



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 03:50 PM UTC

PDB ID : 3WF2 / pdb_00003wf2
Title : Crystal structure of human beta-galactosidase in complex with NBT-DGJ
Authors : Suzuki, H.; Ohto, U.; Shimizu, T.
Deposited on : 2013-07-16
Resolution : 2.30 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

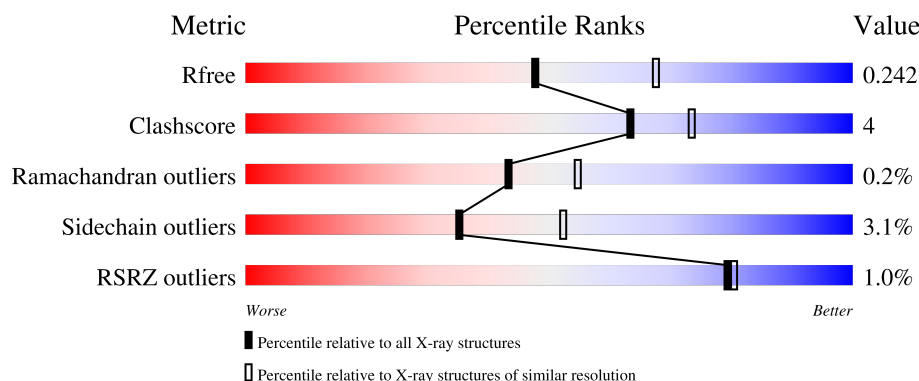
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	79% 9% 11%
1	B	678	78% 11% 11%
1	C	678	78% 11% 11%
1	D	678	76% 12% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	A	710	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20707 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	0	2	0
			4820	3130	794	878	18			
1	B	605	Total	C	N	O	S	0	1	0
			4818	3129	794	878	17			
1	C	603	Total	C	N	O	S	0	4	0
			4805	3121	789	878	17			
1	D	603	Total	C	N	O	S	0	4	0
			4800	3115	789	879	17			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLU	-	expression tag	UNP P16278
A	1	ALA	-	expression tag	UNP P16278
A	2	GLU	-	expression tag	UNP P16278
A	3	ALA	-	expression tag	UNP P16278
A	4	TYR	-	expression tag	UNP P16278
A	5	VAL	-	expression tag	UNP P16278
A	6	GLU	-	expression tag	UNP P16278
A	7	PHE	-	expression tag	UNP P16278
A	8	HIS	-	expression tag	UNP P16278
A	9	HIS	-	expression tag	UNP P16278
A	10	HIS	-	expression tag	UNP P16278
A	11	HIS	-	expression tag	UNP P16278
A	12	HIS	-	expression tag	UNP P16278
A	13	HIS	-	expression tag	UNP P16278
A	14	ASP	-	expression tag	UNP P16278
A	15	TYR	-	expression tag	UNP P16278
A	16	LYS	-	expression tag	UNP P16278
A	17	ASP	-	expression tag	UNP P16278
A	18	ASP	-	expression tag	UNP P16278
A	19	ASP	-	expression tag	UNP P16278
A	20	ASP	-	expression tag	UNP P16278

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	LYS	-	expression tag	UNP P16278
A	22	THR	-	expression tag	UNP P16278
A	23	SER	-	expression tag	UNP P16278
B	0	GLU	-	expression tag	UNP P16278
B	1	ALA	-	expression tag	UNP P16278
B	2	GLU	-	expression tag	UNP P16278
B	3	ALA	-	expression tag	UNP P16278
B	4	TYR	-	expression tag	UNP P16278
B	5	VAL	-	expression tag	UNP P16278
B	6	GLU	-	expression tag	UNP P16278
B	7	PHE	-	expression tag	UNP P16278
B	8	HIS	-	expression tag	UNP P16278
B	9	HIS	-	expression tag	UNP P16278
B	10	HIS	-	expression tag	UNP P16278
B	11	HIS	-	expression tag	UNP P16278
B	12	HIS	-	expression tag	UNP P16278
B	13	HIS	-	expression tag	UNP P16278
B	14	ASP	-	expression tag	UNP P16278
B	15	TYR	-	expression tag	UNP P16278
B	16	LYS	-	expression tag	UNP P16278
B	17	ASP	-	expression tag	UNP P16278
B	18	ASP	-	expression tag	UNP P16278
B	19	ASP	-	expression tag	UNP P16278
B	20	ASP	-	expression tag	UNP P16278
B	21	LYS	-	expression tag	UNP P16278
B	22	THR	-	expression tag	UNP P16278
B	23	SER	-	expression tag	UNP P16278
C	0	GLU	-	expression tag	UNP P16278
C	1	ALA	-	expression tag	UNP P16278
C	2	GLU	-	expression tag	UNP P16278
C	3	ALA	-	expression tag	UNP P16278
C	4	TYR	-	expression tag	UNP P16278
C	5	VAL	-	expression tag	UNP P16278
C	6	GLU	-	expression tag	UNP P16278
C	7	PHE	-	expression tag	UNP P16278
C	8	HIS	-	expression tag	UNP P16278
C	9	HIS	-	expression tag	UNP P16278
C	10	HIS	-	expression tag	UNP P16278
C	11	HIS	-	expression tag	UNP P16278
C	12	HIS	-	expression tag	UNP P16278
C	13	HIS	-	expression tag	UNP P16278
C	14	ASP	-	expression tag	UNP P16278

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Chain	Residue	Modelled	Actual	Comment	Reference
C	15	TYR	-	expression tag	UNP P16278
C	16	LYS	-	expression tag	UNP P16278
C	17	ASP	-	expression tag	UNP P16278
C	18	ASP	-	expression tag	UNP P16278
C	19	ASP	-	expression tag	UNP P16278
C	20	ASP	-	expression tag	UNP P16278
C	21	LYS	-	expression tag	UNP P16278
C	22	THR	-	expression tag	UNP P16278
C	23	SER	-	expression tag	UNP P16278
D	0	GLU	-	expression tag	UNP P16278
D	1	ALA	-	expression tag	UNP P16278
D	2	GLU	-	expression tag	UNP P16278
D	3	ALA	-	expression tag	UNP P16278
D	4	TYR	-	expression tag	UNP P16278
D	5	VAL	-	expression tag	UNP P16278
D	6	GLU	-	expression tag	UNP P16278
D	7	PHE	-	expression tag	UNP P16278
D	8	HIS	-	expression tag	UNP P16278
D	9	HIS	-	expression tag	UNP P16278
D	10	HIS	-	expression tag	UNP P16278
D	11	HIS	-	expression tag	UNP P16278
D	12	HIS	-	expression tag	UNP P16278
D	13	HIS	-	expression tag	UNP P16278
D	14	ASP	-	expression tag	UNP P16278
D	15	TYR	-	expression tag	UNP P16278
D	16	LYS	-	expression tag	UNP P16278
D	17	ASP	-	expression tag	UNP P16278
D	18	ASP	-	expression tag	UNP P16278
D	19	ASP	-	expression tag	UNP P16278
D	20	ASP	-	expression tag	UNP P16278
D	21	LYS	-	expression tag	UNP P16278
D	22	THR	-	expression tag	UNP P16278
D	23	SER	-	expression tag	UNP P16278

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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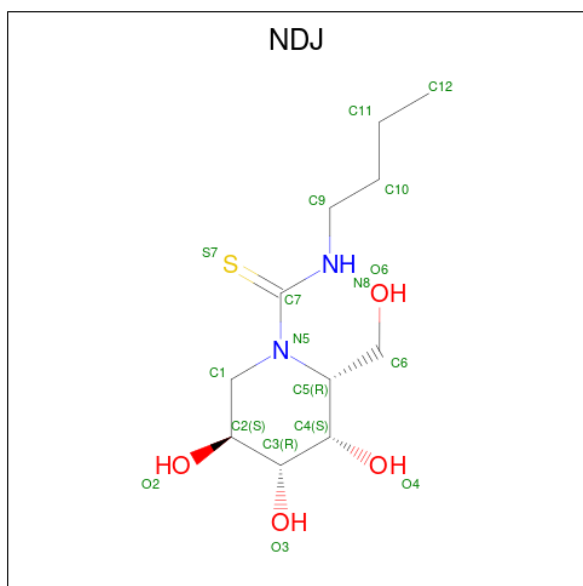
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is (2R,3S,4R,5S)-N-butyl-3,4,5-trihydroxy-2-(hydroxymethyl)piperidine-1-carboxamide (CCD ID: NDJ) (formula: C₁₁H₂₂N₂O₄S).



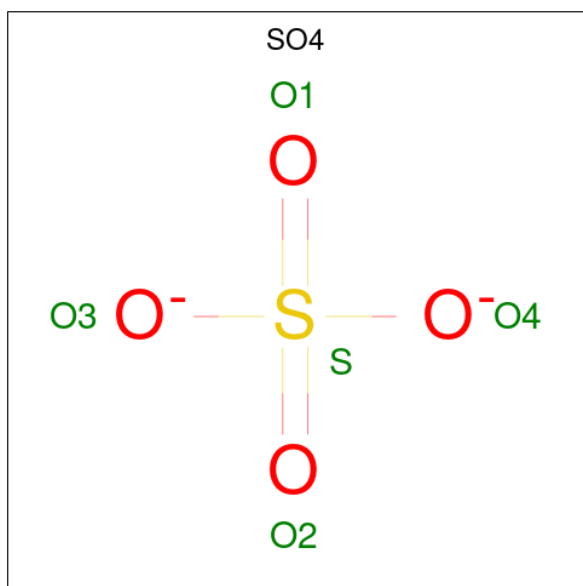
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			18	11	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			18	11	2	4	1		
4	C	1	Total	C	N	O	S	0	0
			18	11	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			18	11	2	4	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

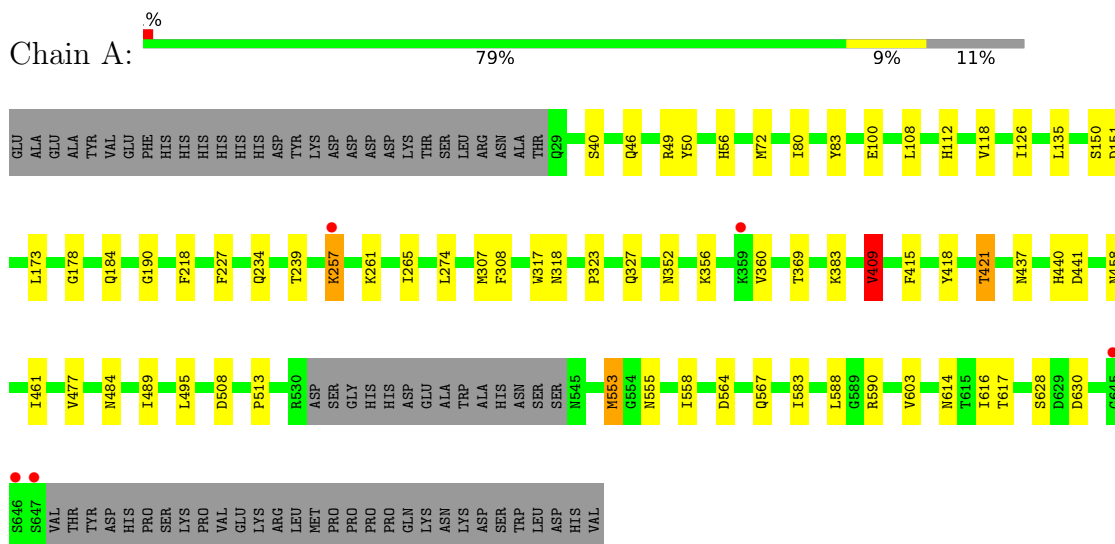
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	288	Total	O	0	0
			288	288		
7	B	288	Total	O	0	0
			288	288		
7	C	279	Total	O	0	0
			279	279		
7	D	237	Total	O	0	0
			237	237		

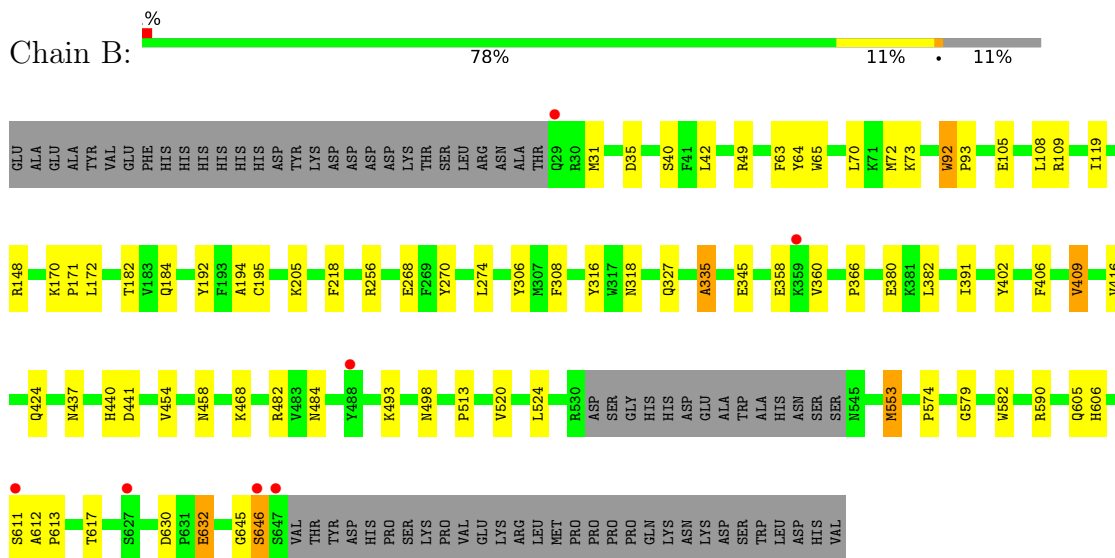
3 Residue-property plots

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.

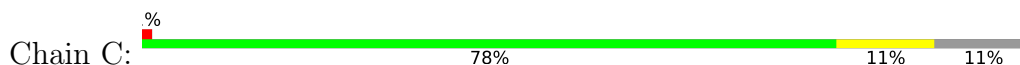
- Molecule 1: Beta-galactosidase

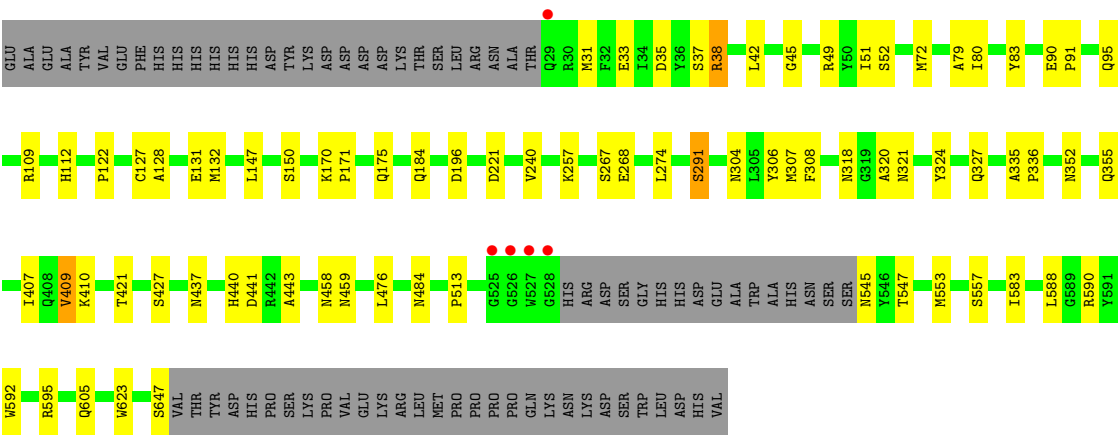


- Molecule 1: Beta-galactosidase

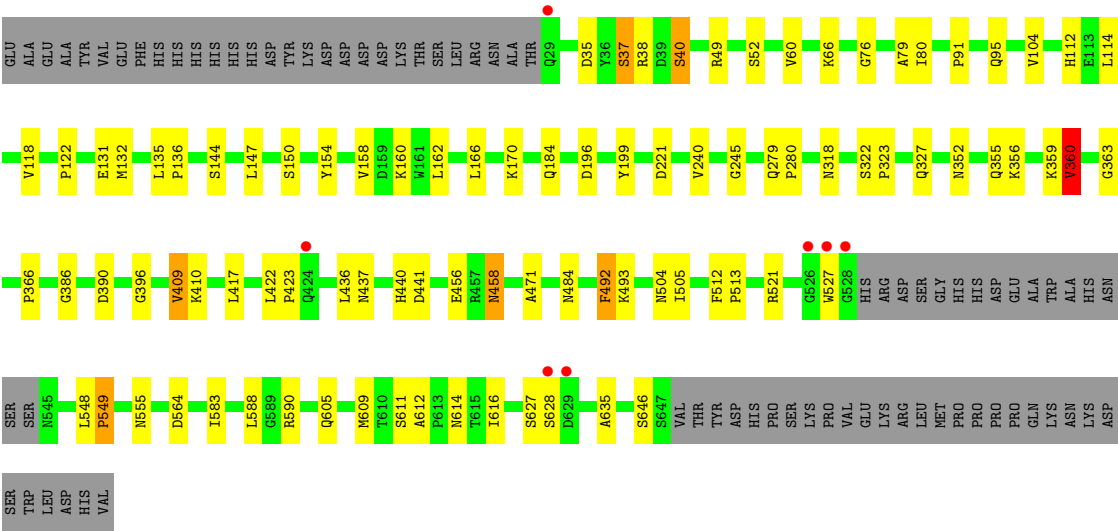
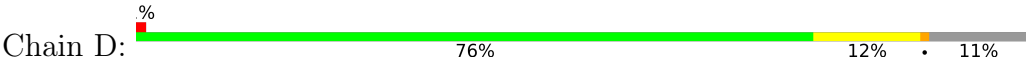


- Molecule 1: Beta-galactosidase





● Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.12Å 116.26Å 141.77Å 90.00° 92.41° 90.00°	Depositor
Resolution (Å)	25.98 – 2.30 25.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (25.98-2.30) 97.5 (25.98-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.175 , 0.240 0.182 , 0.242	Depositor DCC
R_{free} test set	6716 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20707	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: NAG, CL, SO4, NDJ, 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	1.08	2/4982 (0.0%)	1.09	12/6796 (0.2%)
1	B	1.11	1/4974 (0.0%)	1.09	11/6786 (0.2%)
1	C	1.06	1/4977 (0.0%)	1.06	5/6790 (0.1%)
1	D	1.03	3/4971 (0.1%)	1.09	16/6782 (0.2%)
All	All	1.07	7/19904 (0.0%)	1.08	44/27154 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	489	ILE	CA-C	7.47	1.60	1.52
1	A	100	GLU	C-O	-6.06	1.19	1.24
1	B	316	TYR	N-CA	5.60	1.52	1.46
1	D	166	LEU	C-O	-5.54	1.17	1.24
1	D	144	SER	N-CA	5.45	1.53	1.46
1	C	109	ARG	N-CA	5.30	1.52	1.46
1	D	170	LYS	C-O	-5.01	1.19	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	VAL	CB-CA-C	7.68	122.40	111.88
1	A	178	GLY	CA-C-N	7.48	128.47	120.47
1	A	178	GLY	C-N-CA	7.48	128.47	120.47
1	B	335	ALA	CA-C-N	6.70	126.96	119.32
1	B	335	ALA	C-N-CA	6.70	126.96	119.32
1	D	366	PRO	O-C-N	6.59	124.34	121.31
1	A	603	VAL	CA-C-N	6.56	126.48	119.85
1	A	603	VAL	C-N-CA	6.56	126.48	119.85
1	A	46	GLN	CA-C-N	6.11	126.14	119.90
1	A	46	GLN	C-N-CA	6.11	126.14	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ARG	CG-CD-NE	-5.90	99.02	112.00
1	D	635	ALA	N-CA-C	5.80	117.67	108.79
1	B	92	TRP	CA-C-N	-5.77	113.60	119.83
1	B	92	TRP	C-N-CA	-5.77	113.60	119.83
1	C	90	GLU	CA-C-N	5.72	125.57	119.28
1	C	90	GLU	C-N-CA	5.72	125.57	119.28
1	D	612	ALA	CA-C-N	-5.67	114.76	120.31
1	D	612	ALA	C-N-CA	-5.67	114.76	120.31
1	B	579	GLY	N-CA-C	5.64	118.47	110.74
1	A	383	LYS	CB-CA-C	-5.61	99.77	109.86
1	D	360	VAL	CA-C-N	-5.59	114.49	120.03
1	D	360	VAL	C-N-CA	-5.59	114.49	120.03
1	D	49	ARG	CG-CD-NE	-5.58	99.73	112.00
1	D	60	VAL	CA-C-N	-5.58	114.04	119.78
1	D	60	VAL	C-N-CA	-5.58	114.04	119.78
1	C	407	ILE	CB-CA-C	-5.57	104.84	111.97
1	D	458	ASN	N-CA-C	5.56	122.64	110.80
1	D	396	GLY	CA-C-N	5.38	125.36	120.03
1	D	396	GLY	C-N-CA	5.38	125.36	120.03
1	C	45	GLY	N-CA-C	5.38	122.51	115.47
1	B	498	ASN	N-CA-C	5.35	117.98	110.23
1	D	492	PHE	N-CA-C	5.31	116.75	111.07
1	D	104	VAL	N-CA-C	5.23	115.95	110.62
1	D	616	ILE	CB-CA-C	-5.23	103.73	110.84
1	B	553	MET	N-CA-C	5.19	117.70	109.50
1	A	135	LEU	CA-C-N	-5.19	114.57	119.76
1	A	135	LEU	C-N-CA	-5.19	114.57	119.76
1	D	40	SER	N-CA-C	5.18	116.17	108.60
1	A	558	ILE	CA-C-N	-5.18	114.65	120.14
1	A	558	ILE	C-N-CA	-5.18	114.65	120.14
1	B	402	TYR	CA-C-N	-5.14	114.66	119.85
1	B	402	TYR	C-N-CA	-5.14	114.66	119.85
1	C	291	SER	CB-CA-C	-5.07	102.92	110.88
1	B	454	VAL	N-CA-C	5.07	115.57	108.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4820	0	4688	37	0
1	B	4818	0	4687	38	0
1	C	4805	0	4670	37	0
1	D	4800	0	4666	41	0
2	A	56	0	52	0	0
2	B	56	0	52	0	0
2	C	56	0	52	0	0
2	D	56	0	52	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	18	0	22	0	0
4	B	18	0	22	1	0
4	C	18	0	22	1	0
4	D	18	0	22	1	0
5	A	10	0	0	1	0
5	B	10	0	0	0	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
6	A	8	0	12	4	0
6	B	8	0	12	0	0
6	C	8	0	12	0	0
6	D	8	0	12	1	0
7	A	288	0	0	5	0
7	B	288	0	0	5	0
7	C	279	0	0	3	0
7	D	237	0	0	4	0
All	All	20707	0	19055	153	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 4.

All (153) 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:409:VAL:HG13	1:A:513:PRO:HG3	1.62	0.81
1:B:437:ASN:HD21	1:B:458:ASN:H	1.29	0.80
1:D:555:ASN:HB2	2:D:704:NAG:O5	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ASP:HB3	7:D:1006:HOH:O	1.82	0.78
1:C:318:ASN:HD21	1:C:590:ARG:HH21	1.31	0.77
1:B:553:MET:HE3	1:B:617:THR:HG23	1.68	0.76
1:C:437:ASN:HD21	1:C:458:ASN:H	1.33	0.74
1:A:437:ASN:HD21	1:A:458:ASN:H	1.37	0.72
1:B:318:ASN:HD21	1:B:590:ARG:HH21	1.39	0.71
1:D:437:ASN:HD21	1:D:458:ASN:H	1.36	0.70
1:C:112:HIS:CD2	7:C:1050:HOH:O	2.48	0.67
1:B:409:VAL:HG13	1:B:513:PRO:HG3	1.75	0.66
1:C:38:ARG:HH11	1:C:38:ARG:HG3	1.60	0.66
1:A:327:GLN:HE22	1:A:484:ASN:HD21	1.47	0.62
1:B:612:ALA:HB1	1:B:613:PRO:HD2	1.82	0.61
1:D:91:PRO:HD2	1:D:95:GLN:O	2.01	0.61
1:A:257:LYS:HD3	7:A:1059:HOH:O	2.01	0.61
1:B:382:LEU:HD23	1:B:524:LEU:HD12	1.81	0.61
1:A:317:TRP:CZ2	6:A:710:EDO:H11	2.37	0.59
1:A:112:HIS:HD2	7:A:1063:HOH:O	1.84	0.59
1:D:327:GLN:HE22	1:D:484:ASN:HD21	1.50	0.59
1:B:574:PRO:CD	7:B:1068:HOH:O	2.52	0.58
1:B:553:MET:HE3	1:B:617:THR:CG2	2.32	0.57
1:B:574:PRO:HD2	7:B:1068:HOH:O	2.03	0.57
1:B:105:GLU:O	1:B:109:ARG:HG3	2.04	0.57
1:C:583:ILE:HD12	1:C:588:LEU:HD11	1.87	0.56
1:D:422:LEU:HD12	1:D:471:ALA:HB3	1.87	0.56
1:A:421:THR:HB	7:A:1070:HOH:O	2.06	0.55
1:D:112:HIS:HD2	7:D:1005:HOH:O	1.89	0.55
1:D:352[A]:ASN:OD1	1:D:355:GLN:NE2	2.39	0.55
1:B:318:ASN:HD21	1:B:590:ARG:NH2	2.03	0.55
1:C:112:HIS:HD2	7:C:1050:HOH:O	1.87	0.55
1:A:553:MET:HE3	1:A:617:THR:OG1	2.07	0.54
1:C:409:VAL:HG13	1:C:513:PRO:HG3	1.88	0.54
1:A:628:SER:O	1:A:630:ASP:N	2.40	0.54
1:B:73:LYS:HE3	7:B:1059:HOH:O	2.07	0.54
1:C:91:PRO:HD2	1:C:95:GLN:O	2.08	0.53
1:C:122:PRO:HD2	1:C:184:GLN:O	2.08	0.53
1:D:555:ASN:CB	2:D:704:NAG:O5	2.54	0.53
1:A:108:LEU:HD22	1:A:118:VAL:HG11	1.90	0.53
1:B:612:ALA:HB1	1:B:613:PRO:CD	2.39	0.53
1:C:268:GLU:OE1	4:C:705:NDJ:H5	2.09	0.53
1:C:327:GLN:HE22	1:C:484:ASN:HD21	1.55	0.52
1:C:83:TYR:CE2	1:C:128:ALA:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LYS:HE3	7:C:1061:HOH:O	2.09	0.51
1:D:132:MET:HE3	1:D:147:LEU:HD11	1.91	0.51
1:D:150:SER:OG	1:D:196:ASP:OD2	2.28	0.51
1:D:318:ASN:HD21	1:D:590:ARG:HH21	1.57	0.51
1:D:417:LEU:HB3	1:D:512:PHE:HB2	1.92	0.51
1:A:369:THR:HG22	1:D:564:ASP:OD2	2.10	0.51
1:D:52:SER:HA	1:D:79:ALA:O	2.11	0.50
1:D:38:ARG:HB2	7:D:1006:HOH:O	2.12	0.50
1:C:267:SER:O	1:C:304:ASN:HB3	2.12	0.50
1:A:72:MET:HG2	1:A:308:PHE:CD2	2.48	0.49
1:C:150:SER:OG	1:C:196:ASP:OD2	2.30	0.49
1:A:83:TYR:CD1	1:A:126:ILE:HB	2.48	0.48
1:D:555:ASN:HB2	2:D:704:NAG:H61	1.95	0.48
1:A:323:PRO:HA	5:A:708:SO4:O3	2.13	0.48
1:D:322:SER:HA	1:D:323:PRO:C	2.38	0.48
1:B:630:ASP:OD1	1:B:632:GLU:HB3	2.13	0.48
1:B:406:PHE:CZ	1:B:416:VAL:HG23	2.49	0.48
1:C:170:LYS:HB3	1:C:171:PRO:CD	2.43	0.47
1:B:268:GLU:OE1	4:B:706:NDJ:H5	2.15	0.47
1:B:645:GLY:O	1:B:646:SER:C	2.57	0.47
1:D:66:LYS:HE3	1:D:114:LEU:HD21	1.97	0.47
1:A:553:MET:HA	1:A:616:ILE:O	2.14	0.47
1:A:564:ASP:O	1:A:567:GLN:HG3	2.15	0.47
1:B:308:PHE:O	1:B:335:ALA:HB1	2.15	0.47
1:A:184:GLN:HB2	1:A:218:PHE:CZ	2.51	0.46
1:B:184:GLN:HB2	1:B:218:PHE:CZ	2.51	0.46
1:B:119:ILE:HG23	1:B:182:THR:OG1	2.15	0.46
1:B:482:ARG:HG2	1:B:493:LYS:HE2	1.98	0.46
1:A:317:TRP:CE2	6:A:710:EDO:C1	2.98	0.46
1:D:440:HIS:HA	1:D:441:ASP:HA	1.77	0.46
1:A:352:ASN:HB3	7:A:1076:HOH:O	2.16	0.46
1:B:35:ASP:HB2	1:B:42:LEU:HG	1.97	0.45
1:A:190:GLY:HA3	1:A:227:PHE:O	2.16	0.45
1:B:327:GLN:HE22	1:B:484:ASN:HD21	1.64	0.45
1:C:592:TRP:CE2	1:C:595:ARG:HG3	2.52	0.45
1:D:363:GLY:HA3	7:D:1000:HOH:O	2.15	0.45
1:C:38:ARG:HH11	1:C:38:ARG:CG	2.27	0.45
1:A:56:HIS:CE1	1:A:307:MET:HE1	2.52	0.45
1:A:440:HIS:HA	1:A:441:ASP:HA	1.80	0.45
1:C:35:ASP:OD2	1:C:38:ARG:HB2	2.17	0.45
1:C:592:TRP:CZ2	1:C:595:ARG:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ASN:ND2	1:B:590:ARG:HH21	2.10	0.44
1:D:279:GLN:HE21	1:D:280:PRO:HD2	1.83	0.44
1:D:583:ILE:HD12	1:D:588:LEU:HD11	2.00	0.44
1:A:80:ILE:HD11	1:A:118:VAL:HG22	1.99	0.44
1:D:154:TYR:HE2	1:D:199:TYR:CE1	2.35	0.44
1:D:492:PHE:O	1:D:493:LYS:HB2	2.17	0.44
1:D:76:GLY:CA	1:D:360:VAL:HG22	2.48	0.44
1:A:239:THR:HG22	1:A:265:ILE:HD12	2.00	0.44
1:D:504:ASN:O	1:D:505:ILE:C	2.59	0.44
1:A:49:ARG:HG2	1:A:50:TYR:N	2.18	0.43
1:A:150:SER:O	1:A:151:ASP:C	2.61	0.43
1:C:72:MET:HE3	1:C:308:PHE:HB3	2.00	0.43
1:A:555:ASN:HA	1:A:614:ASN:O	2.19	0.43
1:B:170:LYS:N	1:B:171:PRO:HD2	2.34	0.43
1:D:158:VAL:O	1:D:162:LEU:HG	2.18	0.43
1:C:52:SER:HA	1:C:79:ALA:O	2.18	0.43
1:B:92:TRP:O	1:B:93:PRO:C	2.61	0.43
1:D:80:ILE:HD11	1:D:118:VAL:HG22	1.99	0.43
1:D:555:ASN:HA	1:D:614:ASN:O	2.18	0.43
1:A:437:ASN:ND2	1:A:458:ASN:H	2.12	0.42
4:D:708:NDJ:N8	4:D:708:NDJ:H9	2.34	0.42
1:B:63:PHE:CD2	1:B:606:HIS:HB3	2.55	0.42
1:B:194:ALA:O	1:B:195:CYS:C	2.61	0.42
1:C:320:ALA:H	1:C:484:ASN:HD22	1.67	0.42
1:C:409:VAL:O	1:C:410:LYS:HB2	2.20	0.42
1:B:64:TYR:O	1:B:65:TRP:C	2.60	0.42
1:A:318:ASN:HD21	1:A:590:ARG:HH21	1.67	0.42
1:A:415:PHE:HA	1:A:477:VAL:O	2.20	0.42
1:B:72:MET:HG2	1:B:308:PHE:CD2	2.55	0.42
1:C:547:THR:OG1	1:C:623:TRP:HA	2.20	0.42
1:B:108:LEU:HD12	1:B:172:LEU:HD13	2.01	0.42
1:B:31:MET:HA	7:B:890:HOH:O	2.20	0.41
1:C:132:MET:HE3	1:C:147:LEU:HD11	2.00	0.41
1:D:135:LEU:HA	1:D:136:PRO:HD3	1.91	0.41
1:A:583:ILE:HD12	1:A:588:LEU:HD11	2.02	0.41
1:B:148:ARG:HB2	1:B:192:TYR:CE2	2.54	0.41
1:A:173:LEU:HD23	1:A:173:LEU:HA	1.86	0.41
1:C:35:ASP:HB2	1:C:42:LEU:HG	2.02	0.41
1:D:122:PRO:HD2	1:D:184:GLN:O	2.20	0.41
1:D:245:GLY:H	6:D:706:EDO:H22	1.84	0.41
1:C:352[A]:ASN:OD1	1:C:355:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:HIS:HA	1:C:441:ASP:HA	1.85	0.41
1:D:221:ASP:O	1:D:240:VAL:HA	2.21	0.41
1:A:317:TRP:CE2	6:A:710:EDO:H11	2.56	0.41
1:B:70:LEU:HD23	1:B:366:PRO:HG2	2.02	0.41
1:C:321:ASN:O	1:C:324:TYR:HA	2.21	0.41
1:C:409:VAL:O	1:C:410:LYS:CB	2.69	0.41
1:D:437:ASN:OD1	1:D:458:ASN:OD1	2.39	0.41
1:A:317:TRP:CZ2	6:A:710:EDO:C1	3.02	0.41
1:B:520:VAL:HG11	1:B:582:TRP:CG	2.56	0.41
1:C:221:ASP:O	1:C:240:VAL:HA	2.20	0.41
1:C:306:TYR:HA	1:C:307:MET:HA	1.93	0.41
1:A:461:ILE:HD13	1:A:461:ILE:HG21	1.87	0.41
1:B:270:TYR:HA	1:B:306:TYR:O	2.21	0.41
1:B:440:HIS:HA	1:B:441:ASP:HA	1.86	0.41
1:A:112:HIS:CD2	7:A:1063:HOH:O	2.65	0.40
1:C:409:VAL:O	1:C:409:VAL:CG1	2.68	0.40
1:C:335:ALA:HB1	1:C:336:PRO:HD2	2.03	0.40
1:D:37:SER:HB2	1:D:38:ARG:HG2	2.02	0.40
1:D:409:VAL:O	1:D:410:LYS:HB2	2.20	0.40
1:A:418:TYR:CD2	1:A:495:LEU:HD12	2.55	0.40
1:B:574:PRO:HG2	7:B:1068:HOH:O	2.22	0.40
1:C:443:ALA:HA	1:C:476:LEU:O	2.22	0.40
1:D:409:VAL:HG13	1:D:513:PRO:HG3	2.03	0.40
1:D:436:LEU:O	1:D:437:ASN:HB3	2.21	0.40
1:D:548:LEU:O	1:D:549:PRO:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	603/678 (89%)	570 (94%)	32 (5%)	1 (0%)	43 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	602/678 (89%)	575 (96%)	26 (4%)	1 (0%)	43	55
1	C	603/678 (89%)	576 (96%)	26 (4%)	1 (0%)	43	55
1	D	603/678 (89%)	569 (94%)	32 (5%)	2 (0%)	36	46
All	All	2411/2712 (89%)	2290 (95%)	116 (5%)	5 (0%)	43	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	646	SER
1	A	508	ASP
1	C	127	CYS
1	D	423	PRO
1	D	386	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	520/585 (89%)	510 (98%)	10 (2%)	50	69
1	B	519/585 (89%)	504 (97%)	15 (3%)	37	55
1	C	520/585 (89%)	498 (96%)	22 (4%)	26	40
1	D	520/585 (89%)	499 (96%)	21 (4%)	28	42
All	All	2079/2340 (89%)	2011 (97%)	68 (3%)	35	50

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	234	GLN
1	A	257	LYS
1	A	261	LYS
1	A	274	LEU
1	A	356	LYS

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Mol	Chain	Res	Type
1	A	360	VAL
1	A	409	VAL
1	A	421	THR
1	A	553	MET
1	B	40	SER
1	B	205	LYS
1	B	256	ARG
1	B	274	LEU
1	B	345	GLU
1	B	358	GLU
1	B	360	VAL
1	B	380	GLU
1	B	391	ILE
1	B	409	VAL
1	B	424	GLN
1	B	468	LYS
1	B	605	GLN
1	B	611	SER
1	B	632	GLU
1	C	31	MET
1	C	33	GLU
1	C	37	SER
1	C	38	ARG
1	C	49	ARG
1	C	51	ILE
1	C	80	ILE
1	C	131	GLU
1	C	175[A]	GLN
1	C	175[B]	GLN
1	C	257	LYS
1	C	274	LEU
1	C	291	SER
1	C	409	VAL
1	C	421	THR
1	C	427	SER
1	C	459	ASN
1	C	545	ASN
1	C	553	MET
1	C	557	SER
1	C	605	GLN
1	C	647	SER
1	D	37	SER

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Mol	Chain	Res	Type
1	D	40	SER
1	D	131	GLU
1	D	160	LYS
1	D	356	LYS
1	D	359	LYS
1	D	360	VAL
1	D	390	ASP
1	D	409	VAL
1	D	456	GLU
1	D	521	ARG
1	D	527	TRP
1	D	549	PRO
1	D	605	GLN
1	D	609[A]	MET
1	D	609[B]	MET
1	D	611[A]	SER
1	D	611[B]	SER
1	D	627	SER
1	D	628	SER
1	D	646	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	102	HIS
1	A	112	HIS
1	A	204	GLN
1	A	318	ASN
1	A	321	ASN
1	A	412	HIS
1	A	437	ASN
1	A	484	ASN
1	B	95	GLN
1	B	318	ASN
1	B	321	ASN
1	B	355	GLN
1	B	437	ASN
1	B	484	ASN
1	B	523	HIS
1	B	605	GLN
1	C	95	GLN

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Mol	Chain	Res	Type
1	C	102	HIS
1	C	204	GLN
1	C	209	HIS
1	C	318	ASN
1	C	321	ASN
1	C	355	GLN
1	C	437	ASN
1	C	484	ASN
1	D	29	GLN
1	D	204	GLN
1	D	279	GLN
1	D	318	ASN
1	D	321	ASN
1	D	355	GLN
1	D	437	ASN
1	D	484	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 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 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
6	EDO	B	710	-	3,3,3	0.45	0	2,2,2	0.28	0
6	EDO	C	710	-	3,3,3	0.56	0	2,2,2	0.28	0
2	NAG	D	705	1	14,14,15	0.94	0	17,19,21	1.56	4 (23%)
5	SO4	A	707	-	4,4,4	0.53	0	6,6,6	0.29	0
2	NAG	B	704	1	14,14,15	0.50	0	17,19,21	0.77	0
5	SO4	B	708	-	4,4,4	0.60	0	6,6,6	0.87	0
5	SO4	B	707	-	4,4,4	0.51	0	6,6,6	0.20	0
2	NAG	A	703	1	14,14,15	1.56	3 (21%)	17,19,21	3.20	10 (58%)
2	NAG	D	703	1	14,14,15	0.67	0	17,19,21	1.68	4 (23%)
5	SO4	C	706	-	4,4,4	0.48	0	6,6,6	0.23	0
5	SO4	D	709	-	4,4,4	0.39	0	6,6,6	0.50	0
2	NAG	A	702	1	14,14,15	0.50	0	17,19,21	2.47	5 (29%)
2	NAG	B	703	1	14,14,15	0.88	1 (7%)	17,19,21	2.32	3 (17%)
6	EDO	B	709	-	3,3,3	0.42	0	2,2,2	0.62	0
2	NAG	D	701	1	14,14,15	0.29	0	17,19,21	0.56	0
2	NAG	C	704	1	14,14,15	0.71	0	17,19,21	1.77	6 (35%)
2	NAG	C	701	1	14,14,15	0.69	0	17,19,21	1.94	3 (17%)
2	NAG	A	704	1	14,14,15	0.86	1 (7%)	17,19,21	1.51	3 (17%)
4	NDJ	B	706	-	18,18,18	2.05	5 (27%)	20,24,24	1.88	5 (25%)
2	NAG	A	701	1	14,14,15	0.98	2 (14%)	17,19,21	2.00	3 (17%)
2	NAG	B	702	1	14,14,15	0.81	0	17,19,21	1.53	2 (11%)
2	NAG	D	704	1	14,14,15	0.68	0	17,19,21	2.70	5 (29%)
4	NDJ	C	705	-	18,18,18	1.84	3 (16%)	20,24,24	1.96	4 (20%)
5	SO4	A	708	-	4,4,4	0.71	0	6,6,6	0.73	0
6	EDO	D	706	-	3,3,3	0.30	0	2,2,2	1.68	1 (50%)
6	EDO	A	709	-	3,3,3	0.41	0	2,2,2	0.74	0
4	NDJ	D	708	-	18,18,18	1.68	3 (16%)	20,24,24	1.77	4 (20%)
2	NAG	C	703	1	14,14,15	0.78	0	17,19,21	1.70	5 (29%)
5	SO4	D	710	-	4,4,4	0.63	0	6,6,6	1.00	0
6	EDO	C	709	-	3,3,3	0.70	0	2,2,2	0.26	0
4	NDJ	A	706	-	18,18,18	1.79	5 (27%)	20,24,24	1.79	5 (25%)
2	NAG	C	702	1	14,14,15	0.74	1 (7%)	17,19,21	1.85	3 (17%)
2	NAG	B	701	1	14,14,15	0.61	0	17,19,21	1.43	1 (5%)
5	SO4	C	707	-	4,4,4	0.54	0	6,6,6	0.74	0
6	EDO	A	710	-	3,3,3	0.33	0	2,2,2	0.21	0
6	EDO	D	707	-	3,3,3	0.52	0	2,2,2	0.23	0

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
6	EDO	B	710	-	-	1/1/1/1	-
6	EDO	C	710	-	-	1/1/1/1	-
2	NAG	D	705	1	-	0/6/23/26	0/1/1/1
2	NAG	B	704	1	-	2/6/23/26	0/1/1/1
2	NAG	A	703	1	-	1/6/23/26	0/1/1/1
2	NAG	D	703	1	-	2/6/23/26	0/1/1/1
2	NAG	A	702	1	-	2/6/23/26	0/1/1/1
2	NAG	B	703	1	-	0/6/23/26	0/1/1/1
6	EDO	B	709	-	-	1/1/1/1	-
2	NAG	D	701	1	-	2/6/23/26	0/1/1/1
2	NAG	C	704	1	-	1/6/23/26	0/1/1/1
2	NAG	C	701	1	-	0/6/23/26	0/1/1/1
2	NAG	A	704	1	-	2/6/23/26	0/1/1/1
4	NDJ	B	706	-	-	6/11/31/31	0/1/1/1
2	NAG	A	701	1	-	2/6/23/26	0/1/1/1
2	NAG	B	702	1	-	0/6/23/26	0/1/1/1
2	NAG	D	704	1	-	3/6/23/26	0/1/1/1
4	NDJ	C	705	-	-	5/11/31/31	0/1/1/1
6	EDO	D	706	-	-	0/1/1/1	-
6	EDO	A	709	-	-	0/1/1/1	-
4	NDJ	D	708	-	-	8/11/31/31	0/1/1/1
2	NAG	C	703	1	-	1/6/23/26	0/1/1/1
6	EDO	C	709	-	-	1/1/1/1	-
4	NDJ	A	706	-	-	5/11/31/31	0/1/1/1
2	NAG	C	702	1	-	0/6/23/26	0/1/1/1
2	NAG	B	701	1	-	1/6/23/26	0/1/1/1
6	EDO	A	710	-	-	1/1/1/1	-
6	EDO	D	707	-	-	1/1/1/1	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	705	NDJ	C7-N5	5.70	1.42	1.34
4	D	708	NDJ	C7-N5	4.67	1.40	1.34
4	A	706	NDJ	C7-N5	4.59	1.40	1.34
4	B	706	NDJ	C7-N5	4.38	1.40	1.34
4	D	708	NDJ	C7-S7	-4.30	1.60	1.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	706	NDJ	C7-S7	-4.04	1.61	1.67
4	C	705	NDJ	C7-S7	-3.75	1.61	1.67
2	A	703	NAG	C2-N2	3.73	1.52	1.46
4	B	706	NDJ	C1-C2	3.44	1.56	1.52
4	B	706	NDJ	C2-C3	3.03	1.57	1.52
4	B	706	NDJ	C7-N8	2.90	1.38	1.34
4	A	706	NDJ	C1-C2	2.83	1.56	1.52
2	A	703	NAG	C3-C2	2.72	1.58	1.52
4	A	706	NDJ	C5-N5	2.64	1.51	1.48
4	A	706	NDJ	C7-S7	-2.59	1.63	1.67
2	A	701	NAG	O5-C1	-2.56	1.39	1.43
4	A	706	NDJ	C7-N8	2.48	1.37	1.34
2	C	702	NAG	C1-C2	2.33	1.55	1.52
2	B	703	NAG	C1-C2	2.29	1.55	1.52
2	A	703	NAG	C1-C2	2.27	1.55	1.52
4	C	705	NDJ	C7-N8	2.20	1.37	1.34
2	A	701	NAG	C2-N2	-2.19	1.42	1.46
4	D	708	NDJ	C7-N8	2.16	1.37	1.34
2	A	704	NAG	C1-C2	2.09	1.55	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	704	NAG	C1-O5-C5	8.17	123.14	112.19
2	A	702	NAG	C1-O5-C5	7.99	122.89	112.19
2	B	703	NAG	C1-O5-C5	7.49	122.22	112.19
2	A	703	NAG	C1-O5-C5	6.56	120.98	112.19
2	A	701	NAG	C1-C2-N2	-5.91	101.12	110.43
2	C	702	NAG	C1-O5-C5	5.38	119.39	112.19
2	A	703	NAG	O3-C3-C2	5.38	120.57	109.40
2	D	704	NAG	O5-C1-C2	5.33	119.54	111.29
2	A	703	NAG	O7-C7-C8	-5.20	112.80	122.05
4	B	706	NDJ	C2-C1-N5	-4.90	102.68	110.30
4	A	706	NDJ	C6-C5-C4	-4.74	105.79	112.93
2	C	701	NAG	C4-C3-C2	4.58	117.72	111.02
2	A	703	NAG	O3-C3-C4	-4.51	99.75	110.38
2	A	704	NAG	C1-O5-C5	4.28	117.93	112.19
4	C	705	NDJ	S7-C7-N8	-4.24	114.54	122.47
4	C	705	NDJ	C1-N5-C5	-4.23	103.70	115.29
2	A	703	NAG	C2-N2-C7	4.20	128.53	122.90
2	D	703	NAG	C1-O5-C5	4.19	117.81	112.19
4	D	708	NDJ	N8-C7-N5	4.15	123.36	116.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	NAG	C1-O5-C5	4.04	117.60	112.19
4	C	705	NDJ	N8-C7-N5	3.81	122.76	116.15
2	B	701	NAG	C1-O5-C5	3.74	117.20	112.19
4	D	708	NDJ	S7-C7-N8	-3.67	115.61	122.47
2	C	701	NAG	C1-O5-C5	3.67	117.10	112.19
4	C	705	NDJ	C2-C1-N5	-3.63	104.64	110.30
2	C	701	NAG	C3-C4-C5	3.60	116.75	110.23
2	C	704	NAG	C1-C2-N2	-3.56	104.82	110.43
2	D	705	NAG	C3-C4-C5	-3.53	103.83	110.23
2	A	702	NAG	C1-C2-N2	-3.33	105.18	110.43
2	B	703	NAG	C3-C4-C5	3.33	116.27	110.23
2	A	703	NAG	C8-C7-N2	3.33	121.64	116.12
4	B	706	NDJ	C1-N5-C5	-3.25	106.38	115.29
4	D	708	NDJ	C2-C1-N5	-3.11	105.46	110.30
4	A	706	NDJ	S7-C7-N8	-3.02	116.82	122.47
4	D	708	NDJ	C1-N5-C5	-3.02	107.01	115.29
4	B	706	NDJ	S7-C7-N8	-3.01	116.85	122.47
4	B	706	NDJ	N8-C7-N5	2.99	121.34	116.15
2	A	701	NAG	C8-C7-N2	-2.98	111.18	116.12
2	C	703	NAG	O3-C3-C4	2.96	117.36	110.38
2	C	703	NAG	C1-O5-C5	2.91	116.09	112.19
2	A	702	NAG	O5-C5-C4	2.91	117.90	110.83
4	A	706	NDJ	C1-N5-C5	-2.77	107.70	115.29
4	A	706	NDJ	C2-C1-N5	-2.74	106.04	110.30
2	D	705	NAG	O4-C4-C3	-2.73	103.94	110.38
2	D	703	NAG	C2-N2-C7	-2.69	119.30	122.90
2	C	703	NAG	C1-C2-N2	2.67	114.63	110.43
2	C	703	NAG	C8-C7-N2	2.66	120.53	116.12
2	C	704	NAG	O7-C7-C8	-2.66	117.32	122.05
2	A	704	NAG	C4-C3-C2	2.60	114.83	111.02
2	D	704	NAG	C4-C3-C2	-2.59	107.22	111.02
2	D	703	NAG	C1-C2-N2	-2.56	106.40	110.43
2	B	703	NAG	C6-C5-C4	-2.55	106.77	113.02
4	A	706	NDJ	C1-C2-C3	2.52	113.16	110.17
2	D	704	NAG	O7-C7-C8	-2.50	117.60	122.05
2	D	705	NAG	C1-O5-C5	2.50	115.53	112.19
2	C	704	NAG	C1-O5-C5	2.47	115.49	112.19
4	B	706	NDJ	O3-C3-C2	2.45	115.06	110.05
2	D	703	NAG	C3-C4-C5	-2.45	105.80	110.23
2	C	704	NAG	O5-C5-C6	2.41	112.35	107.66
2	A	702	NAG	C6-C5-C4	-2.38	107.16	113.02
2	A	703	NAG	O5-C1-C2	2.38	114.97	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	704	NAG	O7-C7-N2	2.36	126.16	121.98
2	B	702	NAG	O7-C7-N2	2.32	126.08	121.98
2	C	703	NAG	O3-C3-C2	-2.31	104.61	109.40
2	A	701	NAG	O7-C7-N2	2.28	126.02	121.98
2	A	704	NAG	C3-C4-C5	2.27	114.35	110.23
6	D	706	EDO	O2-C2-C1	-2.25	95.28	112.39
2	C	702	NAG	C1-C2-N2	2.20	113.91	110.43
2	A	703	NAG	C4-C3-C2	-2.17	107.83	111.02
2	A	702	NAG	O6-C6-C5	-2.13	104.08	111.33
2	C	702	NAG	C2-N2-C7	-2.10	120.08	122.90
2	D	705	NAG	C2-N2-C7	-2.08	120.11	122.90
2	C	704	NAG	O3-C3-C2	-2.06	105.12	109.40
2	A	703	NAG	C1-C2-N2	2.05	113.66	110.43
2	A	703	NAG	O7-C7-N2	2.03	125.56	121.98
2	D	704	NAG	O5-C5-C6	2.01	111.57	107.66

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	706	NDJ	N8-C7-N5-C1
4	A	706	NDJ	N8-C7-N5-C5
4	A	706	NDJ	S7-C7-N5-C5
4	B	706	NDJ	N8-C7-N5-C1
4	B	706	NDJ	S7-C7-N5-C1
4	B	706	NDJ	N8-C7-N5-C5
4	B	706	NDJ	S7-C7-N5-C5
4	D	708	NDJ	N8-C7-N5-C5
4	D	708	NDJ	S7-C7-N5-C5
2	A	702	NAG	O5-C5-C6-O6
2	D	704	NAG	O5-C5-C6-O6
2	A	702	NAG	C4-C5-C6-O6
2	D	704	NAG	C4-C5-C6-O6
2	B	704	NAG	O5-C5-C6-O6
4	D	708	NDJ	C10-C9-N8-C7
2	A	704	NAG	C4-C5-C6-O6
2	A	701	NAG	C4-C5-C6-O6
2	A	704	NAG	O5-C5-C6-O6
2	B	704	NAG	C4-C5-C6-O6
2	D	701	NAG	O5-C5-C6-O6
2	D	701	NAG	C4-C5-C6-O6
4	A	706	NDJ	S7-C7-N5-C1

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Mol	Chain	Res	Type	Atoms
4	D	708	NDJ	C9-C10-C11-C12
6	B	710	EDO	O1-C1-C2-O2
4	B	706	NDJ	C11-C10-C9-N8
4	D	708	NDJ	N8-C7-N5-C1
2	A	701	NAG	O5-C5-C6-O6
2	A	703	NAG	O5-C5-C6-O6
4	C	705	NDJ	C11-C10-C9-N8
6	C	710	EDO	O1-C1-C2-O2
4	D	708	NDJ	C11-C10-C9-N8
6	D	707	EDO	O1-C1-C2-O2
2	D	703	NAG	C4-C5-C6-O6
4	A	706	NDJ	N5-C5-C6-O6
4	B	706	NDJ	N5-C5-C6-O6
4	C	705	NDJ	N5-C5-C6-O6
4	D	708	NDJ	N5-C5-C6-O6
4	D	708	NDJ	S7-C7-N5-C1
2	C	703	NAG	O5-C5-C6-O6
2	D	703	NAG	O5-C5-C6-O6
6	A	710	EDO	O1-C1-C2-O2
6	C	709	EDO	O1-C1-C2-O2
4	C	705	NDJ	N8-C7-N5-C1
2	D	704	NAG	C1-C2-N2-C7
4	C	705	NDJ	S7-C7-N5-C1
2	C	704	NAG	C4-C5-C6-O6
6	B	709	EDO	O1-C1-C2-O2
2	B	701	NAG	C4-C5-C6-O6
4	C	705	NDJ	C9-C10-C11-C12

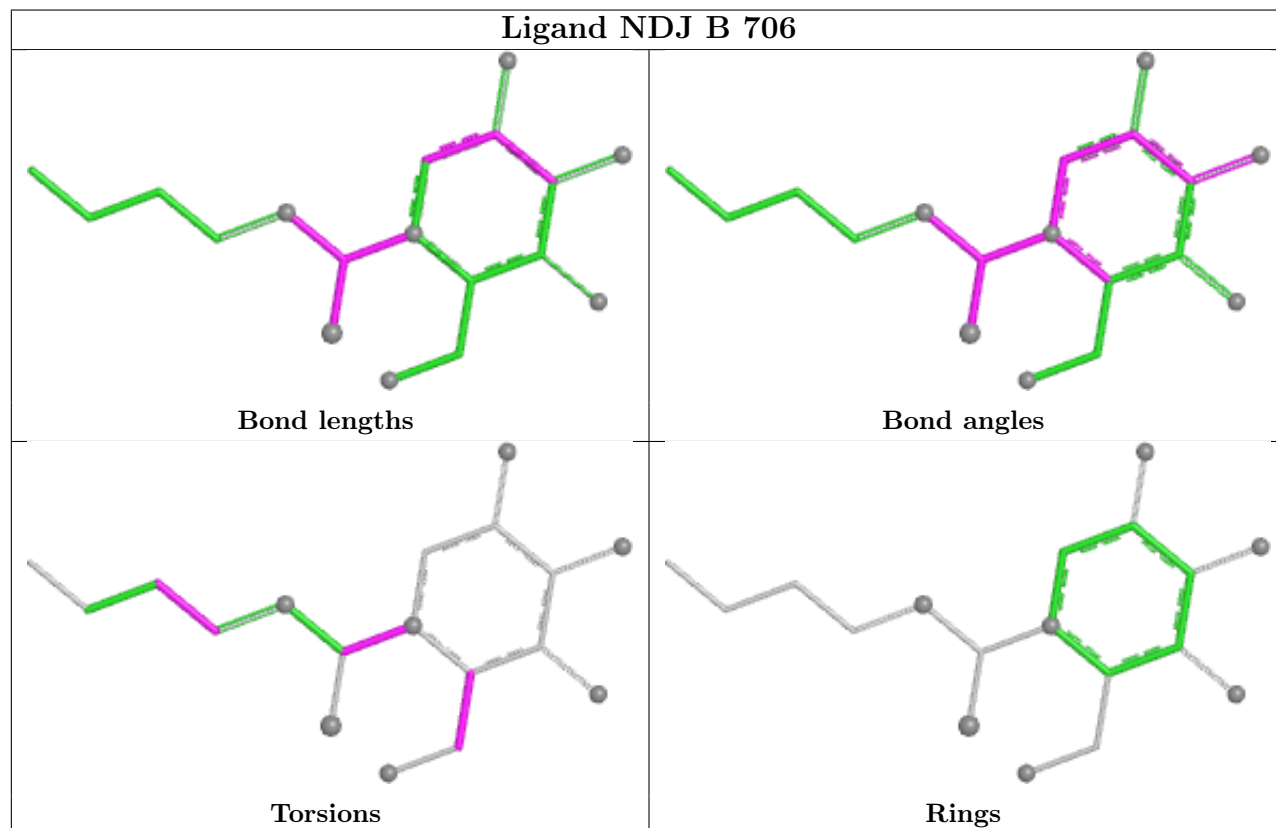
There are no ring outliers.

7 monomers are involved in 12 short contacts:

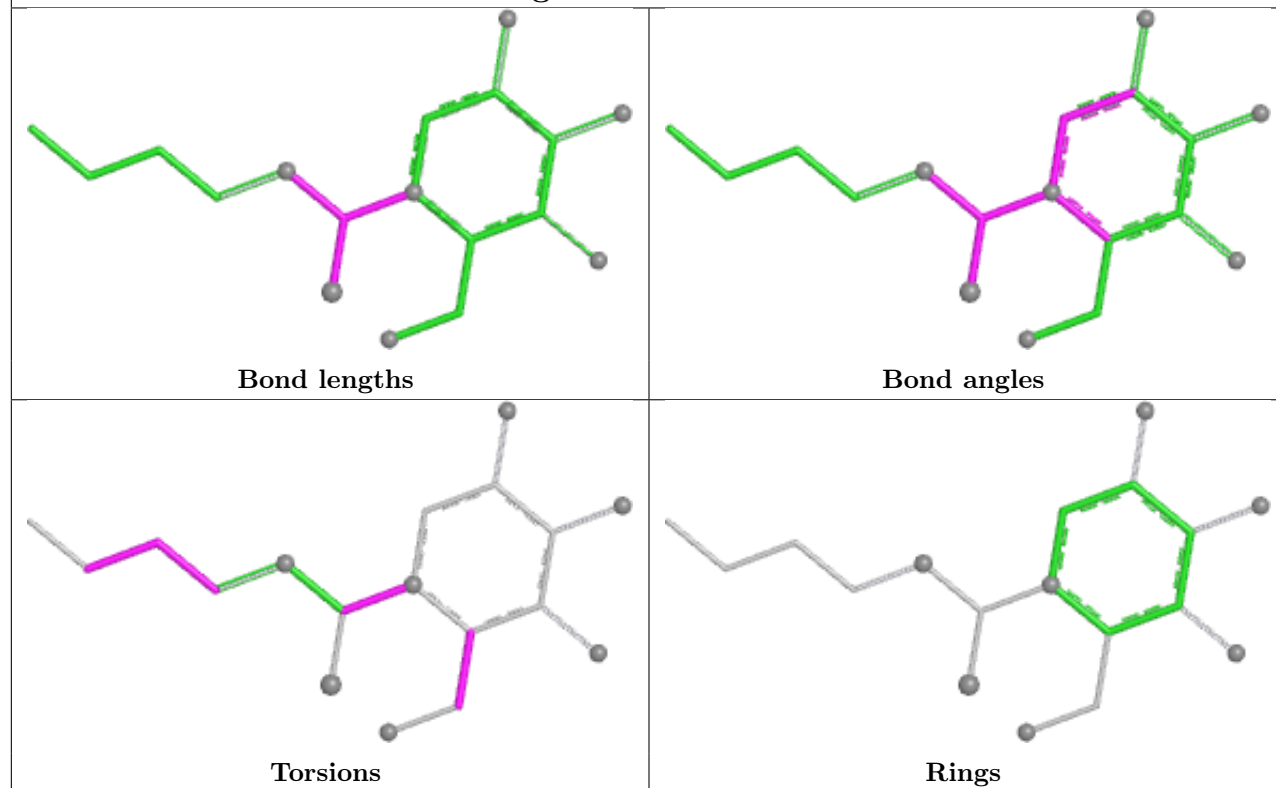
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	706	NDJ	1	0
2	D	704	NAG	3	0
4	C	705	NDJ	1	0
5	A	708	SO4	1	0
6	D	706	EDO	1	0
4	D	708	NDJ	1	0
6	A	710	EDO	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

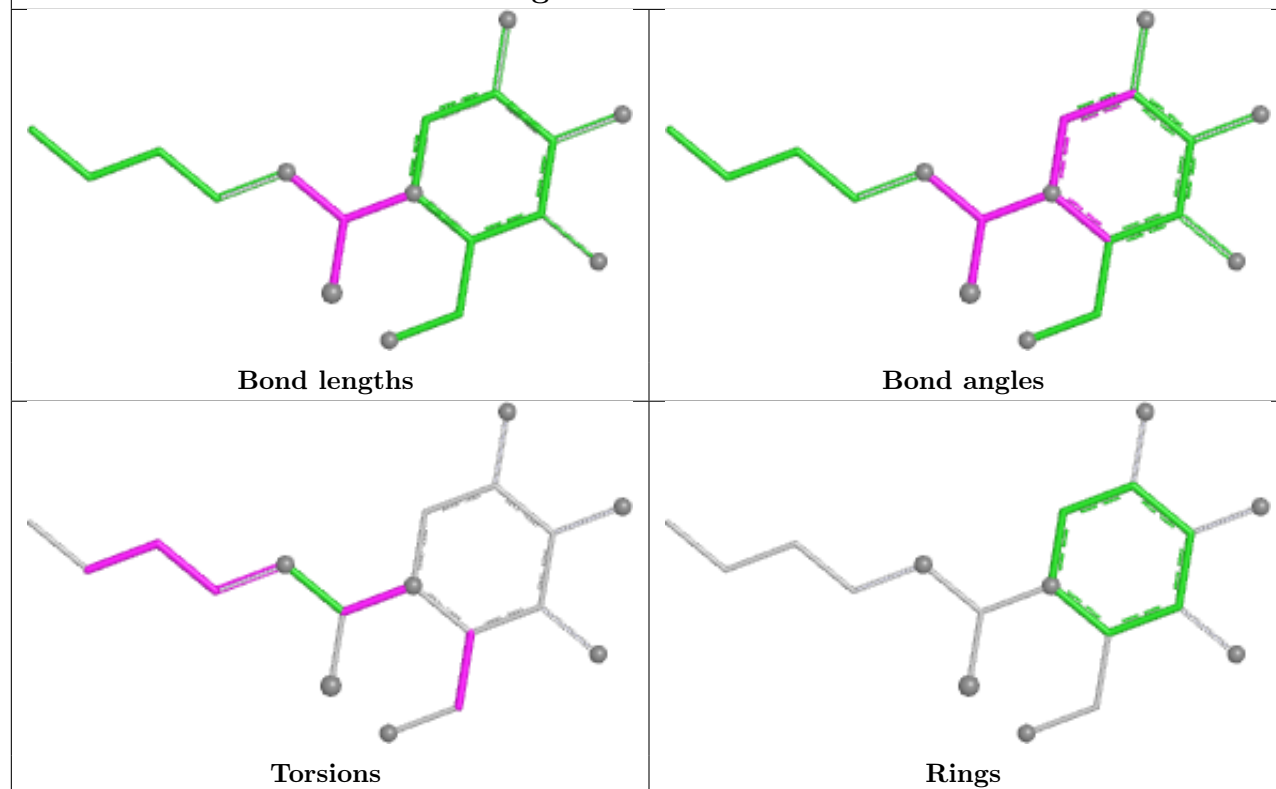
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

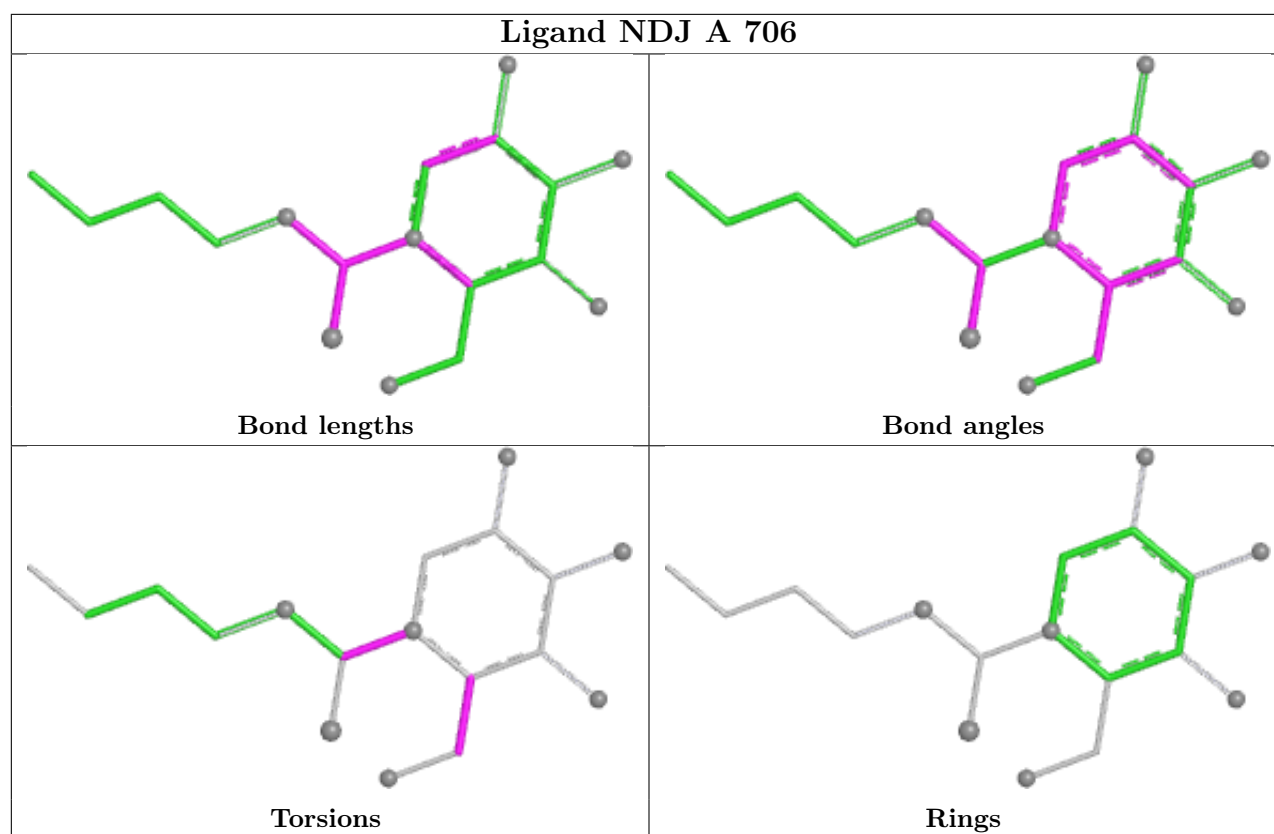


Ligand NDJ C 705



Ligand NDJ D 708





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	605/678 (89%)	-0.28	5 (0%) 82 83	13, 29, 48, 104	2 (0%)
1	B	605/678 (89%)	-0.33	7 (1%) 76 77	13, 27, 46, 93	1 (0%)
1	C	603/678 (88%)	-0.25	5 (0%) 82 83	14, 29, 56, 87	4 (0%)
1	D	603/678 (88%)	-0.21	7 (1%) 76 77	17, 30, 58, 97	4 (0%)
All	All	2416/2712 (89%)	-0.26	24 (0%) 79 80	13, 28, 54, 104	11 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	647	SER	5.3
1	C	528	GLY	4.7
1	C	527	TRP	4.6
1	B	646	SER	4.0
1	D	527	TRP	3.5
1	D	29	GLN	3.1
1	C	526	GLY	3.0
1	A	646	SER	2.7
1	D	526	GLY	2.7
1	C	525	GLY	2.7
1	B	647	SER	2.6
1	D	628	SER	2.6
1	A	257	LYS	2.5
1	B	29	GLN	2.4
1	D	629	ASP	2.2
1	B	488	TYR	2.2
1	D	528	GLY	2.2
1	A	359	LYS	2.1
1	B	611	SER	2.1
1	B	627	SER	2.1
1	C	29	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	645	GLY	2.1
1	B	359	LYS	2.0
1	D	424	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	701	14/15	0.63	0.15	78,83,85,86	0
2	NAG	A	704	14/15	0.65	0.16	59,71,84,84	0
2	NAG	C	701	14/15	0.68	0.16	75,92,97,100	0
2	NAG	D	704	14/15	0.68	0.18	72,93,100,101	0
2	NAG	A	703	14/15	0.74	0.15	43,50,55,55	0
5	SO4	D	710	5/5	0.77	0.14	54,59,70,70	0
2	NAG	C	702	14/15	0.80	0.12	53,58,61,63	0
6	EDO	A	709	4/4	0.80	0.19	42,47,53,58	0
2	NAG	C	703	14/15	0.81	0.12	40,52,55,58	0
5	SO4	A	707	5/5	0.82	0.12	65,69,76,83	0
5	SO4	C	706	5/5	0.82	0.19	70,73,82,83	0
6	EDO	B	709	4/4	0.82	0.21	47,51,53,55	0
5	SO4	D	709	5/5	0.83	0.14	68,76,78,87	0
2	NAG	D	703	14/15	0.86	0.10	42,53,62,63	0
6	EDO	C	710	4/4	0.86	0.17	37,46,54,55	0
5	SO4	C	707	5/5	0.87	0.12	58,58,62,62	0
2	NAG	A	702	14/15	0.87	0.10	25,36,42,45	0
2	NAG	B	703	14/15	0.87	0.11	46,52,61,61	0
2	NAG	B	704	14/15	0.88	0.10	59,67,70,71	0
5	SO4	B	708	5/5	0.88	0.13	57,58,61,66	0

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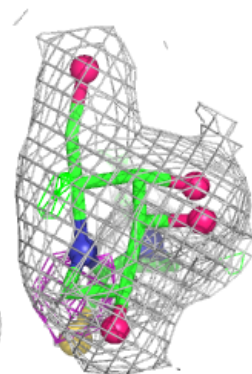
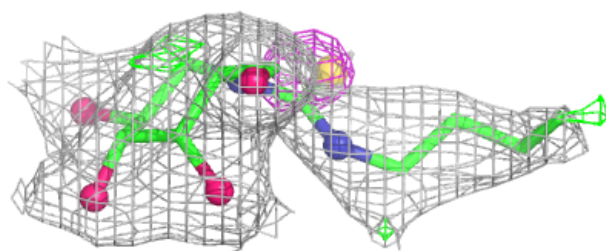
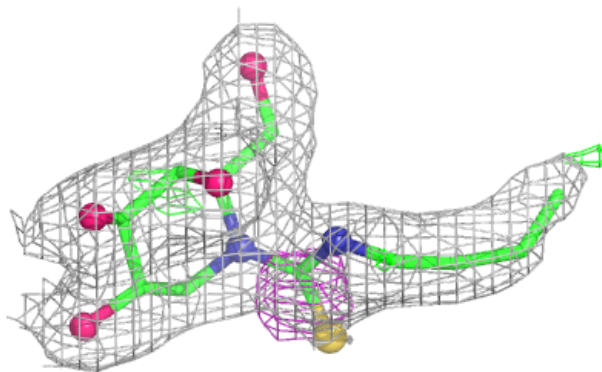
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NDJ	D	708	18/18	0.88	0.13	27,35,58,77	0
6	EDO	D	706	4/4	0.88	0.12	35,38,39,40	0
5	SO4	B	707	5/5	0.89	0.13	73,74,81,82	0
5	SO4	A	708	5/5	0.89	0.14	47,48,59,62	0
4	NDJ	B	706	18/18	0.90	0.14	22,29,81,83	0
4	NDJ	A	706	18/18	0.90	0.12	25,29,59,66	0
2	NAG	B	701	14/15	0.91	0.07	35,40,49,49	0
6	EDO	B	710	4/4	0.92	0.13	43,43,47,48	0
4	NDJ	C	705	18/18	0.92	0.12	19,31,63,77	0
2	NAG	D	705	14/15	0.92	0.07	32,36,39,44	0
2	NAG	C	704	14/15	0.93	0.07	27,31,34,34	0
2	NAG	A	701	14/15	0.93	0.07	26,30,34,38	0
6	EDO	C	709	4/4	0.94	0.12	30,34,35,35	0
2	NAG	B	702	14/15	0.94	0.07	31,35,38,39	0
6	EDO	A	710	4/4	0.94	0.10	34,45,46,47	0
6	EDO	D	707	4/4	0.95	0.09	35,44,47,49	0
3	CL	A	705	1/1	0.99	0.08	21,21,21,21	0
3	CL	B	705	1/1	0.99	0.03	21,21,21,21	0
3	CL	C	708	1/1	1.00	0.04	19,19,19,19	0
3	CL	D	702	1/1	1.00	0.02	22,22,22,22	0

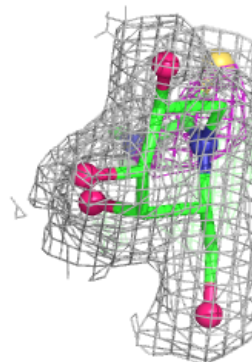
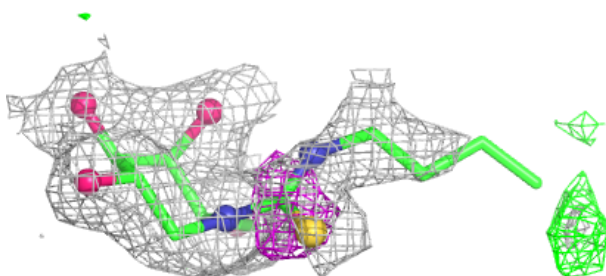
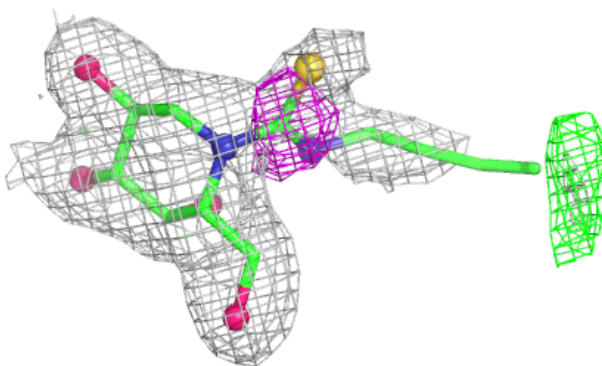
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDJ D 708:

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

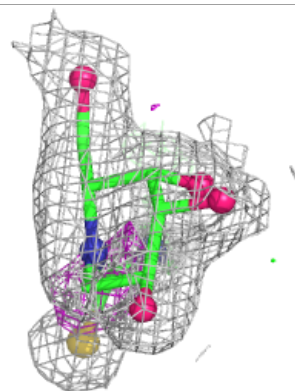
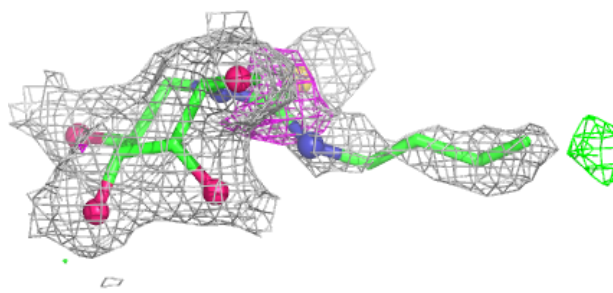
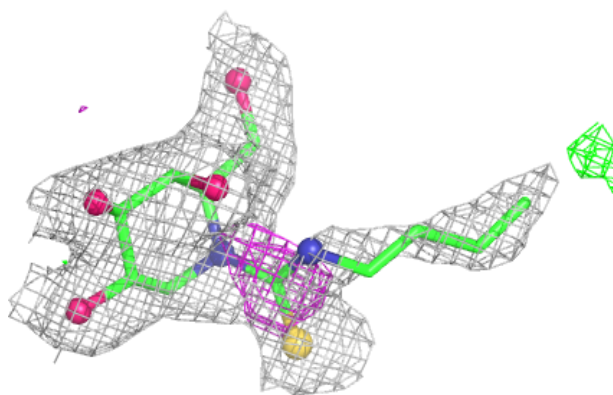
**Electron density around NDJ B 706:**

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



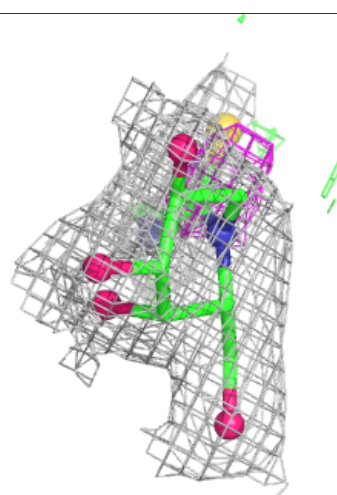
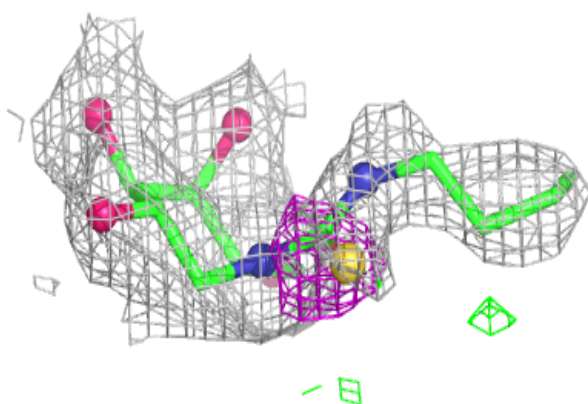
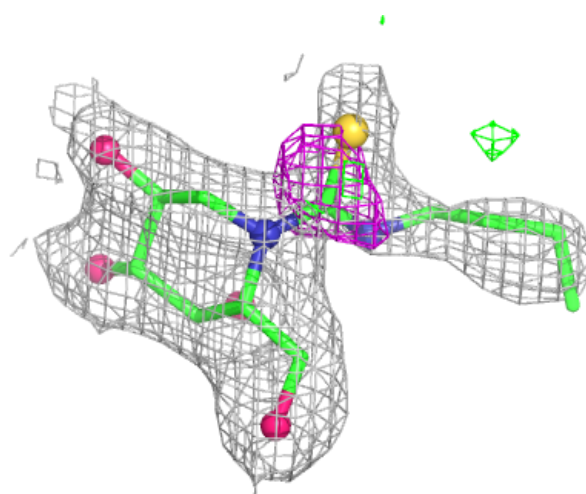
Electron density around NDJ A 706:

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



Electron density around NDJ C 705:

$2mF_o-DF_c$ (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.