Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2025 – 02:33 PM JST

PDB ID	:	8YVR
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:

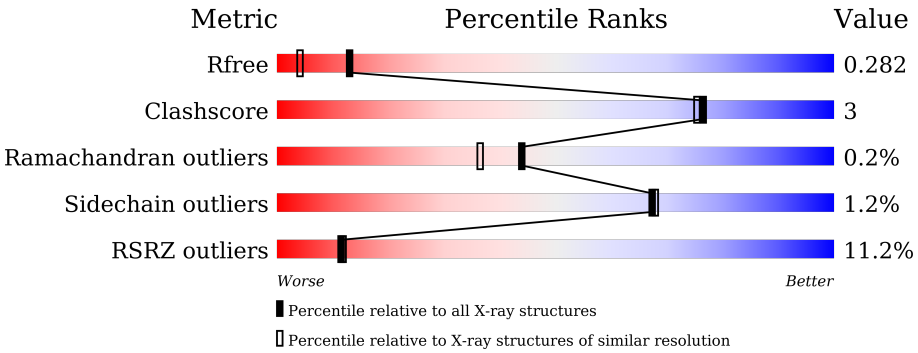
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (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 <=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	3% 89% 7%
1	B	678	27% 89% 7%
1	C	678	3% 91% 6%

2 Entry composition (i)

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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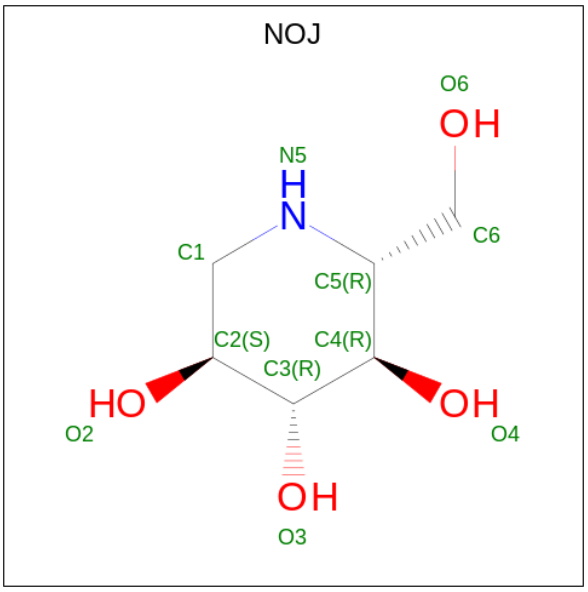
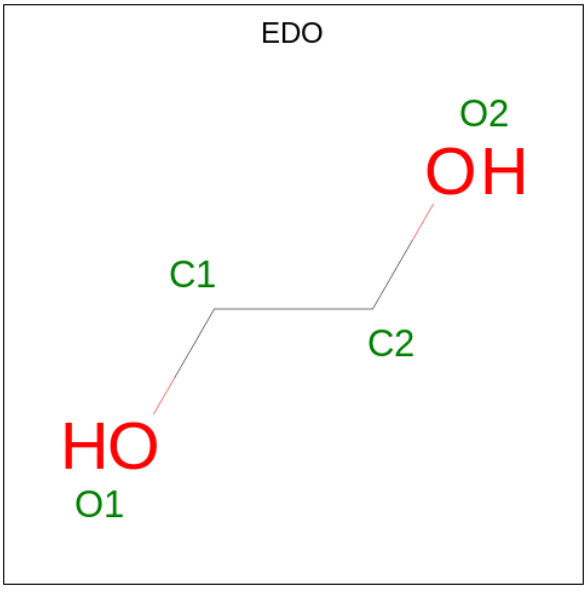
Chain	Residue	Modelled	Actual	Comment	Reference
B	6	SER	-	expression tag	UNP A5FBJ5
B	7	SER	-	expression tag	UNP A5FBJ5
B	8	HIS	-	expression tag	UNP A5FBJ5
B	9	HIS	-	expression tag	UNP A5FBJ5
B	10	HIS	-	expression tag	UNP A5FBJ5
B	11	HIS	-	expression tag	UNP A5FBJ5
B	12	HIS	-	expression tag	UNP A5FBJ5
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 (three-letter code: NOJ) (formula: $C_6H_{13}NO_4$) (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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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.

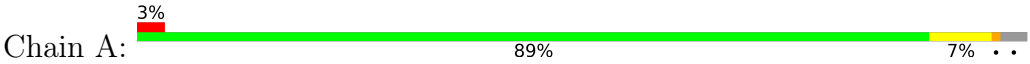
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	329	Total	O	0	0
			329	329		
4	B	207	Total	O	0	0
			207	207		
4	C	350	Total	O	0	0
			350	350		

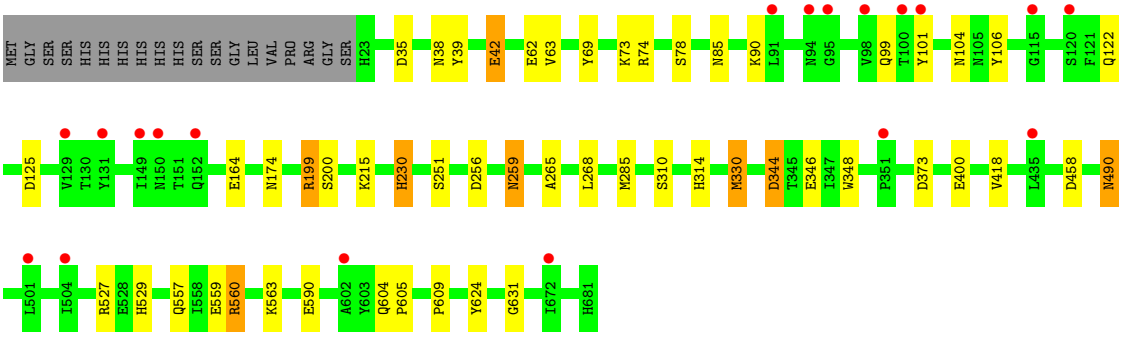
3 Residue-property plots (i)

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

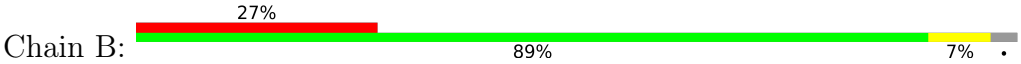
Chain A:

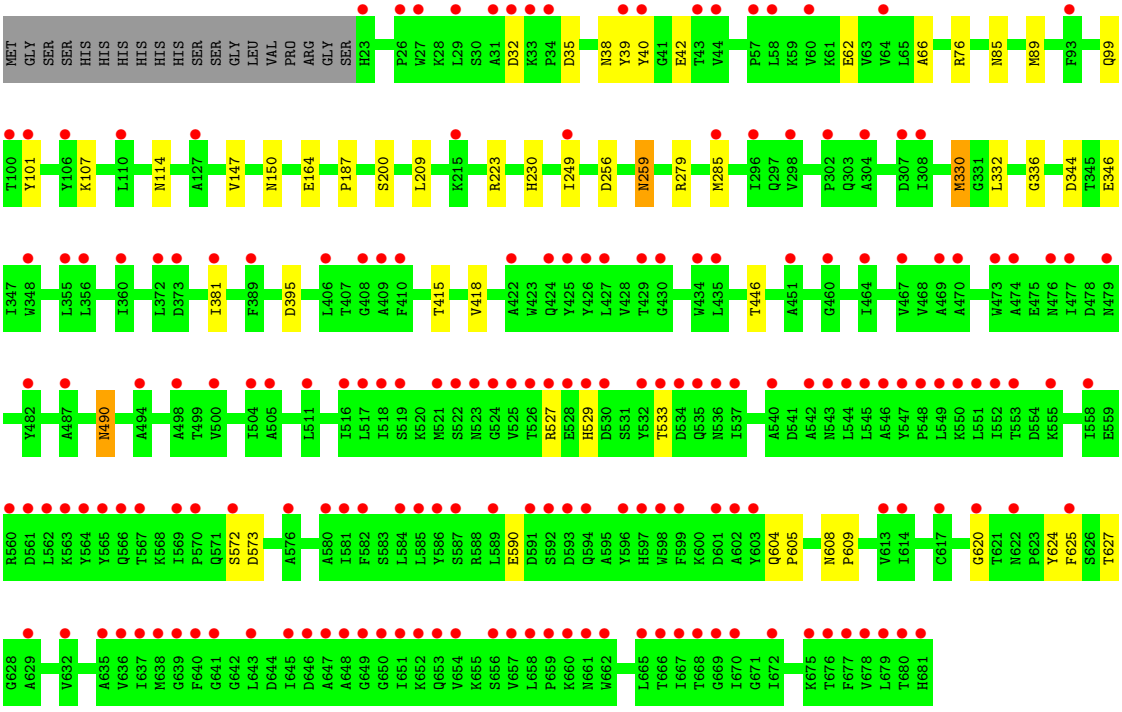




• Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65

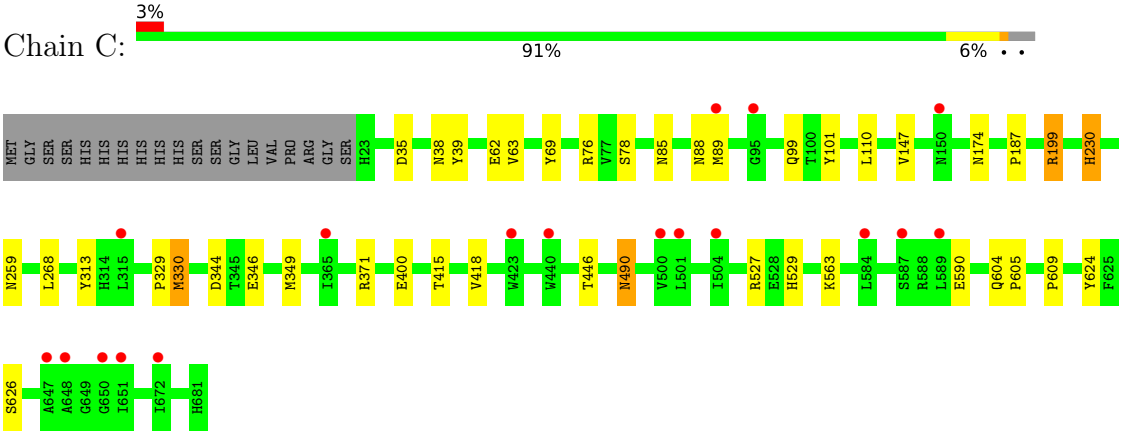
Chain B:





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

Chain C:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	9250 reflections (5.02%)	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]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, NOJ

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	0.47	0/5376	0.80	4/7296 (0.1%)
1	B	0.42	1/5376 (0.0%)	0.76	2/7296 (0.0%)
1	C	0.45	0/5376	0.79	5/7296 (0.1%)
All	All	0.45	1/16128 (0.0%)	0.79	11/21888 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	GLU	CD-OE1	-5.74	1.19	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	330	MET	CG-SD-CE	8.17	113.28	100.20
1	B	187	PRO	N-CD-CG	-6.33	93.70	103.20
1	C	199	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	199	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	400	GLU	OE1-CD-OE2	5.61	130.03	123.30
1	A	199	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	285	MET	CG-SD-CE	5.26	108.61	100.20
1	C	400	GLU	CG-CD-OE1	-5.15	108.01	118.30
1	C	76	ARG	NE-CZ-NH2	-5.14	117.73	120.30
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 (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	5247	5156	5139	34	0
1	B	5247	5156	5139	30	0
1	C	5247	5156	5139	23	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	86	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 (86) 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: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:268:LEU:HD12	4:A:1102:HOH:O	2.07	0.53
1:A:164:GLU:CD	4:A:868:HOH:O	2.47	0.53
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:A:490:ASN:HD22	1:A:490:ASN:C	2.17	0.48
1:C:490:ASN:C	1:C:490:ASN:HD22	2.16	0.48
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:89:MET:HE1	1:C:147:VAL:HG21	1.96	0.47
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:B:490:ASN:C	1:B:490:ASN:HD22	2.17	0.47
1:C:199:ARG:NH2	4:C:811:HOH:O	2.41	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:200:SER:OG	1:B:256:ASP:OD2	2.29	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:B:259:ASN:ND2	1:B:259:ASN:H	2.14	0.44
1:A:38:ASN:HD21	1:A:609:PRO:HG3	1.82	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:A:62:GLU:HA	1:A:85:ASN:HD21	1.83	0.43
1:B:89:MET:HE1	1:B:147:VAL:HG21	2.01	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: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:200:SER:OG	1:A:256:ASP:OD2	2.29	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: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
1:C:415:THR:HG23	1:C:446:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:GLY:HA3	4:A:982:HOH:O	2.21	0.41
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%)	44	36
1	B	657/678 (97%)	633 (96%)	23 (4%)	1 (0%)	44	36
1	C	657/678 (97%)	635 (97%)	21 (3%)	1 (0%)	44	36
All	All	1971/2034 (97%)	1899 (96%)	69 (4%)	3 (0%)	44	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%)	556 (98%)	9 (2%)	58	56
1	B	565/581 (97%)	559 (99%)	6 (1%)	70	71
1	C	565/581 (97%)	560 (99%)	5 (1%)	75	77
All	All	1695/1743 (97%)	1675 (99%)	20 (1%)	67	68

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	90	LYS
1	A	215	LYS
1	A	230	HIS
1	A	259	ASN
1	A	330	MET
1	A	344	ASP
1	A	458	ASP
1	A	490	ASN
1	B	42	GLU
1	B	230	HIS
1	B	259	ASN
1	B	344	ASP
1	B	490	ASN
1	B	533	THR
1	C	230	HIS
1	C	330	MET
1	C	344	ASP
1	C	490	ASN
1	C	563	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	85	ASN
1	A	122	GLN
1	A	158	ASN
1	A	259	ASN
1	A	282	ASN
1	A	314	HIS
1	B	38	ASN
1	B	85	ASN

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Mol	Chain	Res	Type
1	B	158	ASN
1	B	259	ASN
1	C	23	HIS
1	C	38	ASN
1	C	85	ASN
1	C	282	ASN
1	C	293	GLN
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	$\#\|Z\| > 2$
2	NOJ	C	701	-	11,11,11	0.77	0	13,15,15	1.28	2 (15%)
2	NOJ	A	701	-	11,11,11	0.66	0	13,15,15	1.44	4 (30%)
3	EDO	A	702	-	3,3,3	0.40	0	2,2,2	0.30	0
3	EDO	C	702	-	3,3,3	0.20	0	2,2,2	0.08	0
2	NOJ	B	701	-	11,11,11	0.32	0	13,15,15	1.24	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NOJ	C	701	-	-	0/2/19/19	0/1/1/1
2	NOJ	A	701	-	-	0/2/19/19	0/1/1/1
3	EDO	A	702	-	-	0/1/1/1	-
3	EDO	C	702	-	-	0/1/1/1	-
2	NOJ	B	701	-	-	0/2/19/19	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	NOJ	C1-N5-C5	2.83	115.72	109.61
2	A	701	NOJ	C1-N5-C5	2.47	114.96	109.61
2	A	701	NOJ	C4-C5-N5	2.44	114.03	109.14
2	B	701	NOJ	C3-C4-C5	2.37	114.49	111.02
2	C	701	NOJ	O4-C4-C5	-2.35	104.61	109.47
2	A	701	NOJ	O2-C2-C1	2.06	113.64	109.61
2	A	701	NOJ	O3-C3-C2	-2.01	106.14	109.99

There are no chirality outliers.

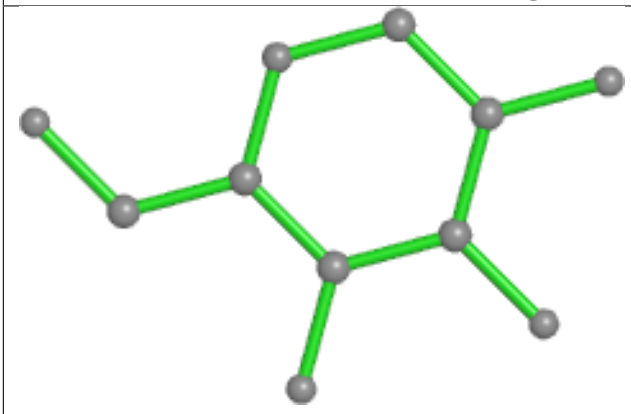
There are no torsion outliers.

There are no ring outliers.

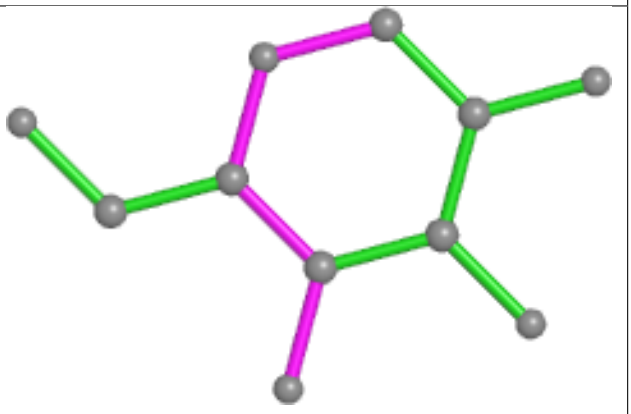
No monomer is involved in short contacts.

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 then 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.

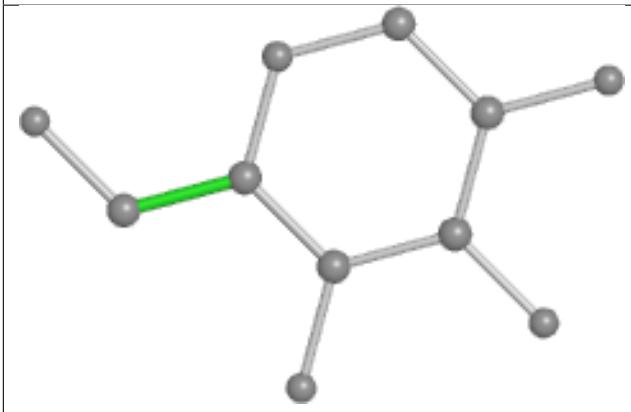
Ligand NOJ C 701



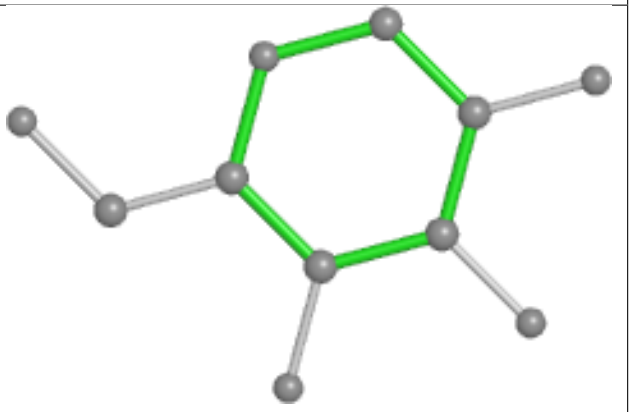
Bond lengths



Bond angles

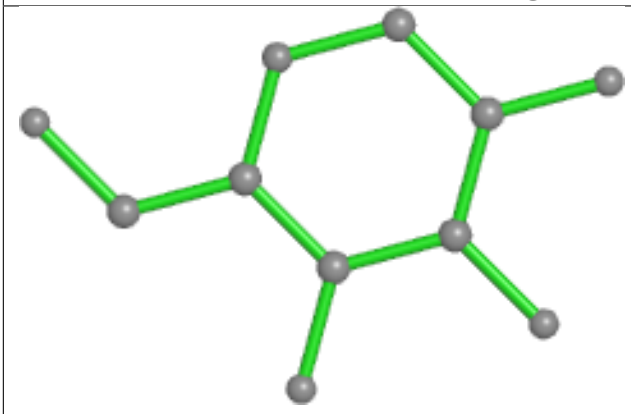


Torsions

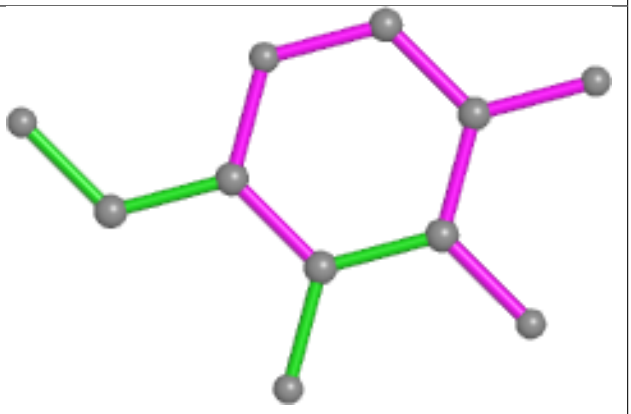


Rings

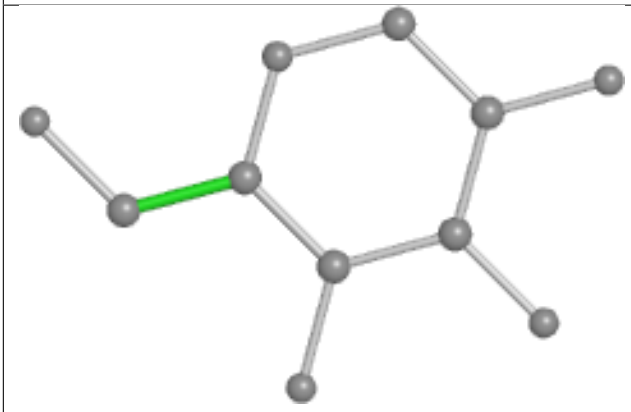
Ligand NOJ A 701



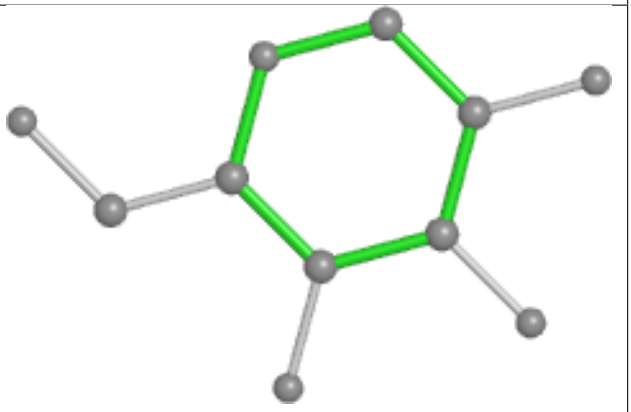
Bond lengths



Bond angles

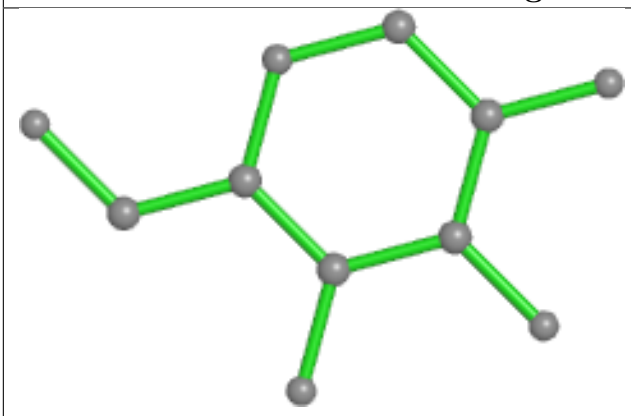


Torsions

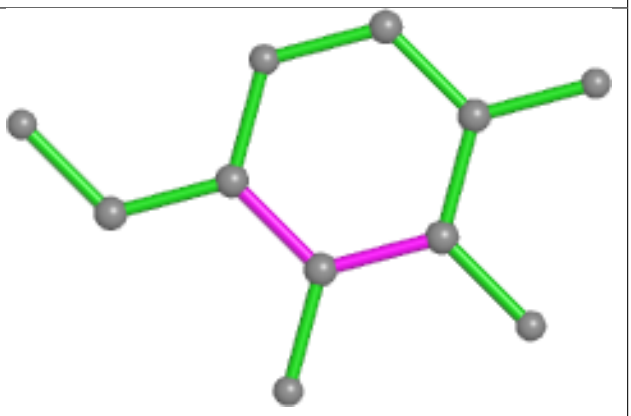


Rings

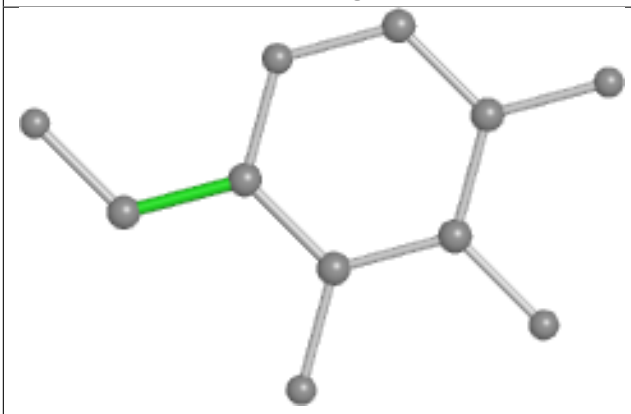
Ligand NOJ B 701



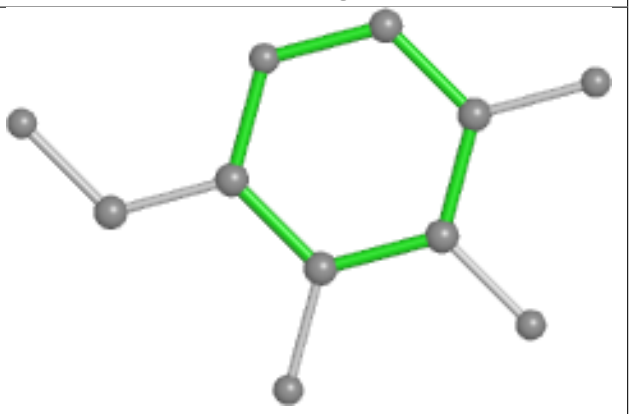
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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%)	0.61	19 (2%) 54 56	22, 34, 53, 73	0
1	B	659/678 (97%)	1.49	184 (27%) 2 1	21, 43, 81, 100	0
1	C	659/678 (97%)	0.63	18 (2%) 56 58	22, 34, 50, 68	0
All	All	1977/2034 (97%)	0.91	221 (11%) 11 12	21, 36, 67, 100	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	ALA	6.7
1	B	565	TYR	5.7
1	B	562	LEU	5.6
1	B	532	TYR	5.5
1	B	632	VAL	5.4
1	B	677	PHE	5.4
1	B	546	ALA	5.3
1	B	552	ILE	5.3
1	B	298	VAL	5.2
1	B	564	TYR	5.0
1	B	533	THR	4.9
1	B	540	ALA	4.6
1	B	558	ILE	4.6
1	B	658	LEU	4.6
1	B	537	ILE	4.5
1	B	584	LEU	4.4
1	B	296	ILE	4.4
1	B	643	LEU	4.4
1	B	589	LEU	4.3
1	B	563	LYS	4.3
1	B	678	VAL	4.3
1	B	636	VAL	4.2
1	B	672	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	467	VAL	4.2
1	B	654	VAL	4.2
1	B	525	VAL	4.2
1	B	599	PHE	4.1
1	B	569	ILE	4.0
1	B	679	LEU	4.0
1	B	647	ALA	3.9
1	B	670	ILE	3.9
1	B	524	GLY	3.9
1	B	586	TYR	3.8
1	B	523	ASN	3.8
1	B	477	ILE	3.7
1	C	504	ILE	3.6
1	B	582	PHE	3.6
1	B	521	MET	3.6
1	B	473	TRP	3.6
1	B	522	SER	3.6
1	B	542	ALA	3.5
1	A	672	ILE	3.5
1	B	517	LEU	3.5
1	B	519	SER	3.5
1	B	662	TRP	3.4
1	B	543	ASN	3.4
1	A	98	VAL	3.4
1	B	355	LEU	3.4
1	B	518	ILE	3.4
1	B	640	PHE	3.4
1	B	660	LYS	3.4
1	B	553	THR	3.4
1	B	657	VAL	3.4
1	B	635	ALA	3.3
1	A	101	TYR	3.3
1	B	430	GLY	3.3
1	B	665	LEU	3.2
1	B	598	TRP	3.2
1	B	581	ILE	3.2
1	B	592	SER	3.2
1	B	668	THR	3.2
1	B	637	ILE	3.2
1	B	551	LEU	3.2
1	B	667	ILE	3.2
1	B	527	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	648	ALA	3.2
1	B	516	ILE	3.1
1	B	34	PRO	3.1
1	B	639	GLY	3.1
1	B	567	THR	3.1
1	B	545	LEU	3.1
1	B	464	ILE	3.0
1	B	106	TYR	3.0
1	B	651	ILE	3.0
1	B	470	ALA	3.0
1	B	64	VAL	3.0
1	B	504	ILE	3.0
1	B	487	ALA	3.0
1	B	482	TYR	3.0
1	B	58	LEU	3.0
1	B	40	TYR	2.9
1	B	547	TYR	2.9
1	B	544	LEU	2.9
1	B	348	TRP	2.9
1	A	115	GLY	2.9
1	B	596	TYR	2.9
1	B	534	ASP	2.9
1	B	529	HIS	2.9
1	B	652	LYS	2.9
1	B	500	VAL	2.9
1	B	650	GLY	2.8
1	A	152	GLN	2.8
1	B	566	GLN	2.8
1	B	659	PRO	2.8
1	B	474	ALA	2.8
1	A	100	THR	2.8
1	B	555	LYS	2.8
1	B	661	ASN	2.8
1	B	406	LEU	2.8
1	C	584	LEU	2.8
1	B	603	TYR	2.8
1	B	27	TRP	2.8
1	B	356	LEU	2.7
1	B	597	HIS	2.7
1	B	585	LEU	2.7
1	B	669	GLY	2.7
1	B	381	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	645	ILE	2.7
1	B	561	ASP	2.7
1	B	646	ASP	2.7
1	C	589	LEU	2.7
1	C	89	MET	2.7
1	C	648	ALA	2.7
1	B	591	ASP	2.7
1	B	649	GLY	2.6
1	B	23	HIS	2.6
1	B	526	THR	2.6
1	B	469	ALA	2.6
1	C	672	ILE	2.6
1	A	435	LEU	2.6
1	B	680	THR	2.6
1	B	505	ALA	2.6
1	B	580	ALA	2.6
1	B	410	PHE	2.5
1	B	426	TYR	2.5
1	B	570	PRO	2.5
1	C	501	LEU	2.5
1	B	629	ALA	2.5
1	A	91	LEU	2.5
1	B	435	LEU	2.5
1	B	511	LEU	2.5
1	B	602	ALA	2.5
1	B	587	SER	2.5
1	B	33	LYS	2.5
1	A	501	LEU	2.5
1	A	149	ILE	2.4
1	A	504	ILE	2.4
1	B	549	LEU	2.4
1	B	666	THR	2.4
1	B	653	GLN	2.4
1	A	129	VAL	2.4
1	B	26	PRO	2.4
1	B	427	LEU	2.4
1	B	536	ASN	2.4
1	B	498	ALA	2.4
1	B	302	PRO	2.4
1	B	613	VAL	2.4
1	B	249	ILE	2.4
1	B	304	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	620	GLY	2.4
1	B	372	LEU	2.3
1	B	593	ASP	2.3
1	B	535	GLN	2.3
1	A	95	GLY	2.3
1	B	479	ASN	2.3
1	B	43	THR	2.3
1	C	651	ILE	2.3
1	B	601	ASP	2.3
1	B	434	TRP	2.3
1	B	548	PRO	2.3
1	B	617	CYS	2.3
1	B	31	ALA	2.3
1	B	576	ALA	2.3
1	B	57	PRO	2.3
1	B	560	ARG	2.3
1	C	150	ASN	2.3
1	B	681	HIS	2.3
1	C	647	ALA	2.2
1	B	424	GLN	2.2
1	B	676	THR	2.2
1	B	307	ASP	2.2
1	B	389	PHE	2.2
1	C	365	ILE	2.2
1	B	528	GLU	2.2
1	C	587	SER	2.2
1	B	625	PHE	2.2
1	B	29	LEU	2.2
1	B	425	TYR	2.2
1	B	308	ILE	2.2
1	C	500	VAL	2.2
1	B	93	PHE	2.2
1	B	638	MET	2.2
1	C	650	GLY	2.2
1	B	451	ALA	2.2
1	B	494	ALA	2.2
1	B	594	GLN	2.2
1	A	351	PRO	2.2
1	B	39	TYR	2.2
1	B	101	TYR	2.2
1	B	656	SER	2.1
1	B	285	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	641	GLY	2.1
1	B	422	ALA	2.1
1	C	423	TRP	2.1
1	B	360	ILE	2.1
1	B	530	ASP	2.1
1	B	675	LYS	2.1
1	B	614	ILE	2.1
1	B	100	THR	2.1
1	A	150	ASN	2.1
1	B	60	VAL	2.1
1	A	120	SER	2.1
1	B	572	SER	2.1
1	A	131	TYR	2.1
1	B	429	THR	2.1
1	C	440	TRP	2.1
1	A	94	ASN	2.1
1	B	460	GLY	2.1
1	C	95	GLY	2.1
1	B	32	ASP	2.0
1	A	602	ALA	2.0
1	C	315	LEU	2.0
1	B	215	LYS	2.0
1	B	476	ASN	2.0
1	B	622	ASN	2.0
1	B	408	GLY	2.0
1	B	373	ASP	2.0
1	B	44	VAL	2.0
1	B	550	LYS	2.0
1	B	127	ALA	2.0
1	B	110	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

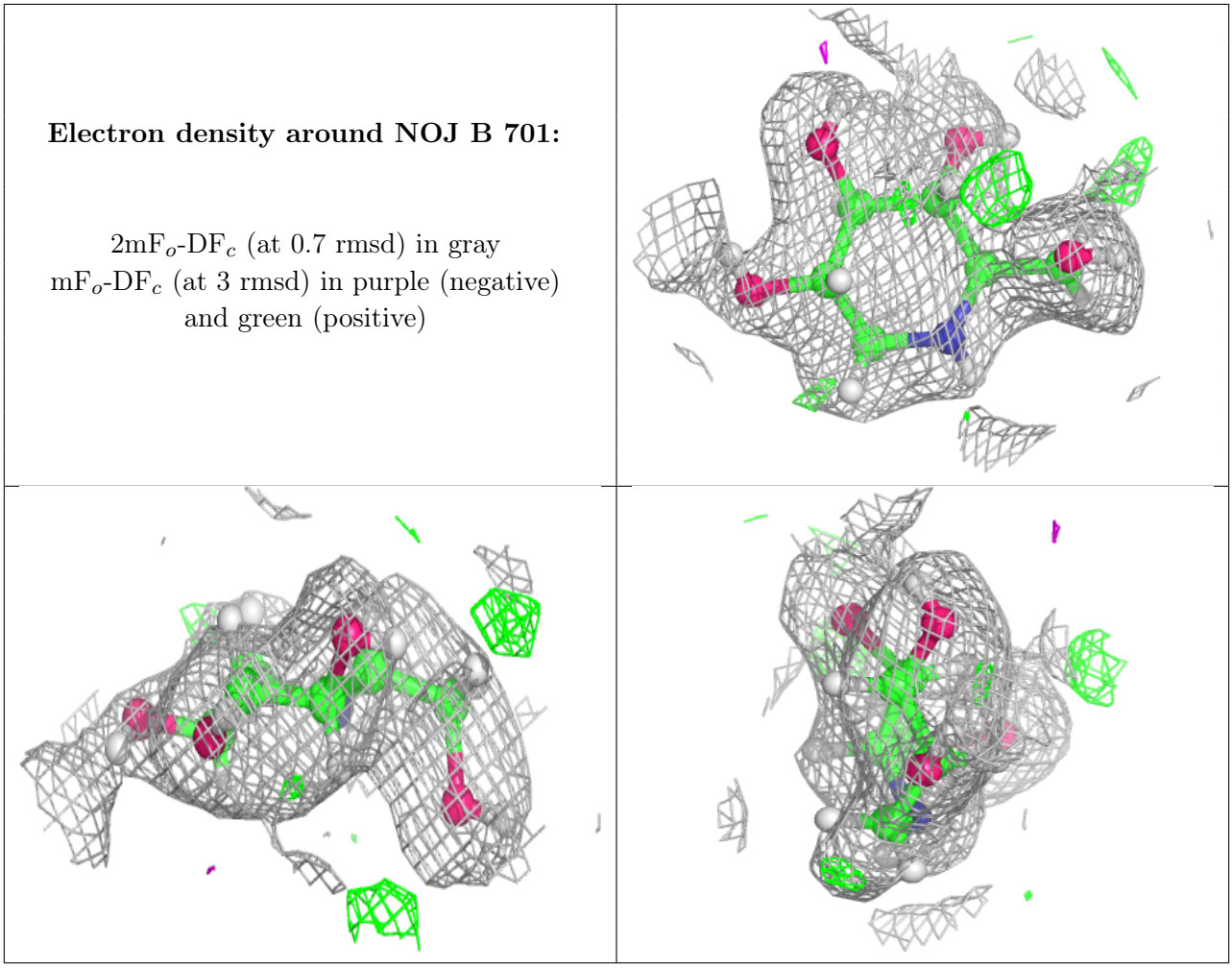
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

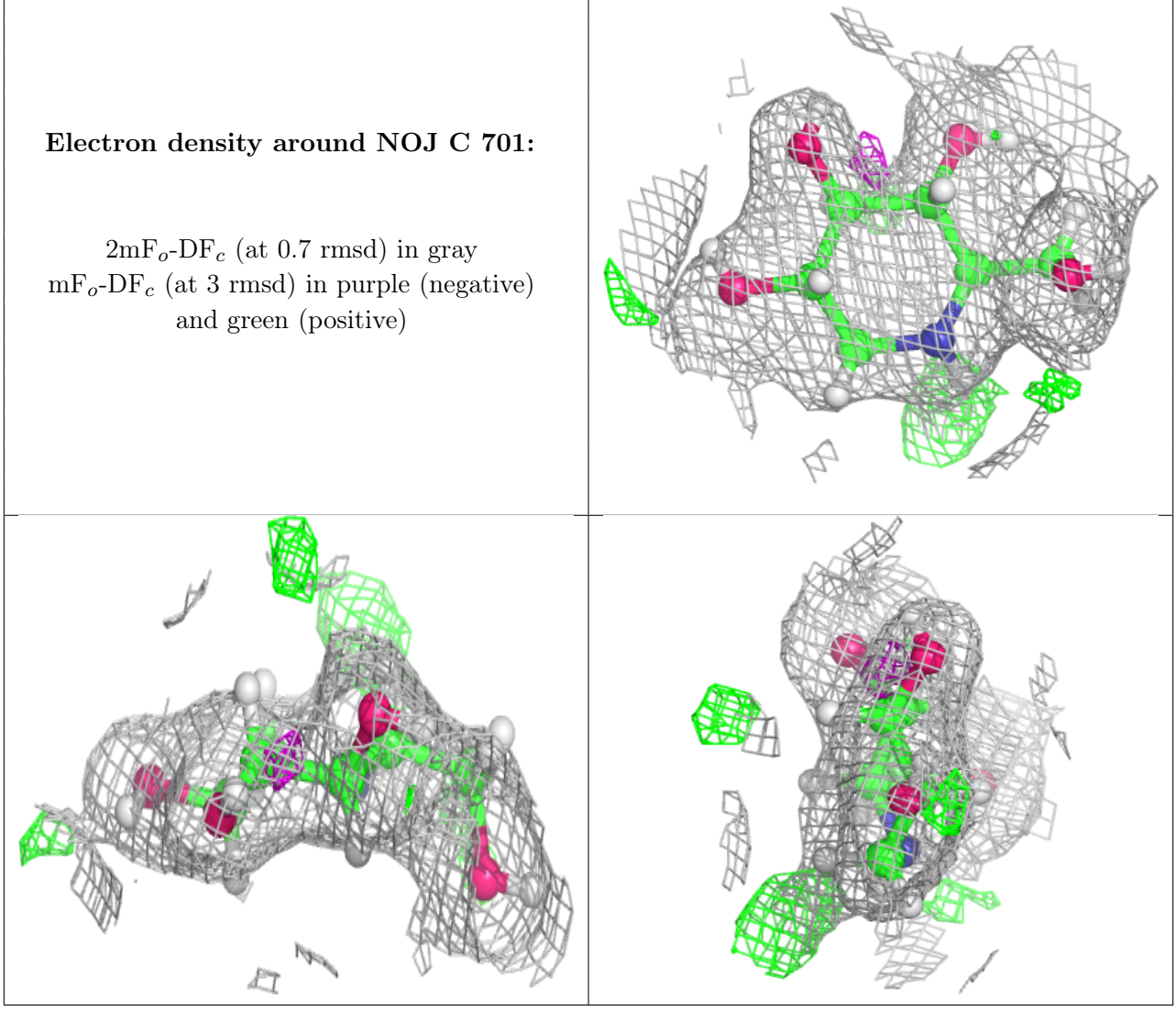
Electron density around NOJ B 701:

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



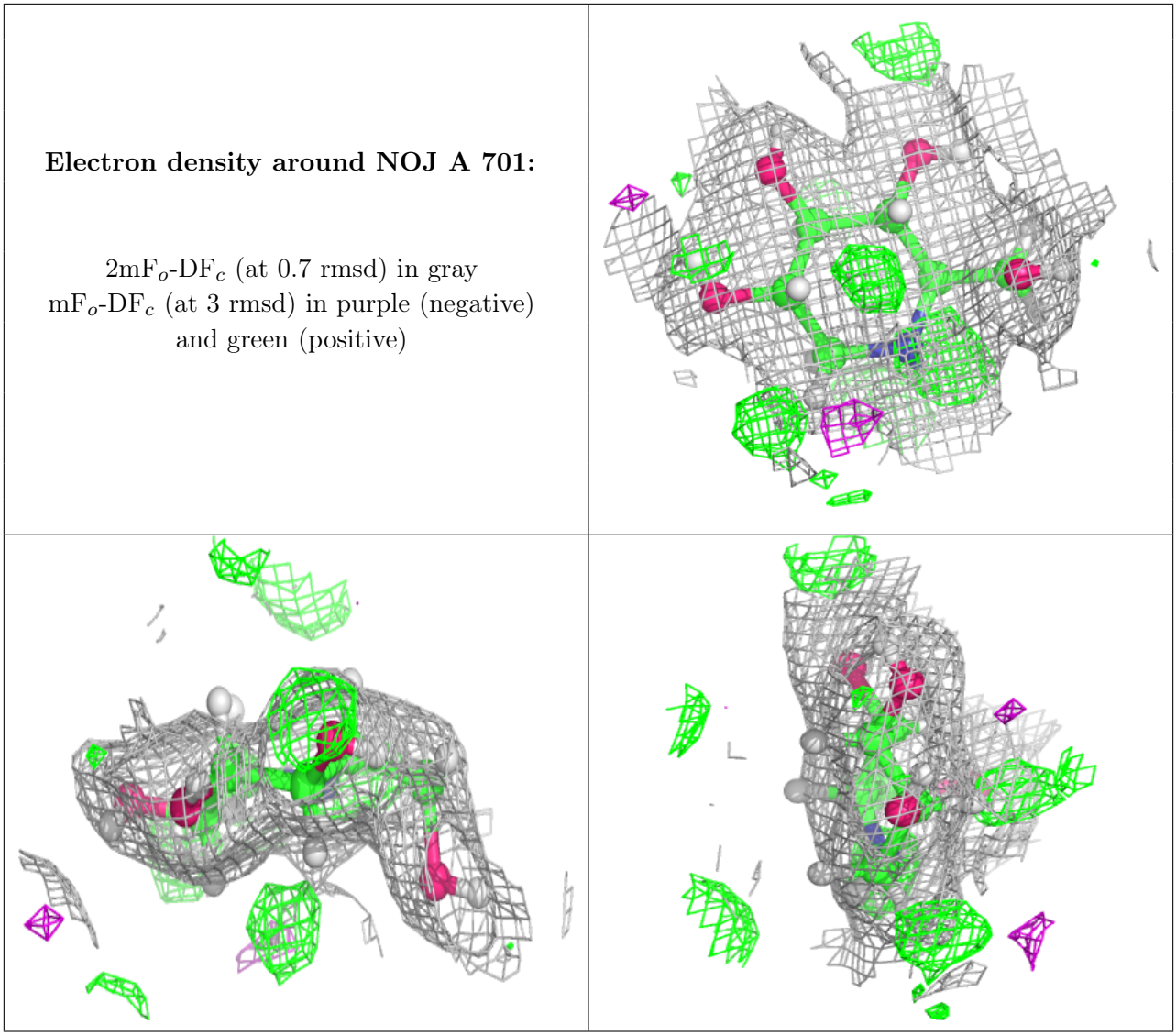
Electron density around NOJ C 701:

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



Electron density around NOJ A 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 (i)

There are no such residues in this entry.