



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:28 AM UTC

PDB ID : 6FJ1 / pdb_00006fj1
Title : Structure of the Ldtfm-avibactam carbamoyl enzyme
Authors : Li de la Sierra Gallay, I.; Iannazzo, L.; Compain, F.; Fonvielle, M.; van Tilbeurgh, H.; Edoo, Z.; Arthur, M.; Etheve-Quelquejeu, M.; Hugonnet, J.
Deposited on : 2018-01-19
Resolution : 2.69 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

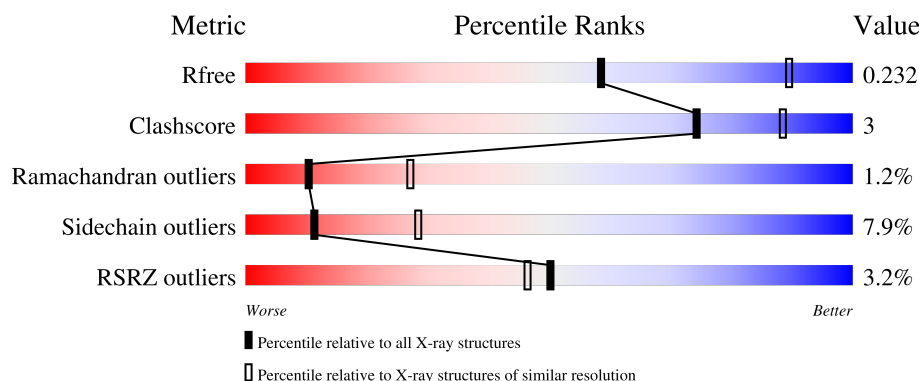
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	258	4% 84% 11% ...
1	B	258	3% 82% 14% ...
1	C	258	3% 84% 12% ...

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
4	GOL	A	503	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6192 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 L,D-TRANSPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1980	1254	320	399	7			
1	B	253	Total	C	N	O	S	0	0	0
			1980	1254	320	399	7			
1	C	253	Total	C	N	O	S	0	0	0
			1980	1254	320	399	7			

There are 33 discrepancies between the modelled and reference sequences:

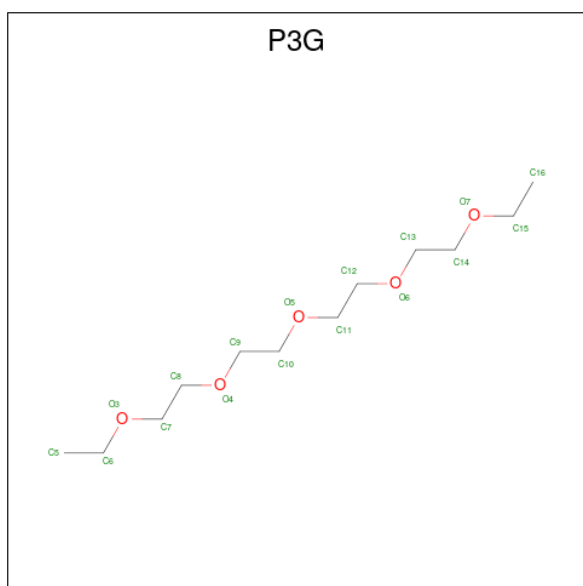
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	GLY	-	expression tag	UNP A0A2D0BNR1
A	?	-	ASP	deletion	UNP A0A2D0BNR1
A	?	-	ASP	deletion	UNP A0A2D0BNR1
A	467	GLY	-	expression tag	UNP A0A2D0BNR1
A	468	SER	-	expression tag	UNP A0A2D0BNR1
A	469	HIS	-	expression tag	UNP A0A2D0BNR1
A	470	HIS	-	expression tag	UNP A0A2D0BNR1
A	471	HIS	-	expression tag	UNP A0A2D0BNR1
A	472	HIS	-	expression tag	UNP A0A2D0BNR1
A	473	HIS	-	expression tag	UNP A0A2D0BNR1
A	474	HIS	-	expression tag	UNP A0A2D0BNR1
B	217	GLY	-	expression tag	UNP A0A2D0BNR1
B	?	-	ASP	deletion	UNP A0A2D0BNR1
B	?	-	ASP	deletion	UNP A0A2D0BNR1
B	467	GLY	-	expression tag	UNP A0A2D0BNR1
B	468	SER	-	expression tag	UNP A0A2D0BNR1
B	469	HIS	-	expression tag	UNP A0A2D0BNR1
B	470	HIS	-	expression tag	UNP A0A2D0BNR1
B	471	HIS	-	expression tag	UNP A0A2D0BNR1
B	472	HIS	-	expression tag	UNP A0A2D0BNR1
B	473	HIS	-	expression tag	UNP A0A2D0BNR1
B	474	HIS	-	expression tag	UNP A0A2D0BNR1
C	217	GLY	-	expression tag	UNP A0A2D0BNR1

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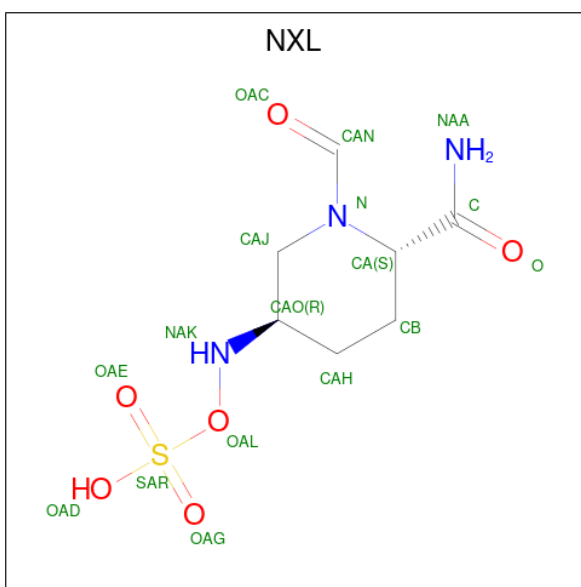
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	deletion	UNP A0A2D0BNR1
C	?	-	ASP	deletion	UNP A0A2D0BNR1
C	467	GLY	-	expression tag	UNP A0A2D0BNR1
C	468	SER	-	expression tag	UNP A0A2D0BNR1
C	469	HIS	-	expression tag	UNP A0A2D0BNR1
C	470	HIS	-	expression tag	UNP A0A2D0BNR1
C	471	HIS	-	expression tag	UNP A0A2D0BNR1
C	472	HIS	-	expression tag	UNP A0A2D0BNR1
C	473	HIS	-	expression tag	UNP A0A2D0BNR1
C	474	HIS	-	expression tag	UNP A0A2D0BNR1

- Molecule 2 is 3,6,9,12,15-PENTAOXAHEPTADECANE (CCD ID: P3G) (formula: $C_{12}H_{26}O_5$).



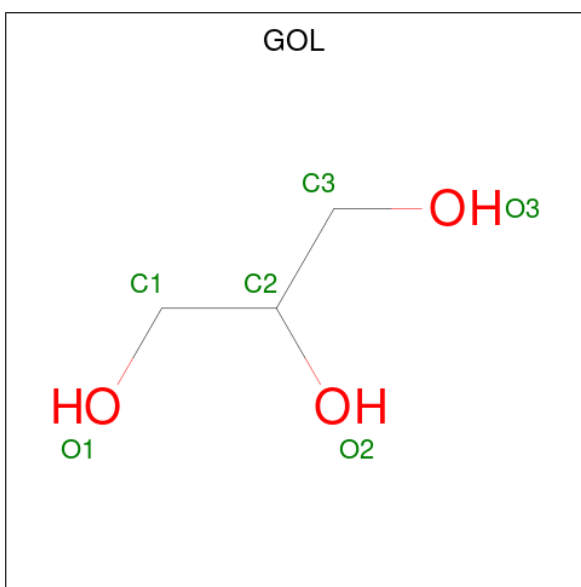
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	12	5		
2	B	1	Total	C	O	0	0
			17	12	5		
2	C	1	Total	C	O	0	0
			17	12	5		

- Molecule 3 is (2S,5R)-1-formyl-5-[(sulfooxy)amino]piperidine-2-carboxamide (CCD ID: NXL) (formula: $C_7H_{13}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			17	7	3	6	1		
3	B	1	Total	C	N	O	S	0	0
			17	7	3	6	1		
3	C	1	Total	C	N	O	S	0	0
			17	7	3	6	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

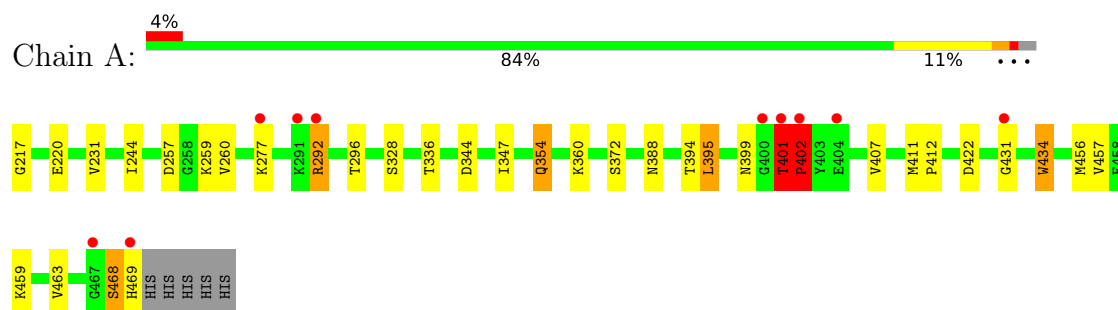
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total	O	0	0
			30	30		
6	B	41	Total	O	0	0
			41	41		
6	C	30	Total	O	0	0
			30	30		

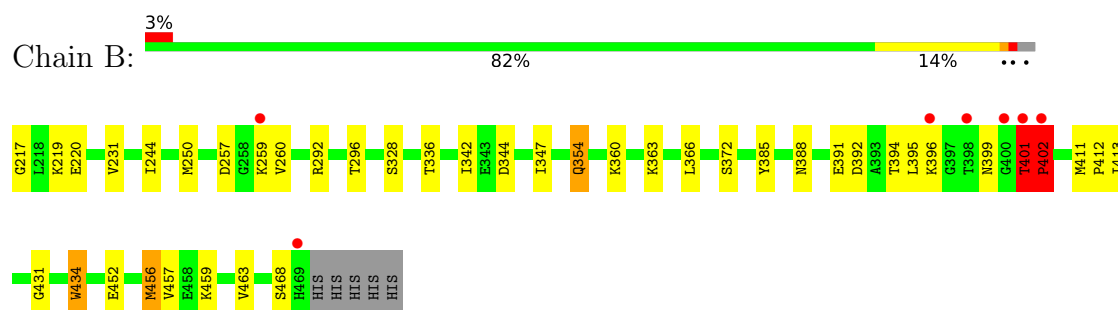
3 Residue-property plots [i](#)

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.

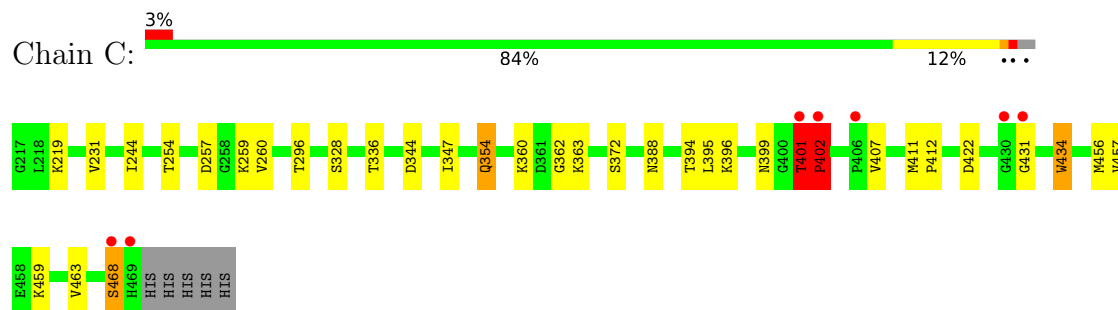
• Molecule 1: L,D-TRANSPEPTIDASE



• Molecule 1: L,D-TRANSPEPTIDASE



• Molecule 1: L,D-TRANSPEPTIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.54Å 131.97Å 70.09Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	48.04 – 2.69 48.04 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.04-2.69) 99.0 (48.04-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.228 0.205 , 0.232	Depositor DCC
R_{free} test set	2602 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6192	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: NXL, P3G, CL, GOL

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	1.09	4/2032 (0.2%)	1.16	9/2773 (0.3%)
1	B	1.09	4/2032 (0.2%)	1.17	9/2773 (0.3%)
1	C	1.10	3/2032 (0.1%)	1.17	8/2773 (0.3%)
All	All	1.09	11/6096 (0.2%)	1.17	26/8319 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	THR	CA-C	8.42	1.63	1.52
1	C	401	THR	CA-C	8.25	1.63	1.52
1	A	401	THR	CA-C	8.21	1.63	1.52
1	B	401	THR	N-CA	6.94	1.55	1.46
1	A	401	THR	N-CA	6.53	1.55	1.46
1	A	468	SER	N-CA	6.25	1.53	1.46
1	C	401	THR	N-CA	6.16	1.54	1.46
1	B	399	ASN	CA-C	5.98	1.60	1.52
1	A	399	ASN	CA-C	5.96	1.60	1.52
1	B	342	ILE	C-O	-5.80	1.17	1.24
1	C	399	ASN	CA-C	5.78	1.60	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	SER	N-CA-C	8.25	122.18	108.73
1	C	468	SER	N-CA-C	7.44	120.86	108.73
1	A	468	SER	N-CA-C	7.19	120.44	108.73
1	A	231	VAL	N-CA-CB	7.10	119.98	110.26
1	C	244	ILE	N-CA-C	-7.05	102.56	108.63
1	C	402	PRO	N-CA-C	6.20	125.25	112.47
1	A	402	PRO	N-CA-C	6.03	124.88	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	VAL	CB-CA-C	-5.86	103.53	111.15
1	B	244	ILE	N-CA-C	-5.74	103.70	108.63
1	C	244	ILE	CB-CA-C	-5.74	105.60	110.94
1	C	328	SER	CA-C-N	-5.72	114.43	120.66
1	C	328	SER	C-N-CA	-5.72	114.43	120.66
1	B	250	MET	CG-SD-CE	5.70	113.44	100.90
1	B	402	PRO	N-CA-C	5.69	124.18	112.47
1	A	244	ILE	CB-CA-C	-5.53	105.80	110.94
1	B	328	SER	CA-C-N	-5.53	114.64	120.66
1	B	328	SER	C-N-CA	-5.53	114.64	120.66
1	A	260	VAL	CB-CA-C	-5.53	103.97	111.15
1	A	244	ILE	N-CA-C	-5.48	103.92	108.63
1	C	434	TRP	N-CA-C	5.42	118.68	111.75
1	A	328	SER	CA-C-N	-5.30	114.89	120.66
1	A	328	SER	C-N-CA	-5.30	114.89	120.66
1	A	434	TRP	N-CA-C	5.30	118.53	111.75
1	B	244	ILE	CB-CA-C	-5.22	106.08	110.94
1	B	434	TRP	N-CA-C	5.17	118.37	111.75
1	C	260	VAL	CB-CA-C	-5.00	104.24	111.34

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	1980	0	1893	14	0
1	B	1980	0	1893	12	0
1	C	1980	0	1893	11	0
2	A	17	0	26	3	0
2	B	17	0	26	0	0
2	C	17	0	26	0	0
3	A	17	0	12	1	0
3	B	17	0	12	0	0
3	C	17	0	12	1	0
4	A	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	32	0	0
4	C	12	0	16	0	0
5	A	1	0	0	0	0
6	A	30	0	0	0	0
6	B	41	0	0	0	0
6	C	30	0	0	1	0
All	All	6192	0	5857	37	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 (37) 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:277:LYS:HG2	2:A:501:P3G:H81	1.72	0.70
1:A:277:LYS:CG	2:A:501:P3G:H81	2.30	0.61
1:A:401:THR:HG22	1:A:402:PRO:HD3	1.84	0.60
1:C:401:THR:HG22	1:C:402:PRO:HD3	1.84	0.59
1:A:277:LYS:HG2	2:A:501:P3G:C8	2.35	0.57
1:C:395:LEU:HD22	3:C:501:NXL:H2	1.88	0.55
1:B:401:THR:HB	1:B:402:PRO:CD	2.40	0.52
1:B:401:THR:HB	1:B:402:PRO:HD2	1.93	0.51
1:B:354:GLN:OE1	1:B:434:TRP:HB3	2.13	0.48
1:B:347:ILE:HB	1:B:463:VAL:HG22	1.95	0.48
1:B:401:THR:HG22	1:B:402:PRO:HD3	1.95	0.48
1:A:354:GLN:OE1	1:A:434:TRP:HB3	2.14	0.48
1:C:395:LEU:HD23	6:C:630:HOH:O	2.14	0.47
1:B:388:ASN:O	1:B:412:PRO:HD2	2.15	0.47
1:C:401:THR:HB	1:C:402:PRO:CD	2.44	0.47
1:C:354:GLN:OE1	1:C:434:TRP:HB3	2.15	0.47
1:A:401:THR:HB	1:A:402:PRO:CD	2.45	0.47
1:B:411:MET:HE1	1:B:457:VAL:HG11	1.98	0.46
1:C:388:ASN:O	1:C:412:PRO:HD2	2.15	0.46
1:A:347:ILE:HB	1:A:463:VAL:HG22	1.98	0.46
1:A:388:ASN:O	1:A:412:PRO:HD2	2.16	0.46
1:C:344:ASP:HB2	1:C:362:GLY:N	2.32	0.45
1:A:401:THR:HB	1:A:402:PRO:HD2	1.99	0.44
1:A:411:MET:HE1	1:A:457:VAL:HG11	1.99	0.44
1:C:347:ILE:HB	1:C:463:VAL:HG22	2.00	0.43
1:A:407:VAL:HG13	1:A:422:ASP:OD1	2.18	0.43
1:C:411:MET:HE1	1:C:457:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:THR:HB	1:C:402:PRO:HD2	2.01	0.42
1:A:217:GLY:HA3	1:A:220:GLU:OE2	2.20	0.41
1:A:395:LEU:CB	3:A:502:NXL:H11	2.50	0.41
1:B:385:TYR:O	1:B:413:ILE:HA	2.21	0.41
1:A:292:ARG:HH11	1:A:292:ARG:HG2	1.86	0.40
1:B:217:GLY:HA3	1:B:220:GLU:OE2	2.21	0.40
1:B:452:GLU:O	1:B:456:MET:HG2	2.22	0.40
1:C:407:VAL:HG13	1:C:422:ASP:OD1	2.20	0.40
1:B:366:LEU:C	1:B:366:LEU:HD23	2.46	0.40
1:B:391:GLU:O	1:B:392:ASP:C	2.65	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	251/258 (97%)	230 (92%)	18 (7%)	3 (1%)	10	27
1	B	251/258 (97%)	230 (92%)	18 (7%)	3 (1%)	10	27
1	C	251/258 (97%)	232 (92%)	16 (6%)	3 (1%)	10	27
All	All	753/774 (97%)	692 (92%)	52 (7%)	9 (1%)	10	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	402	PRO
1	A	402	PRO
1	A	431	GLY
1	B	402	PRO
1	B	431	GLY
1	C	431	GLY
1	B	401	THR

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Mol	Chain	Res	Type
1	A	401	THR
1	C	401	THR

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	219/224 (98%)	203 (93%)	16 (7%)	13	32
1	B	219/224 (98%)	201 (92%)	18 (8%)	10	27
1	C	219/224 (98%)	201 (92%)	18 (8%)	10	27
All	All	657/672 (98%)	605 (92%)	52 (8%)	11	28

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	ASP
1	A	259	LYS
1	A	292	ARG
1	A	296	THR
1	A	336	THR
1	A	344	ASP
1	A	354	GLN
1	A	360	LYS
1	A	372	SER
1	A	394	THR
1	A	395	LEU
1	A	401	THR
1	A	456	MET
1	A	459	LYS
1	A	468	SER
1	A	469	HIS
1	B	219	LYS
1	B	231	VAL
1	B	257	ASP
1	B	259	LYS

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Mol	Chain	Res	Type
1	B	292	ARG
1	B	296	THR
1	B	336	THR
1	B	344	ASP
1	B	354	GLN
1	B	360	LYS
1	B	363	LYS
1	B	372	SER
1	B	394	THR
1	B	395	LEU
1	B	396	LYS
1	B	401	THR
1	B	456	MET
1	B	459	LYS
1	C	219	LYS
1	C	231	VAL
1	C	254	THR
1	C	257	ASP
1	C	259	LYS
1	C	296	THR
1	C	336	THR
1	C	354	GLN
1	C	360	LYS
1	C	363	LYS
1	C	372	SER
1	C	394	THR
1	C	396	LYS
1	C	401	THR
1	C	402	PRO
1	C	456	MET
1	C	459	LYS
1	C	468	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	B	266	GLN
1	B	408	ASN
1	C	221	GLN
1	C	256	ASN
1	C	388	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	$\# Z > 2$
3	NXL	A	502	1	14,17,17	2.63	2 (14%)	16,24,24	1.96	3 (18%)
4	GOL	A	504	-	5,5,5	0.51	0	5,5,5	0.63	0
4	GOL	A	503	-	5,5,5	1.29	0	5,5,5	1.83	2 (40%)
3	NXL	B	501	1	14,17,17	2.67	3 (21%)	16,24,24	2.23	7 (43%)
3	NXL	C	501	1	14,17,17	2.43	2 (14%)	16,24,24	1.80	3 (18%)
4	GOL	B	504	-	5,5,5	0.51	0	5,5,5	1.24	0
4	GOL	B	506	-	5,5,5	0.89	0	5,5,5	0.50	0
4	GOL	C	504	-	5,5,5	0.55	0	5,5,5	0.35	0
2	P3G	A	501	-	16,16,16	1.21	0	15,15,15	1.96	3 (20%)
2	P3G	C	502	-	16,16,16	1.09	0	15,15,15	1.67	2 (13%)
2	P3G	B	502	-	16,16,16	0.92	0	15,15,15	1.50	2 (13%)
4	GOL	C	503	-	5,5,5	0.43	0	5,5,5	0.52	0
4	GOL	B	505	-	5,5,5	1.33	0	5,5,5	1.60	1 (20%)
4	GOL	B	503	-	5,5,5	0.34	0	5,5,5	0.58	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
3	NXL	A	502	1	-	0/5/25/25	0/1/1/1
4	GOL	A	504	-	-	2/4/4/4	-
4	GOL	A	503	-	-	4/4/4/4	-
3	NXL	B	501	1	-	1/5/25/25	0/1/1/1
3	NXL	C	501	1	-	0/5/25/25	0/1/1/1
4	GOL	B	504	-	-	2/4/4/4	-
4	GOL	B	506	-	-	2/4/4/4	-
4	GOL	C	504	-	-	2/4/4/4	-
2	P3G	A	501	-	-	7/14/14/14	-
2	P3G	C	502	-	-	7/14/14/14	-
2	P3G	B	502	-	-	8/14/14/14	-
4	GOL	C	503	-	-	4/4/4/4	-
4	GOL	B	505	-	-	2/4/4/4	-
4	GOL	B	503	-	-	1/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NXL	CAN-N	7.50	1.48	1.34
3	B	501	NXL	C-NAA	6.76	1.48	1.32
3	B	501	NXL	CAN-N	6.73	1.47	1.34
3	C	501	NXL	CAN-N	6.56	1.46	1.34
3	A	502	NXL	C-NAA	5.92	1.46	1.32
3	C	501	NXL	C-NAA	5.77	1.46	1.32
3	B	501	NXL	CAJ-CAO	2.17	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NXL	CB-CAH-CAO	5.61	117.65	111.49
3	C	501	NXL	CB-CAH-CAO	4.85	116.81	111.49
2	C	502	P3G	C6-O3-C7	4.57	129.11	113.06
2	A	501	P3G	C6-O3-C7	4.41	128.55	113.06
3	B	501	NXL	CB-CAH-CAO	4.35	116.26	111.49
3	B	501	NXL	OAC-CAN-N	-3.52	116.74	125.34
2	B	502	P3G	C6-O3-C7	3.45	125.18	113.06
3	B	501	NXL	CA-C-NAA	3.40	124.17	116.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NXL	OAC-CAN-N	-3.39	117.05	125.34
2	A	501	P3G	O6-C13-C14	3.36	125.65	110.35
2	A	501	P3G	O4-C8-C7	3.24	125.12	110.35
2	C	502	P3G	O3-C7-C8	2.99	123.97	110.35
4	B	505	GOL	O3-C3-C2	2.78	122.91	110.38
3	C	501	NXL	OAC-CAN-N	-2.73	118.67	125.34
3	B	501	NXL	OAG-SAR-OAE	-2.67	101.94	112.24
3	A	502	NXL	CAH-CAO-NAK	2.60	115.37	110.08
4	A	503	GOL	O3-C3-C2	2.57	121.93	110.38
3	B	501	NXL	O-C-CA	-2.49	116.07	120.22
3	B	501	NXL	CAO-CAJ-N	-2.49	106.74	110.11
4	A	503	GOL	O1-C1-C2	2.34	120.91	110.38
3	C	501	NXL	CAH-CAO-CAJ	2.20	112.57	109.71
3	B	501	NXL	C-CA-N	2.20	116.79	111.21
2	B	502	P3G	C13-O6-C12	2.09	122.39	113.26

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	GOL	O1-C1-C2-C3
4	A	503	GOL	O2-C2-C3-O3
4	B	505	GOL	O1-C1-C2-C3
4	B	506	GOL	O1-C1-C2-C3
4	C	503	GOL	O1-C1-C2-C3
2	C	502	P3G	C8-C7-O3-C6
2	A	501	P3G	C14-C13-O6-C12
2	C	502	P3G	O3-C7-C8-O4
2	C	502	P3G	O5-C10-C9-O4
2	A	501	P3G	O5-C10-C9-O4
2	A	501	P3G	O5-C11-C12-O6
2	A	501	P3G	O6-C13-C14-O7
2	C	502	P3G	O6-C13-C14-O7
2	B	502	P3G	O3-C7-C8-O4
4	C	503	GOL	O1-C1-C2-O2
2	B	502	P3G	O5-C10-C9-O4
4	A	503	GOL	C1-C2-C3-O3
4	A	504	GOL	C1-C2-C3-O3
4	C	503	GOL	C1-C2-C3-O3
4	C	504	GOL	C1-C2-C3-O3
4	A	503	GOL	O1-C1-C2-O2
4	B	505	GOL	O1-C1-C2-O2

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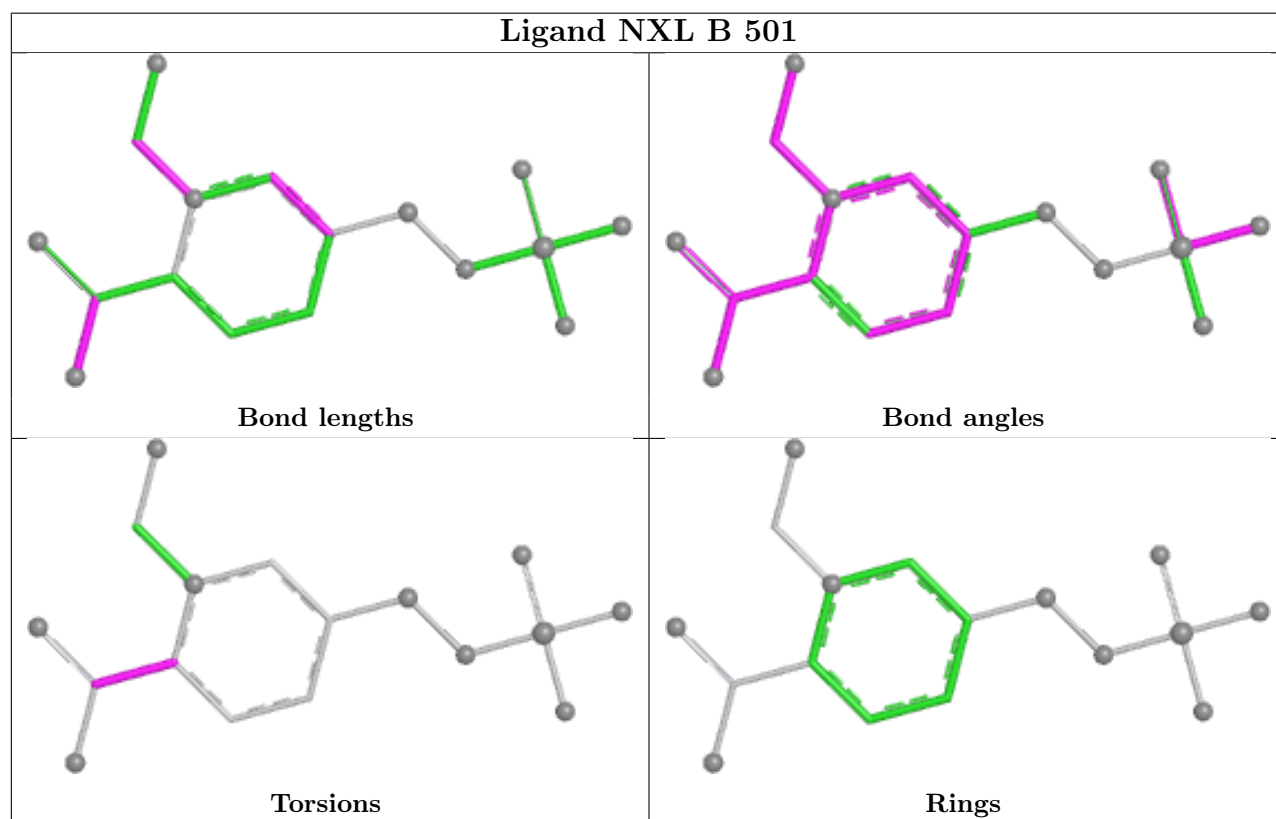
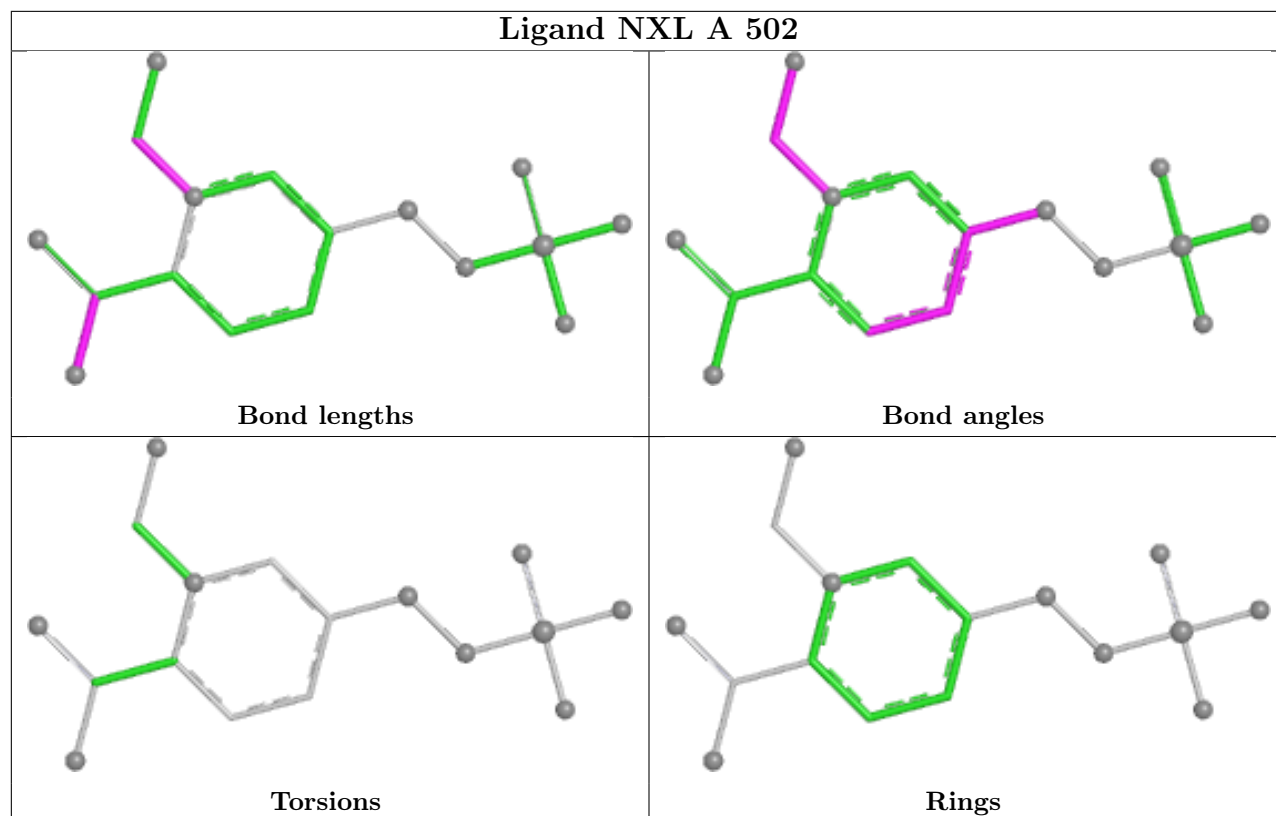
Mol	Chain	Res	Type	Atoms
4	C	503	GOL	O2-C2-C3-O3
4	C	504	GOL	O2-C2-C3-O3
2	B	502	P3G	O6-C13-C14-O7
4	A	504	GOL	O2-C2-C3-O3
4	B	504	GOL	O2-C2-C3-O3
2	C	502	P3G	O5-C11-C12-O6
3	B	501	NXL	O-C-CA-N
2	A	501	P3G	C11-C12-O6-C13
2	A	501	P3G	C10-C9-O4-C8
2	C	502	P3G	C5-C6-O3-C7
2	B	502	P3G	C10-C9-O4-C8
2	B	502	P3G	C8-C7-O3-C6
2	A	501	P3G	C9-C10-O5-C11
4	B	506	GOL	O1-C1-C2-O2
2	B	502	P3G	C16-C15-O7-C14
2	B	502	P3G	C7-C8-O4-C9
4	B	503	GOL	O1-C1-C2-O2
2	B	502	P3G	C12-C11-O5-C10
2	C	502	P3G	C7-C8-O4-C9
4	B	504	GOL	C1-C2-C3-O3

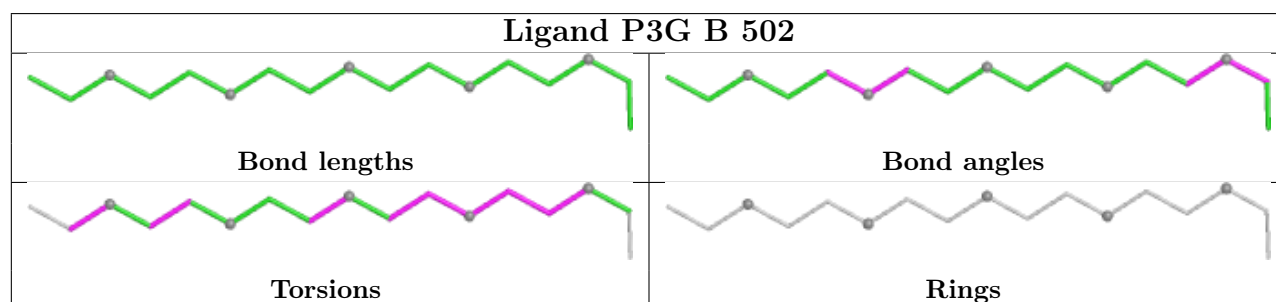
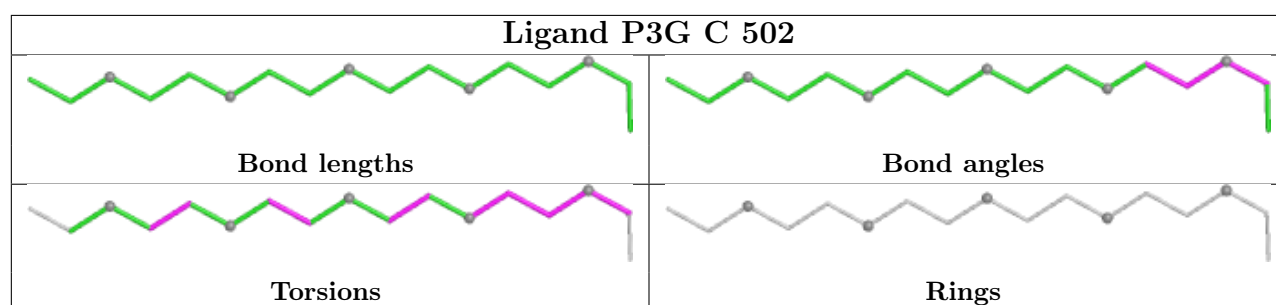
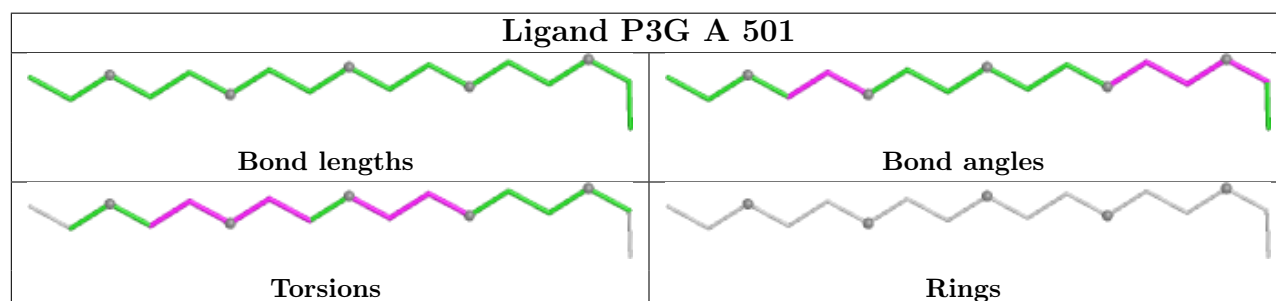
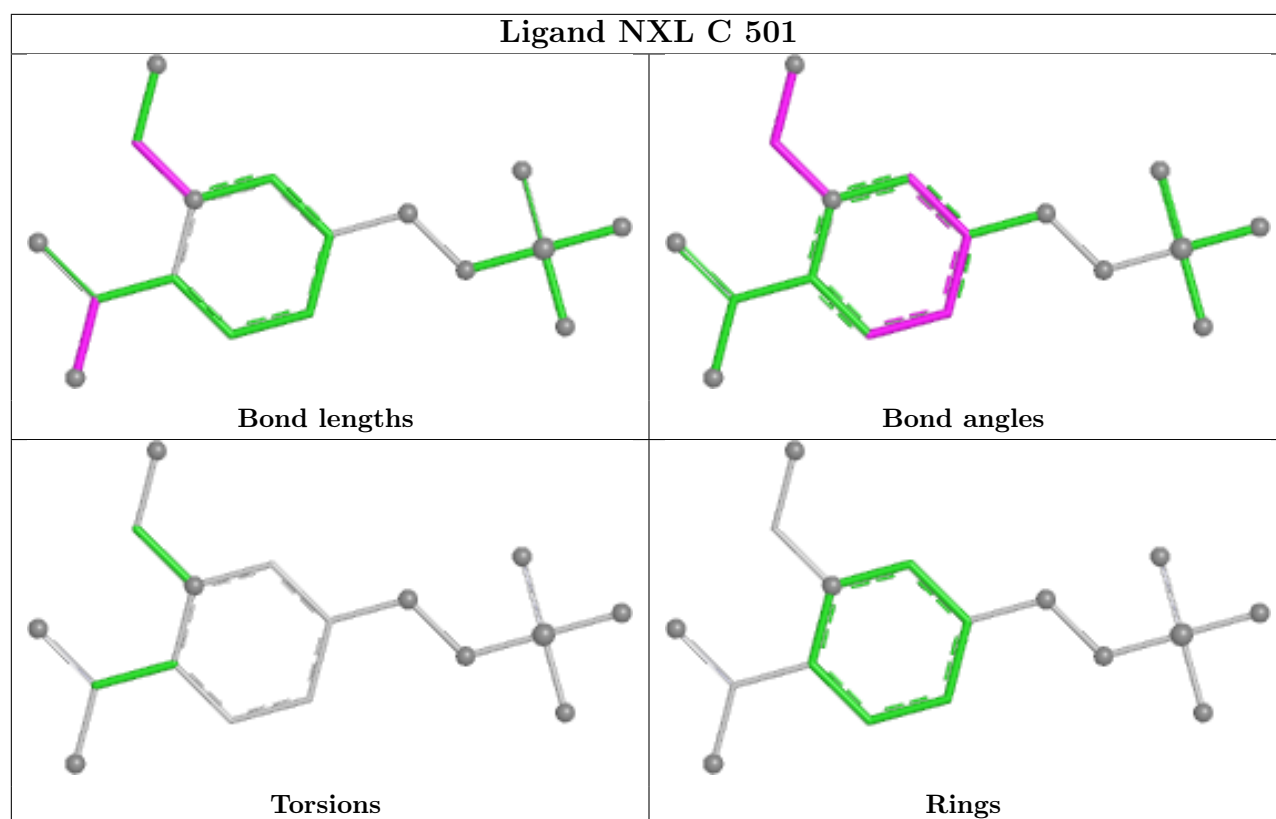
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NXL	1	0
3	C	501	NXL	1	0
2	A	501	P3G	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	253/258 (98%)	-0.02	10 (3%) 42 38	53, 78, 128, 171	0
1	B	253/258 (98%)	-0.05	7 (2%) 55 51	51, 77, 131, 172	0
1	C	253/258 (98%)	-0.01	7 (2%) 55 51	54, 80, 138, 171	0
All	All	759/774 (98%)	-0.03	24 (3%) 50 46	51, 79, 134, 172	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	469	HIS	5.1
1	C	469	HIS	4.7
1	A	469	HIS	4.6
1	B	398	THR	4.0
1	C	402	PRO	3.1
1	A	401	THR	3.0
1	A	400	GLY	2.9
1	A	292	ARG	2.8
1	A	431	GLY	2.8
1	B	400	GLY	2.7
1	C	401	THR	2.6
1	B	259	LYS	2.5
1	A	402	PRO	2.5
1	B	396	LYS	2.4
1	A	291	LYS	2.3
1	C	468	SER	2.3
1	A	467	GLY	2.2
1	A	404	GLU	2.2
1	B	402	PRO	2.1
1	A	277	LYS	2.1
1	C	406	PRO	2.1
1	C	431	GLY	2.1
1	B	401	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	430	GLY	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](#)

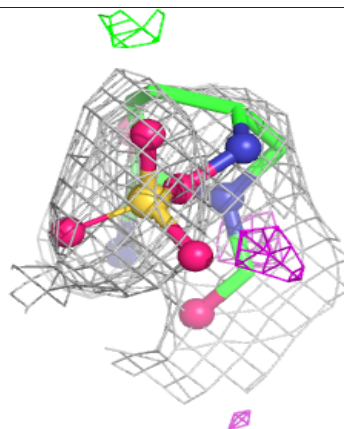
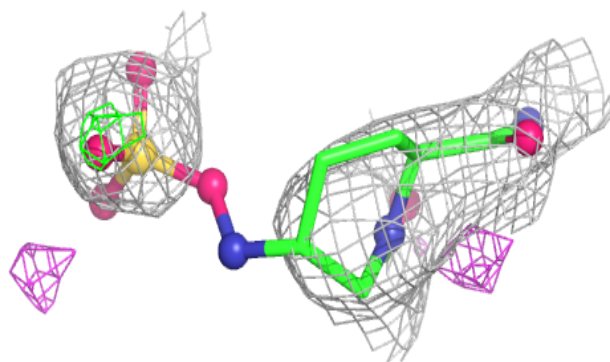
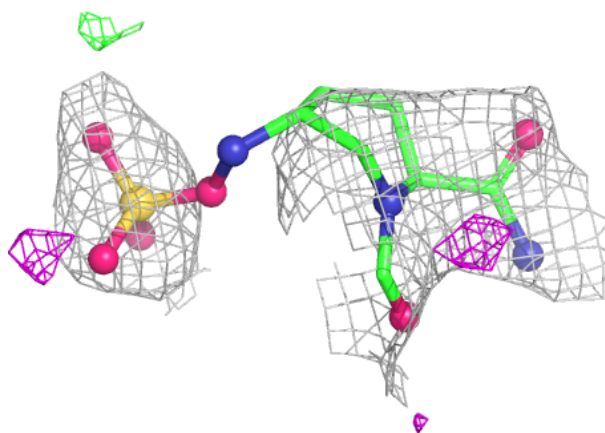
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	503	6/6	0.85	0.23	87,132,150,173	0
4	GOL	B	506	6/6	0.85	0.20	94,110,118,126	0
3	NXL	B	501	17/17	0.86	0.17	115,166,247,251	0
4	GOL	A	504	6/6	0.86	0.15	105,126,135,138	0
5	CL	A	505	1/1	0.88	0.15	112,112,112,112	0
2	P3G	B	502	17/17	0.89	0.27	87,101,129,148	0
3	NXL	C	501	17/17	0.89	0.15	112,171,224,233	0
3	NXL	A	502	17/17	0.89	0.14	130,165,219,232	0
2	P3G	C	502	17/17	0.91	0.20	75,93,110,110	0
4	GOL	C	503	6/6	0.91	0.14	101,106,116,117	0
2	P3G	A	501	17/17	0.91	0.22	75,98,124,140	0
4	GOL	B	505	6/6	0.94	0.19	95,104,125,125	0
4	GOL	B	504	6/6	0.94	0.14	79,87,92,104	0
4	GOL	A	503	6/6	0.95	0.13	78,85,90,96	0
4	GOL	C	504	6/6	0.96	0.12	72,96,100,111	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.

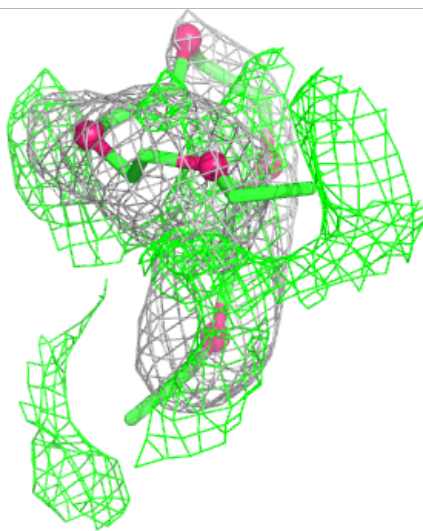
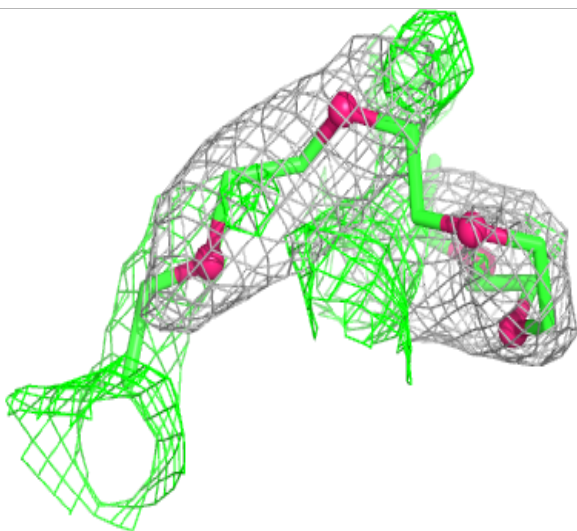
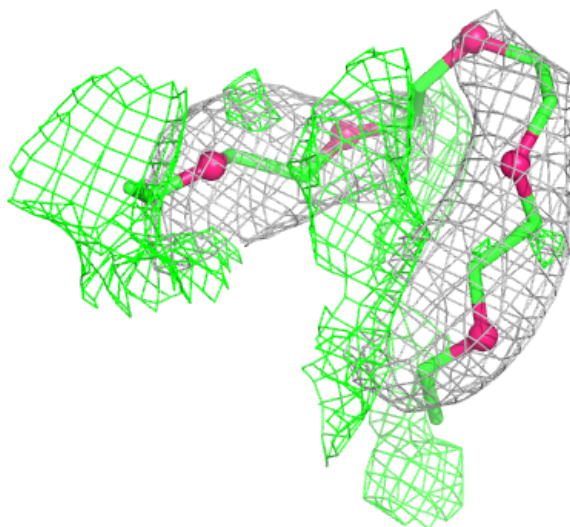
Electron density around NXL B 501:

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



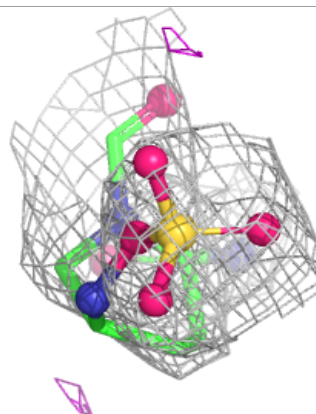
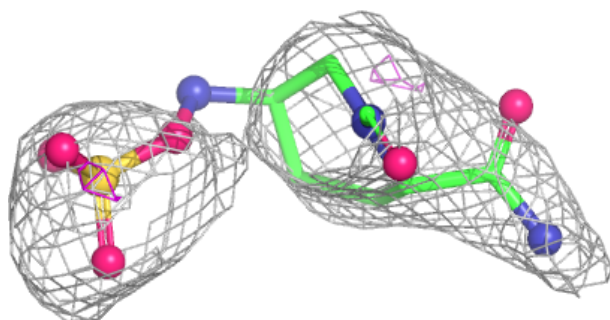
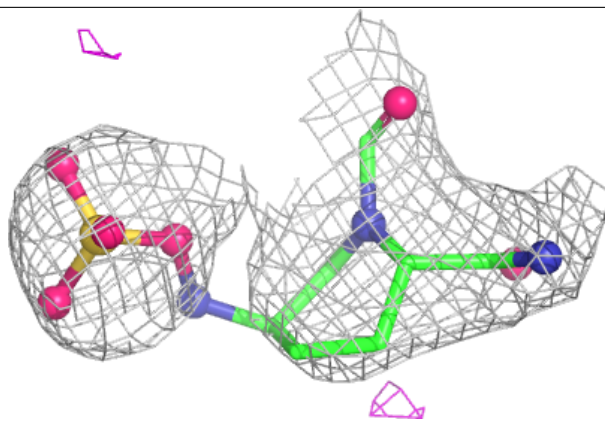
Electron density around P3G B 502:

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

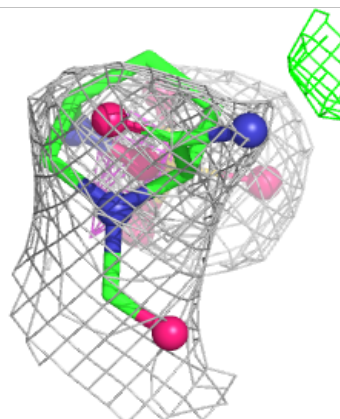
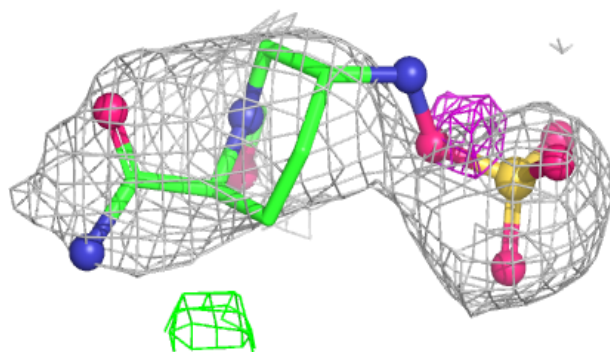
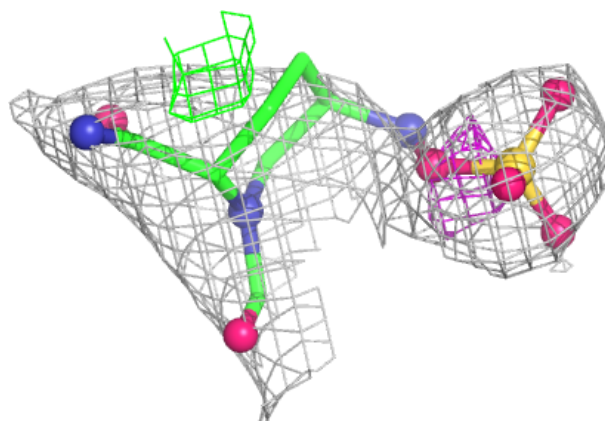


Electron density around NXL C 501:

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

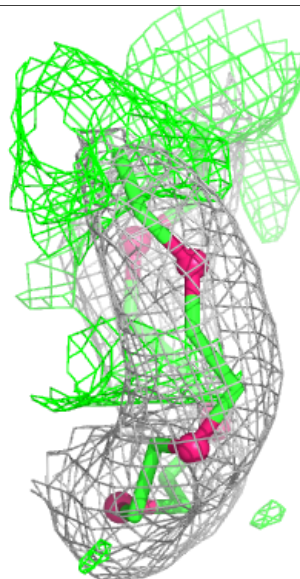
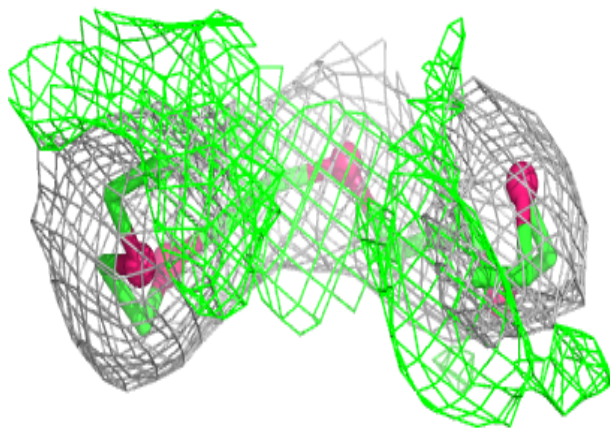
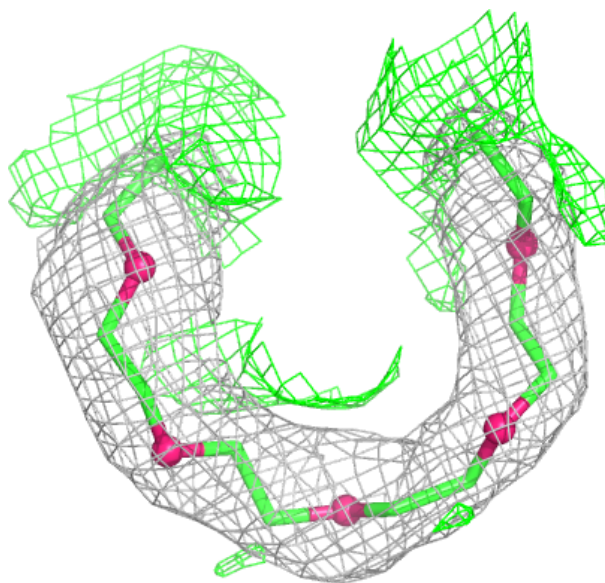
**Electron density around NXL A 502:**

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



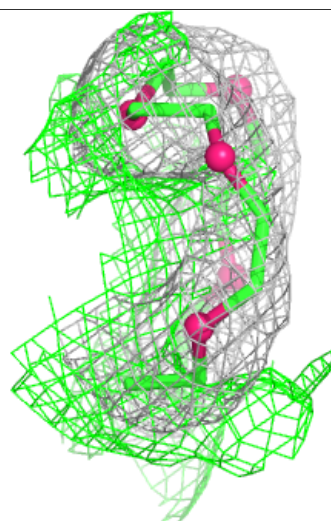
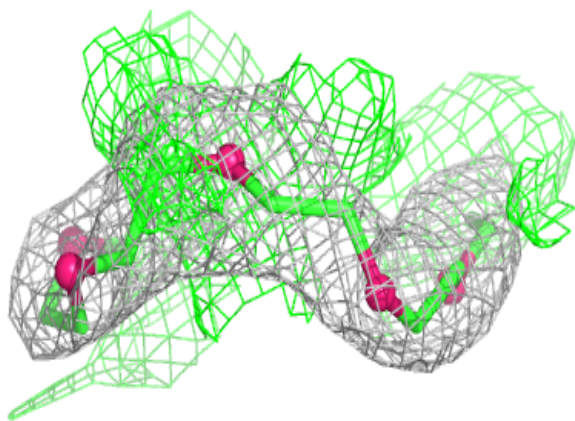
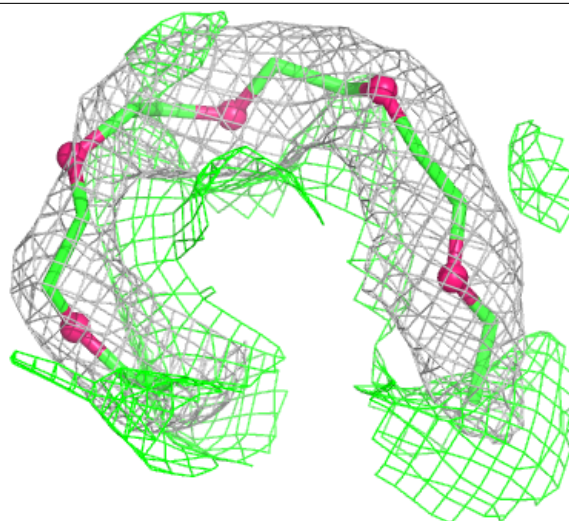
Electron density around P3G C 502:

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



Electron density around P3G A 501:

$2mF_o-DF_c$ (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.