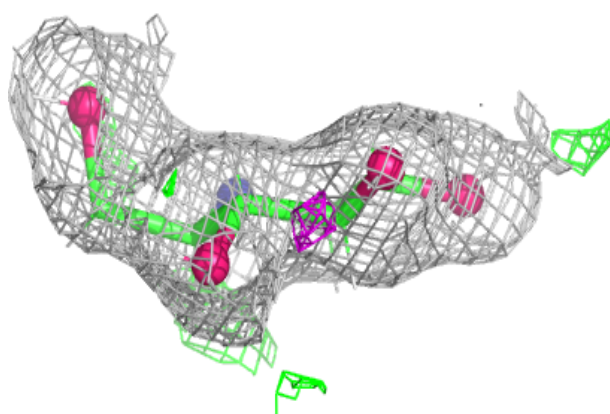
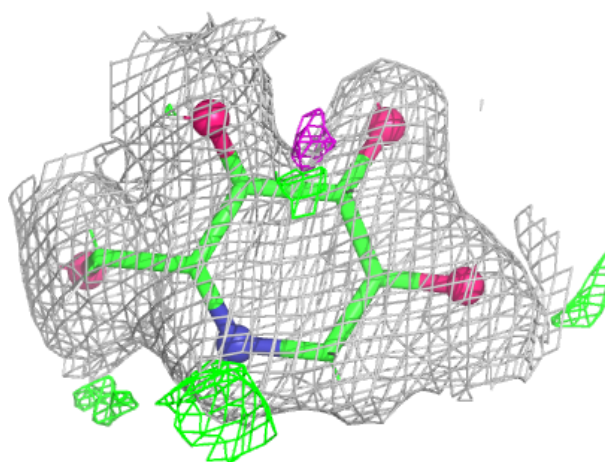
Electron density around NOJ B 701:

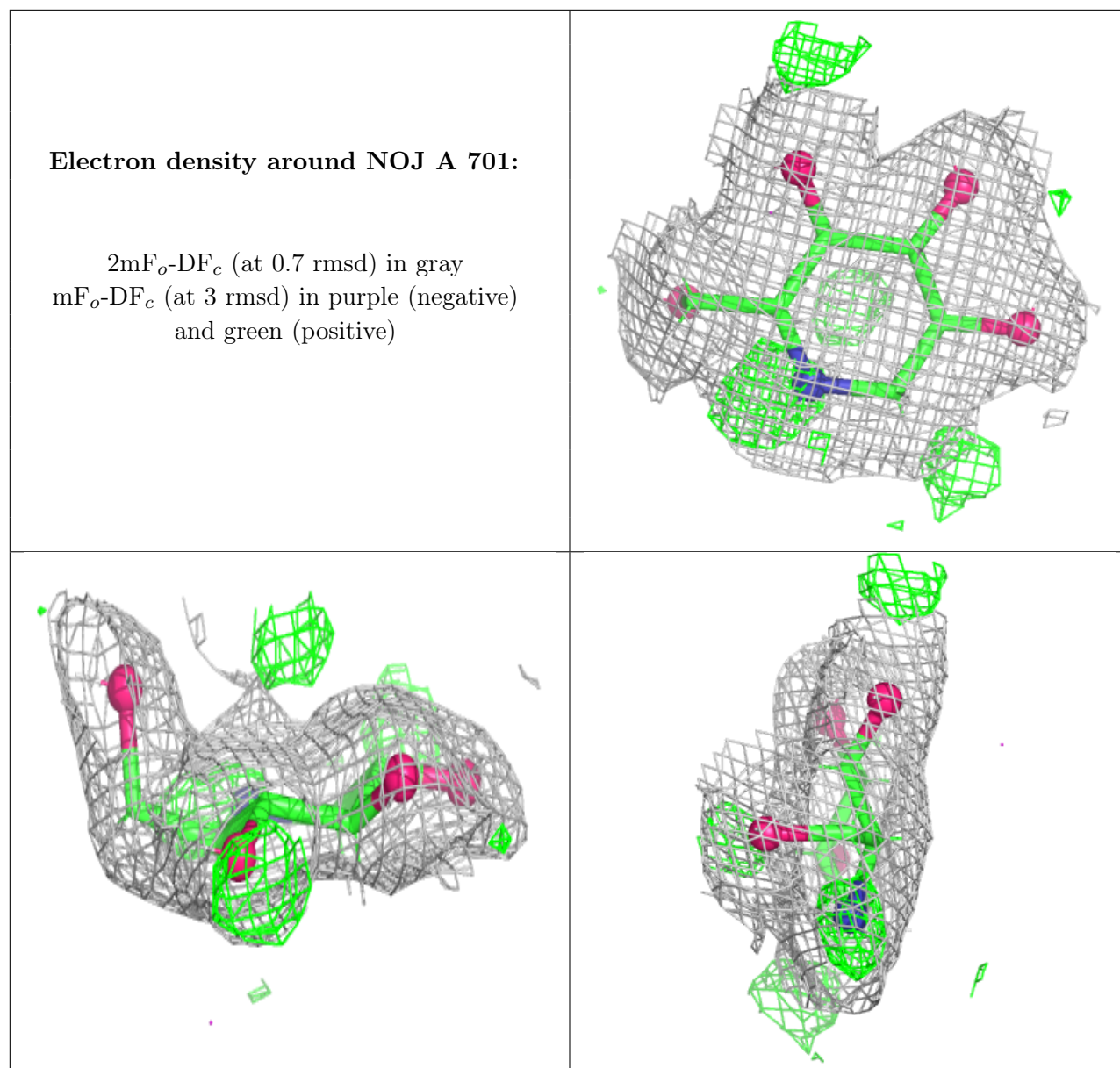
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NOJ C 701:

$2mF_o-DF_c$ (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.