



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2022 – 10:39 AM EDT

PDB ID : 7SOK  
Title : Structure of Nicotinamide N-Methyltransferase (NNMT) in complex with inhibitor II329  
Authors : Yadav, R.; Iyamu, I.D.; Huang, R.; Noinaj, N.  
Deposited on : 2021-10-31  
Resolution : 2.08 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](mailto: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>.

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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)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

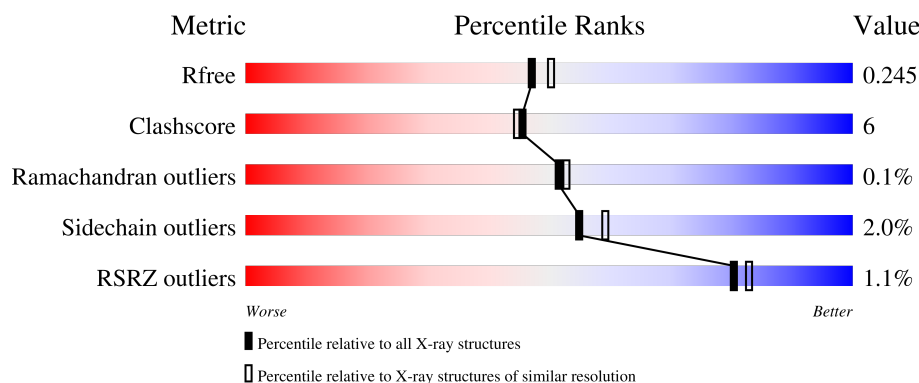
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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))
$R_{free}$	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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  $\geq 3$ , 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	283	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 9%</div> </div> </div>
1	B	283	<div> <div>78%</div> <div>12%</div> <div>10%</div> </div>
1	C	283	<div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
1	D	283	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>• 9%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8572 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 NNMT protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	267	Total	C	N	O	S	0	2	0
			2062	1324	333	392	13			
1	A	258	Total	C	N	O	S	0	3	0
			2015	1296	328	379	12			
1	B	256	Total	C	N	O	S	0	2	0
			1978	1276	318	372	12			
1	D	257	Total	C	N	O	S	0	0	0
			1982	1276	321	374	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	MET	-	expression tag	UNP Q6FH49
C	-17	GLY	-	expression tag	UNP Q6FH49
C	-16	SER	-	expression tag	UNP Q6FH49
C	-15	SER	-	expression tag	UNP Q6FH49
C	-14	HIS	-	expression tag	UNP Q6FH49
C	-13	HIS	-	expression tag	UNP Q6FH49
C	-12	HIS	-	expression tag	UNP Q6FH49
C	-11	HIS	-	expression tag	UNP Q6FH49
C	-10	HIS	-	expression tag	UNP Q6FH49
C	-9	HIS	-	expression tag	UNP Q6FH49
C	-8	SER	-	expression tag	UNP Q6FH49
C	-7	SER	-	expression tag	UNP Q6FH49
C	-6	GLY	-	expression tag	UNP Q6FH49
C	-5	LEU	-	expression tag	UNP Q6FH49
C	-4	VAL	-	expression tag	UNP Q6FH49
C	-3	PRO	-	expression tag	UNP Q6FH49
C	-2	ARG	-	expression tag	UNP Q6FH49
C	-1	GLY	-	expression tag	UNP Q6FH49
C	0	SER	-	expression tag	UNP Q6FH49
C	100	ALA	LYS	engineered mutation	UNP Q6FH49
C	101	ALA	GLU	engineered mutation	UNP Q6FH49

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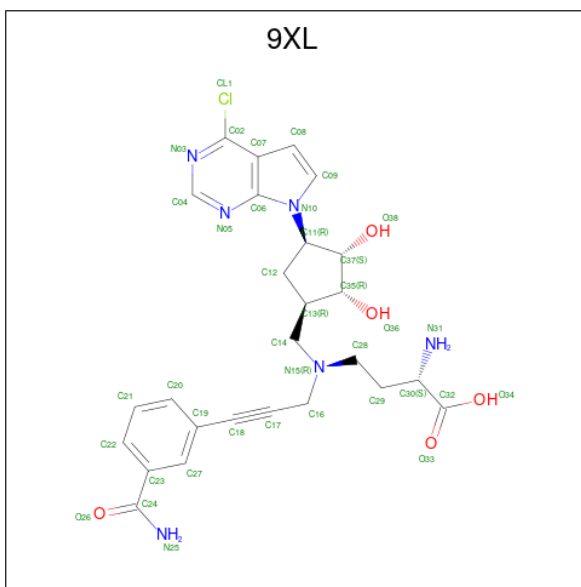
Chain	Residue	Modelled	Actual	Comment	Reference
C	103	ALA	GLU	engineered mutation	UNP Q6FH49
A	-18	MET	-	expression tag	UNP Q6FH49
A	-17	GLY	-	expression tag	UNP Q6FH49
A	-16	SER	-	expression tag	UNP Q6FH49
A	-15	SER	-	expression tag	UNP Q6FH49
A	-14	HIS	-	expression tag	UNP Q6FH49
A	-13	HIS	-	expression tag	UNP Q6FH49
A	-12	HIS	-	expression tag	UNP Q6FH49
A	-11	HIS	-	expression tag	UNP Q6FH49
A	-10	HIS	-	expression tag	UNP Q6FH49
A	-9	HIS	-	expression tag	UNP Q6FH49
A	-8	SER	-	expression tag	UNP Q6FH49
A	-7	SER	-	expression tag	UNP Q6FH49
A	-6	GLY	-	expression tag	UNP Q6FH49
A	-5	LEU	-	expression tag	UNP Q6FH49
A	-4	VAL	-	expression tag	UNP Q6FH49
A	-3	PRO	-	expression tag	UNP Q6FH49
A	-2	ARG	-	expression tag	UNP Q6FH49
A	-1	GLY	-	expression tag	UNP Q6FH49
A	0	SER	-	expression tag	UNP Q6FH49
A	100	ALA	LYS	engineered mutation	UNP Q6FH49
A	101	ALA	GLU	engineered mutation	UNP Q6FH49
A	103	ALA	GLU	engineered mutation	UNP Q6FH49
B	-18	MET	-	expression tag	UNP Q6FH49
B	-17	GLY	-	expression tag	UNP Q6FH49
B	-16	SER	-	expression tag	UNP Q6FH49
B	-15	SER	-	expression tag	UNP Q6FH49
B	-14	HIS	-	expression tag	UNP Q6FH49
B	-13	HIS	-	expression tag	UNP Q6FH49
B	-12	HIS	-	expression tag	UNP Q6FH49
B	-11	HIS	-	expression tag	UNP Q6FH49
B	-10	HIS	-	expression tag	UNP Q6FH49
B	-9	HIS	-	expression tag	UNP Q6FH49
B	-8	SER	-	expression tag	UNP Q6FH49
B	-7	SER	-	expression tag	UNP Q6FH49
B	-6	GLY	-	expression tag	UNP Q6FH49
B	-5	LEU	-	expression tag	UNP Q6FH49
B	-4	VAL	-	expression tag	UNP Q6FH49
B	-3	PRO	-	expression tag	UNP Q6FH49
B	-2	ARG	-	expression tag	UNP Q6FH49
B	-1	GLY	-	expression tag	UNP Q6FH49
B	0	SER	-	expression tag	UNP Q6FH49

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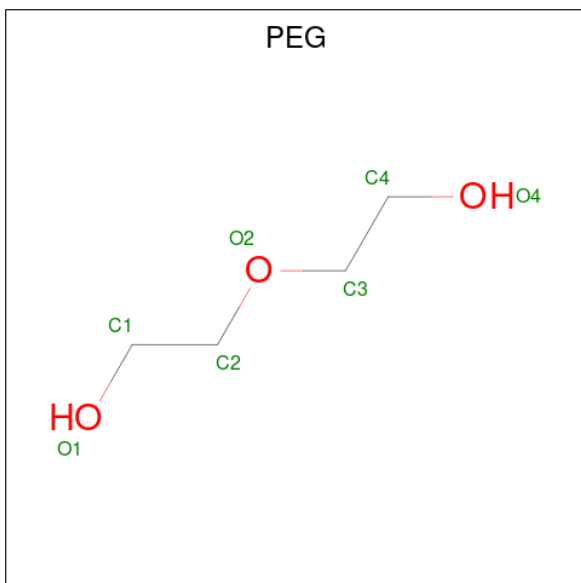
Chain	Residue	Modelled	Actual	Comment	Reference
B	100	ALA	LYS	engineered mutation	UNP Q6FH49
B	101	ALA	GLU	engineered mutation	UNP Q6FH49
B	103	ALA	GLU	engineered mutation	UNP Q6FH49
D	-18	MET	-	expression tag	UNP Q6FH49
D	-17	GLY	-	expression tag	UNP Q6FH49
D	-16	SER	-	expression tag	UNP Q6FH49
D	-15	SER	-	expression tag	UNP Q6FH49
D	-14	HIS	-	expression tag	UNP Q6FH49
D	-13	HIS	-	expression tag	UNP Q6FH49
D	-12	HIS	-	expression tag	UNP Q6FH49
D	-11	HIS	-	expression tag	UNP Q6FH49
D	-10	HIS	-	expression tag	UNP Q6FH49
D	-9	HIS	-	expression tag	UNP Q6FH49
D	-8	SER	-	expression tag	UNP Q6FH49
D	-7	SER	-	expression tag	UNP Q6FH49
D	-6	GLY	-	expression tag	UNP Q6FH49
D	-5	LEU	-	expression tag	UNP Q6FH49
D	-4	VAL	-	expression tag	UNP Q6FH49
D	-3	PRO	-	expression tag	UNP Q6FH49
D	-2	ARG	-	expression tag	UNP Q6FH49
D	-1	GLY	-	expression tag	UNP Q6FH49
D	0	SER	-	expression tag	UNP Q6FH49
D	100	ALA	LYS	engineered mutation	UNP Q6FH49
D	101	ALA	GLU	engineered mutation	UNP Q6FH49
D	103	ALA	GLU	engineered mutation	UNP Q6FH49

- Molecule 2 is (2S)-2-amino-4-([3-(3-carbamoylphenyl)prop-2-yn-1-yl]{[(1R,2R,3S,4R)-4-(4-chloro-7H-pyrrolo[2,3-d]pyrimidin-7-yl)-2,3-dihydroxycyclopentyl]methyl}amino)butanoic acid (three-letter code: 9XL) (formula: C<sub>26</sub>H<sub>29</sub>ClN<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Cl	N	O	0	0
			38	26	1	6	5		
2	A	1	Total	C	Cl	N	O	0	0
			38	26	1	6	5		
2	B	1	Total	C	Cl	N	O	0	0
			38	26	1	6	5		
2	D	1	Total	C	Cl	N	O	0	0
			38	26	1	6	5		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0

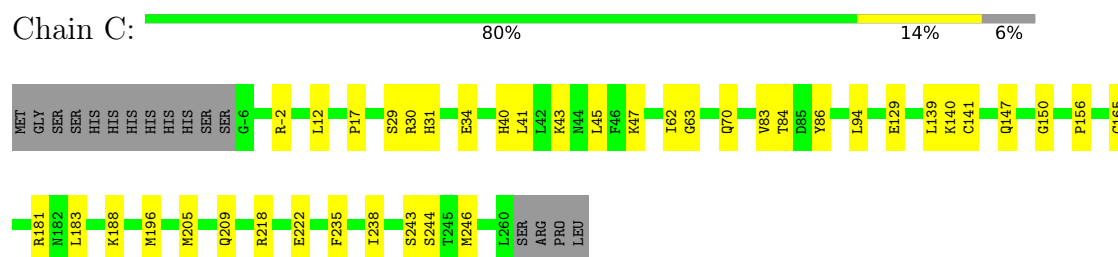
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	115	Total O 115 115	0	0
4	A	85	Total O 85 85	0	0
4	B	74	Total O 74 74	0	0
4	D	53	Total O 53 53	0	0

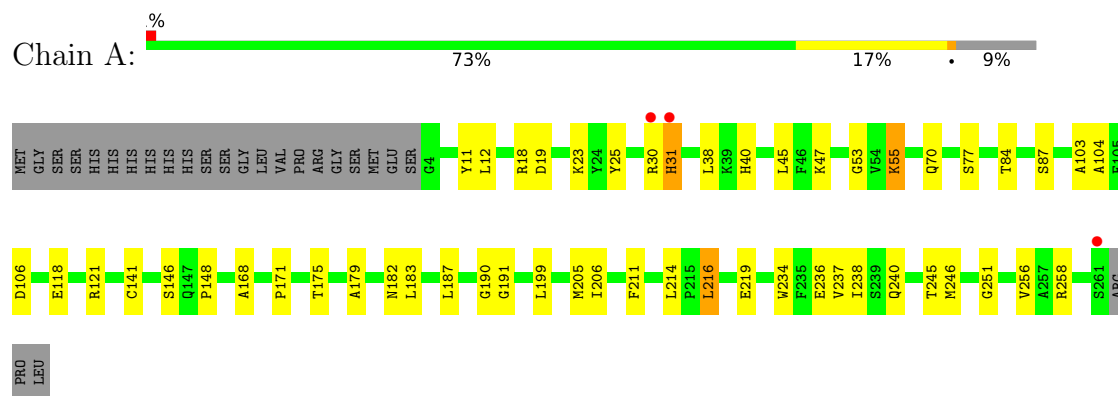
### 3 Residue-property plots [i](#)

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.

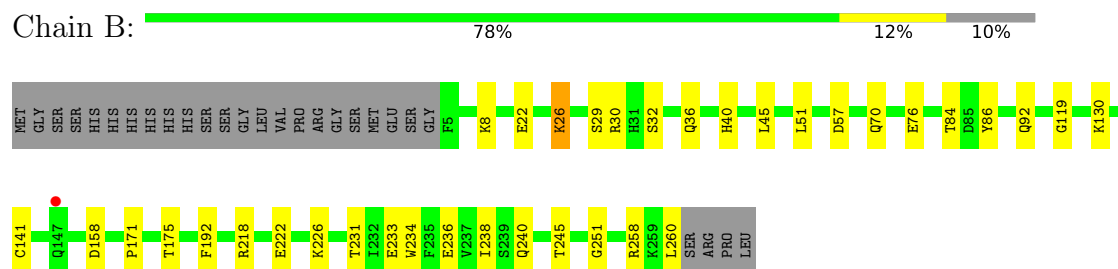
- Molecule 1: NNMT protein



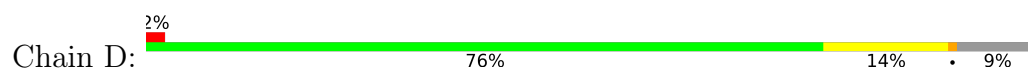
- Molecule 1: NNMT protein



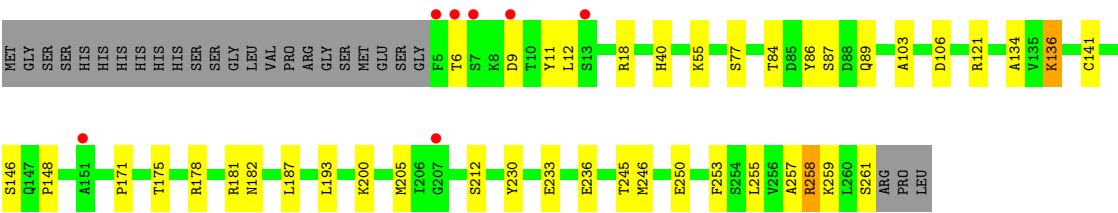
- Molecule 1: NNMT protein



- Molecule 1: NNMT protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.82Å 62.60Å 79.78Å 110.07° 103.82° 103.85°	Depositor
Resolution (Å)	41.14 – 2.08 41.14 – 2.08	Depositor EDS
% Data completeness (in resolution range)	89.4 (41.14-2.08) 89.4 (41.14-2.08)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.08Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.207 , 0.245 0.207 , 0.245	Depositor DCC
$R_{free}$ test set	2012 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-h-k-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, 9XL

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	0.27	0/2064	0.48	0/2796
1	B	0.27	0/2028	0.55	2/2754 (0.1%)
1	C	0.27	0/2113	0.48	0/2867
1	D	0.28	0/2025	0.49	0/2748
All	All	0.27	0/8230	0.50	2/11165 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	B	30	ARG	NE-CZ-NH1	7.77	124.19	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2015	0	2012	35	0
1	B	1978	0	1962	22	0
1	C	2062	0	2045	30	0
1	D	1982	0	1961	23	0
2	A	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	38	0	0	0	0
2	C	38	0	0	0	0
2	D	38	0	0	0	0
3	A	14	0	20	3	0
3	B	7	0	10	0	0
3	C	35	0	50	7	0
4	A	85	0	0	1	0
4	B	74	0	0	1	0
4	C	115	0	0	3	0
4	D	53	0	0	1	0
All	All	8572	0	8060	104	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 6.

All (104) 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:D:9:ASP:HA	1:D:12:LEU:HD23	1.72	0.71
1:A:121:ARG:HB2	3:A:803:PEG:H22	1.74	0.69
1:C:218:ARG:NH1	1:C:222:GLU:OE2	2.27	0.67
1:B:29:SER:HB2	1:D:106:ASP:HB2	1.79	0.64
1:A:55:LYS:HB3	1:A:77:SER:HB3	1.79	0.64
1:D:200:LYS:HE2	1:D:250:GLU:HG3	1.80	0.64
1:C:86:TYR:O	1:C:140:LYS:NZ	2.22	0.63
1:A:30:ARG:HH22	1:B:119:GLY:HA3	1.63	0.62
1:C:205:MET:HB2	1:C:246:MET:HA	1.81	0.62
1:A:118:GLU:HB2	3:A:803:PEG:H11	1.82	0.61
1:C:41:LEU:HD22	1:C:196:MET:HE3	1.82	0.60
1:A:19:ASP:O	1:A:23:LYS:HD2	2.01	0.60
1:A:234:TRP:HE1	1:A:256:VAL:HG23	1.68	0.58
1:C:31:HIS:HE1	3:C:906:PEG:H41	1.68	0.58
1:C:181:ARG:NH1	4:C:1005:HOH:O	2.35	0.57
1:A:234:TRP:HD1	1:A:256:VAL:HB	1.69	0.57
1:D:171:PRO:HD2	1:D:175:THR:HG21	1.85	0.57
1:B:231:THR:HG23	1:B:260:LEU:HD21	1.87	0.57
1:C:83:VAL:HG21	1:C:94:LEU:HD21	1.86	0.57
1:D:12:LEU:HD21	1:D:86:TYR:CE2	2.42	0.55
1:D:12:LEU:HD13	1:D:87:SER:HA	1.88	0.54
1:D:11:TYR:O	1:D:89:GLN:NE2	2.40	0.54
1:D:55:LYS:HB3	1:D:77:SER:HB3	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LYS:HE3	4:B:601:HOH:O	2.09	0.53
1:D:187:LEU:HD23	1:D:259:LYS:HB2	1.91	0.52
1:C:40:HIS:CE1	1:C:238:ILE:HG21	2.45	0.52
1:C:84:THR:HB	1:C:141:CYS:HB3	1.92	0.52
1:D:18:ARG:NH1	1:D:103:ALA:O	2.38	0.52
1:A:240:GLN:O	1:A:251:GLY:HA2	2.11	0.51
1:C:12:LEU:HD11	3:C:902:PEG:H21	1.93	0.51
1:B:84:THR:HB	1:B:141:CYS:HB3	1.92	0.51
1:C:30:ARG:NH2	4:C:1008:HOH:O	2.43	0.51
1:A:121:ARG:H	3:A:803:PEG:H12	1.76	0.51
1:A:18:ARG:NH2	4:A:906:HOH:O	2.45	0.50
1:B:45:LEU:HD13	1:B:70:GLN:HA	1.94	0.50
1:C:218:ARG:HG3	1:C:235:PHE:CE1	2.47	0.50
1:C:147:GLN:HG2	1:C:150:GLY:O	2.13	0.49
1:A:84:THR:HB	1:A:141:CYS:HB3	1.94	0.49
1:D:178:ARG:HG3	1:D:181:ARG:NH1	2.27	0.49
1:B:57:ASP:N	1:B:158:ASP:OD2	2.43	0.49
1:B:171:PRO:HD2	1:B:175:THR:HG21	1.94	0.48
1:C:29:SER:HB2	1:A:106:ASP:HB2	1.96	0.48
1:A:18:ARG:NH2	1:A:103:ALA:O	2.34	0.48
1:D:233:GLU:OE2	1:D:258:ARG:NE	2.39	0.47
1:C:139:LEU:HA	3:C:904:PEG:H32	1.95	0.47
1:C:43:LYS:HD3	1:B:51:LEU:HB3	1.96	0.47
1:D:148:PRO:HG3	1:D:182:ASN:HB3	1.96	0.47
1:B:40:HIS:NE2	1:B:238:ILE:HG21	2.30	0.47
1:D:230:TYR:HB3	1:D:257:ALA:HB1	1.98	0.46
1:B:40:HIS:CD2	1:B:238:ILE:HD13	2.50	0.46
1:D:205:MET:HB2	1:D:246:MET:HA	1.96	0.46
1:C:17:PRO:HG2	3:C:903:PEG:H12	1.98	0.46
1:C:31:HIS:CE1	3:C:906:PEG:H41	2.47	0.46
1:B:192:PHE:CE1	1:B:258:ARG:HD3	2.51	0.46
3:C:906:PEG:H32	3:C:906:PEG:H11	1.47	0.46
1:A:40:HIS:CD2	1:A:238:ILE:HG21	2.51	0.46
1:B:8:LYS:HB3	1:B:86:TYR:CE2	2.51	0.46
1:A:214:LEU:HG	1:A:216:LEU:HD13	1.98	0.45
1:C:156:PRO:HB2	1:C:188:LYS:HG2	1.97	0.45
1:A:53:GLY:O	1:A:55:LYS:HG3	2.16	0.45
1:D:84:THR:HB	1:D:141:CYS:HB3	1.99	0.45
1:A:171:PRO:HD2	1:A:175:THR:HG21	1.99	0.44
1:C:238:ILE:HG22	1:B:234:TRP:HB3	1.99	0.44
1:C:62:ILE:HG13	1:C:183:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HD12	1:A:211:PHE:CE1	2.53	0.44
1:A:199:LEU:HD11	1:A:237:VAL:HG22	2.00	0.44
1:C:29:SER:OG	1:A:104:ALA:O	2.15	0.44
1:C:238:ILE:HG22	1:B:234:TRP:CB	2.48	0.44
1:B:22:GLU:O	1:B:26:LYS:HD3	2.18	0.43
1:D:121:ARG:N	4:D:408:HOH:O	2.51	0.43
1:A:179:ALA:O	1:A:183:LEU:HD13	2.18	0.43
1:A:205:MET:N	1:A:246:MET:O	2.51	0.43
1:A:12:LEU:HD23	1:A:87:SER:HA	2.00	0.43
1:B:76:GLU:HA	1:B:130:LYS:HE3	2.01	0.43
1:B:222:GLU:O	1:B:226:LYS:HG3	2.18	0.43
1:A:205:MET:HB2	1:A:246:MET:HA	2.00	0.43
1:A:148:PRO:HG3	1:A:182:ASN:HB3	2.01	0.43
1:C:-2:ARG:NE	1:C:209:GLN:OE1	2.30	0.42
1:B:234:TRP:HZ3	1:B:236:GLU:HB2	1.85	0.42
1:C:34:GLU:CD	1:C:34:GLU:H	2.23	0.42
1:A:187:LEU:HD22	1:A:191:GLY:HA3	2.01	0.42
1:C:63:GLY:HA3	1:C:165:CYS:SG	2.60	0.41
1:B:32:SER:O	1:B:36:GLN:HG2	2.20	0.41
1:A:45:LEU:HD13	1:A:70:GLN:HA	2.03	0.41
1:A:234:TRP:CD1	1:A:256:VAL:HB	2.51	0.41
1:D:187:LEU:HB3	1:D:259:LYS:HD2	2.03	0.41
1:C:147:GLN:HG3	4:C:1033:HOH:O	2.20	0.41
1:A:30:ARG:O	1:A:31:HIS:C	2.57	0.41
1:B:260:LEU:HA	1:B:260:LEU:HD23	1.87	0.41
1:D:193:LEU:HD22	1:D:230:TYR:CZ	2.55	0.41
1:C:129:GLU:HB2	3:C:905:PEG:H32	2.02	0.41
1:D:253:PHE:CE2	1:D:255:LEU:HD23	2.56	0.41
1:A:190:GLY:O	1:A:258:ARG:HD3	2.21	0.41
1:D:40:HIS:NE2	1:D:236:GLU:OE1	2.42	0.41
1:A:11:TYR:OH	1:A:168:ALA:HB1	2.20	0.41
1:B:8:LYS:HB3	1:B:86:TYR:CZ	2.56	0.41
1:A:25:TYR:HD1	1:A:38:LEU:HD22	1.86	0.40
1:B:240:GLN:O	1:B:251:GLY:HA2	2.20	0.40
1:C:45:LEU:HD13	1:C:70:GLN:HA	2.03	0.40
1:A:219[B]:GLU:CD	1:A:219[B]:GLU:H	2.24	0.40
1:D:134:ALA:O	1:D:136:LYS:HD2	2.22	0.40
1:A:40:HIS:NE2	1:A:238:ILE:HG21	2.35	0.40
1:A:234:TRP:CZ3	1:A:236:GLU:HB2	2.57	0.40
1:D:6:THR:H	1:D:212:SER:CB	2.34	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	258/283 (91%)	253 (98%)	4 (2%)	1 (0%)	34	31
1	B	256/283 (90%)	253 (99%)	3 (1%)	0	100	100
1	C	267/283 (94%)	263 (98%)	4 (2%)	0	100	100
1	D	254/283 (90%)	251 (99%)	3 (1%)	0	100	100
All	All	1035/1132 (91%)	1020 (99%)	14 (1%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	HIS

### 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	221/245 (90%)	216 (98%)	5 (2%)	50	53
1	B	215/245 (88%)	209 (97%)	6 (3%)	43	46
1	C	225/245 (92%)	223 (99%)	2 (1%)	78	83
1	D	215/245 (88%)	210 (98%)	5 (2%)	50	53
All	All	876/980 (89%)	858 (98%)	18 (2%)	55	57

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	243	SER
1	C	244	SER
1	A	47	LYS
1	A	55	LYS
1	A	146	SER
1	A	216	LEU
1	A	245	THR
1	B	26	LYS
1	B	92[A]	GLN
1	B	92[B]	GLN
1	B	218	ARG
1	B	233	GLU
1	B	245	THR
1	D	136	LYS
1	D	146	SER
1	D	245	THR
1	D	258	ARG
1	D	261	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The



Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	A	802	-	6,6,6	0.49	0	5,5,5	0.30	0
2	9XL	B	501	-	36,41,41	3.18	13 (36%)	41,58,58	1.64	8 (19%)
3	PEG	A	803	-	6,6,6	0.49	0	5,5,5	0.21	0
2	9XL	D	301	-	36,41,41	3.29	13 (36%)	41,58,58	1.63	9 (21%)
3	PEG	C	905	-	6,6,6	0.49	0	5,5,5	0.34	0
3	PEG	C	903	-	6,6,6	0.49	0	5,5,5	0.30	0
3	PEG	B	502	-	6,6,6	0.49	0	5,5,5	0.29	0
3	PEG	C	904	-	6,6,6	0.49	0	5,5,5	0.27	0
3	PEG	C	902	-	6,6,6	0.49	0	5,5,5	0.25	0
3	PEG	C	906	-	6,6,6	0.46	0	5,5,5	0.29	0
2	9XL	C	901	-	36,41,41	3.28	13 (36%)	41,58,58	1.37	4 (9%)
2	9XL	A	801	-	36,41,41	3.26	14 (38%)	41,58,58	1.80	9 (21%)

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	PEG	A	802	-	-	2/4/4/4	-
2	9XL	B	501	-	-	9/22/43/43	0/4/4/4
3	PEG	A	803	-	-	1/4/4/4	-
2	9XL	D	301	-	-	8/22/43/43	0/4/4/4
3	PEG	C	905	-	-	4/4/4/4	-
3	PEG	C	903	-	-	3/4/4/4	-
3	PEG	B	502	-	-	4/4/4/4	-
3	PEG	C	904	-	-	3/4/4/4	-
3	PEG	C	902	-	-	2/4/4/4	-
3	PEG	C	906	-	-	2/4/4/4	-
2	9XL	C	901	-	-	3/22/43/43	0/4/4/4
2	9XL	A	801	-	-	8/22/43/43	0/4/4/4

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	9XL	C37-C11	9.67	1.65	1.53
2	D	301	9XL	C37-C11	9.65	1.65	1.53
2	A	801	9XL	C37-C11	9.14	1.64	1.53
2	B	501	9XL	C37-C11	8.72	1.64	1.53
2	A	801	9XL	C37-C35	-7.97	1.31	1.53
2	B	501	9XL	C37-C35	-7.89	1.31	1.53
2	D	301	9XL	C37-C35	-7.69	1.32	1.53
2	C	901	9XL	C37-C35	-7.60	1.32	1.53
2	C	901	9XL	C24-N25	7.28	1.46	1.33
2	D	301	9XL	C24-N25	7.27	1.46	1.33
2	A	801	9XL	C14-C13	-6.89	1.42	1.53
2	B	501	9XL	C24-N25	6.67	1.45	1.33
2	A	801	9XL	C24-N25	6.56	1.45	1.33
2	B	501	9XL	C14-C13	-6.02	1.44	1.53
2	D	301	9XL	C14-C13	-6.01	1.44	1.53
2	C	901	9XL	C19-C18	5.83	1.58	1.44
2	A	801	9XL	C12-C11	-5.77	1.33	1.53
2	B	501	9XL	C12-C11	-5.74	1.33	1.53
2	D	301	9XL	C19-C18	5.74	1.58	1.44
2	C	901	9XL	C14-C13	-5.53	1.44	1.53
2	D	301	9XL	C12-C11	-5.53	1.34	1.53
2	C	901	9XL	C12-C11	-5.50	1.34	1.53
2	B	501	9XL	C19-C18	5.28	1.57	1.44
2	A	801	9XL	C19-C18	5.11	1.56	1.44
2	C	901	9XL	C16-C17	4.34	1.57	1.47
2	D	301	9XL	C16-C17	4.18	1.57	1.47
2	B	501	9XL	C16-C17	3.76	1.56	1.47
2	A	801	9XL	C16-C17	3.65	1.55	1.47
2	A	801	9XL	O26-C24	-3.44	1.17	1.24
2	B	501	9XL	O26-C24	-3.26	1.17	1.24
2	A	801	9XL	C18-C17	-3.08	1.15	1.19
2	D	301	9XL	C14-N15	2.92	1.52	1.47
2	D	301	9XL	C02-CL1	2.87	1.82	1.74
2	C	901	9XL	C14-N15	2.87	1.52	1.47
2	B	501	9XL	C14-N15	2.82	1.52	1.47
2	C	901	9XL	C16-N15	2.76	1.49	1.46
2	C	901	9XL	O26-C24	-2.75	1.18	1.24
2	B	501	9XL	C18-C17	-2.74	1.16	1.19
2	C	901	9XL	C02-CL1	2.70	1.81	1.74
2	D	301	9XL	O26-C24	-2.68	1.19	1.24
2	B	501	9XL	C02-CL1	2.61	1.81	1.74
2	A	801	9XL	C02-CL1	2.56	1.81	1.74
2	A	801	9XL	C09-N10	-2.47	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	9XL	C13-C35	2.46	1.60	1.54
2	A	801	9XL	C14-N15	2.38	1.51	1.47
2	D	301	9XL	C16-N15	2.36	1.49	1.46
2	D	301	9XL	C13-C35	2.35	1.60	1.54
2	B	501	9XL	C09-N10	-2.31	1.33	1.37
2	B	501	9XL	C13-C35	2.21	1.60	1.54
2	A	801	9XL	C27-C19	-2.07	1.36	1.39
2	A	801	9XL	C13-C35	2.04	1.59	1.54
2	C	901	9XL	O33-C32	2.01	1.28	1.22
2	D	301	9XL	O33-C32	2.01	1.28	1.22

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	9XL	C17-C16-N15	-5.10	103.53	113.89
2	C	901	9XL	N05-C04-N03	-4.61	121.48	128.68
2	A	801	9XL	N05-C04-N03	-4.58	121.52	128.68
2	D	301	9XL	N05-C04-N03	-4.55	121.57	128.68
2	D	301	9XL	C17-C16-N15	-4.53	104.68	113.89
2	B	501	9XL	C17-C16-N15	-4.40	104.96	113.89
2	B	501	9XL	N05-C04-N03	-4.29	121.97	128.68
2	A	801	9XL	C04-N03-C02	3.79	121.37	116.26
2	B	501	9XL	C28-N15-C14	3.69	120.75	111.96
2	A	801	9XL	C28-N15-C14	3.56	120.43	111.96
2	B	501	9XL	C04-N03-C02	3.53	121.02	116.26
2	D	301	9XL	C04-N03-C02	3.18	120.54	116.26
2	D	301	9XL	C28-N15-C14	3.07	119.28	111.96
2	C	901	9XL	C04-N03-C02	3.00	120.30	116.26
2	A	801	9XL	C09-N10-C11	2.90	128.26	125.40
2	A	801	9XL	O36-C35-C13	-2.76	105.60	112.75
2	C	901	9XL	CL1-C02-N03	2.73	120.19	115.98
2	B	501	9XL	CL1-C02-N03	2.72	120.16	115.98
2	C	901	9XL	C28-N15-C14	2.68	118.34	111.96
2	D	301	9XL	C29-C28-N15	-2.57	105.48	113.93
2	D	301	9XL	C09-N10-C11	2.54	127.91	125.40
2	D	301	9XL	CL1-C02-N03	2.46	119.77	115.98
2	A	801	9XL	C29-C28-N15	-2.43	105.96	113.93
2	B	501	9XL	O36-C35-C13	-2.40	106.53	112.75
2	A	801	9XL	C23-C24-N25	2.30	120.51	117.75
2	B	501	9XL	C12-C11-N10	-2.20	110.44	113.39
2	B	501	9XL	C29-C28-N15	-2.11	106.99	113.93
2	A	801	9XL	CL1-C02-N03	2.04	119.11	115.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	9XL	C23-C24-N25	2.03	120.19	117.75
2	D	301	9XL	O34-C32-C30	2.01	120.22	113.38

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	9XL	C28-C29-C30-C32
2	C	901	9XL	C28-C29-C30-N31
2	A	801	9XL	N15-C16-C17-C18
2	A	801	9XL	C13-C14-N15-C28
2	A	801	9XL	C13-C14-N15-C16
2	A	801	9XL	C17-C16-N15-C28
2	B	501	9XL	C13-C14-N15-C28
2	B	501	9XL	C13-C14-N15-C16
2	B	501	9XL	C17-C16-N15-C28
2	B	501	9XL	C28-C29-C30-N31
2	D	301	9XL	C13-C14-N15-C28
2	D	301	9XL	C13-C14-N15-C16
2	D	301	9XL	C17-C16-N15-C28
2	D	301	9XL	C28-C29-C30-N31
3	C	906	PEG	C1-C2-O2-C3
3	C	902	PEG	O1-C1-C2-O2
3	C	905	PEG	O2-C3-C4-O4
2	B	501	9XL	C29-C28-N15-C14
2	D	301	9XL	C29-C28-N15-C16
3	C	906	PEG	O1-C1-C2-O2
3	B	502	PEG	O1-C1-C2-O2
3	B	502	PEG	O2-C3-C4-O4
2	B	501	9XL	C29-C28-N15-C16
2	D	301	9XL	C29-C28-N15-C14
3	C	903	PEG	O1-C1-C2-O2
3	C	905	PEG	O1-C1-C2-O2
3	A	802	PEG	O1-C1-C2-O2
3	C	904	PEG	O2-C3-C4-O4
3	A	802	PEG	C4-C3-O2-C2
3	C	905	PEG	C1-C2-O2-C3
2	B	501	9XL	C28-C29-C30-C32
2	D	301	9XL	C28-C29-C30-C32
2	A	801	9XL	C12-C13-C14-N15
2	A	801	9XL	C35-C13-C14-N15
3	C	902	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
2	A	801	9XL	C29-C28-N15-C14
3	C	904	PEG	C4-C3-O2-C2
3	C	903	PEG	C1-C2-O2-C3
3	A	803	PEG	C4-C3-O2-C2
3	B	502	PEG	C4-C3-O2-C2
3	C	904	PEG	O1-C1-C2-O2
3	C	905	PEG	C4-C3-O2-C2
2	A	801	9XL	C17-C16-N15-C14
2	B	501	9XL	C17-C16-N15-C14
2	D	301	9XL	C17-C16-N15-C14
3	B	502	PEG	C1-C2-O2-C3
3	C	903	PEG	C4-C3-O2-C2
2	C	901	9XL	C13-C14-N15-C16
2	B	501	9XL	C22-C23-C24-N25

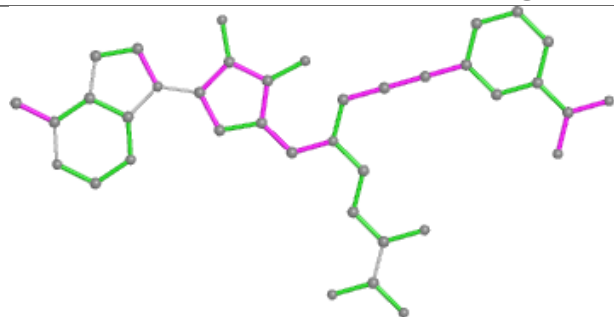
There are no ring outliers.

6 monomers are involved in 10 short contacts:

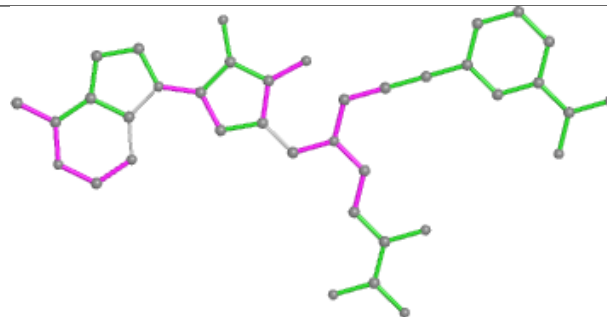
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	PEG	3	0
3	C	905	PEG	1	0
3	C	903	PEG	1	0
3	C	904	PEG	1	0
3	C	902	PEG	1	0
3	C	906	PEG	3	0

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.

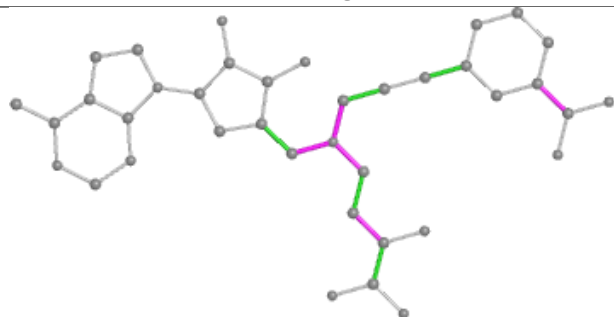
## Ligand 9XL B 501



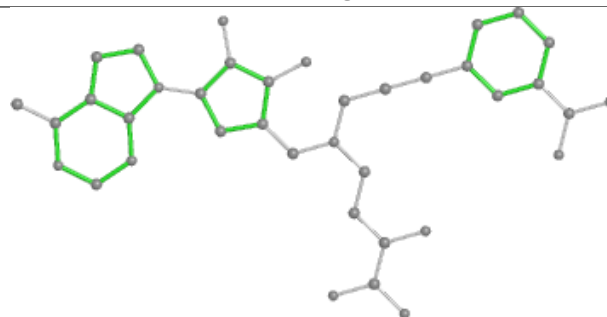
Bond lengths



Bond angles

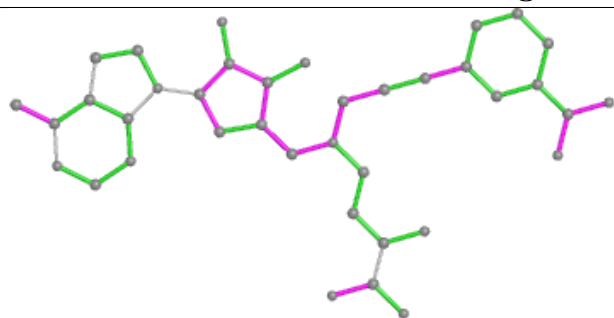


Torsions

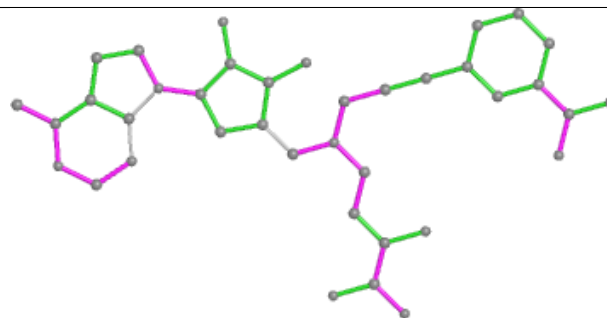


Rings

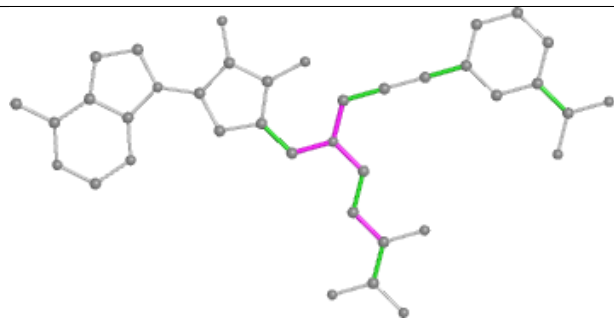
## Ligand 9XL D 301



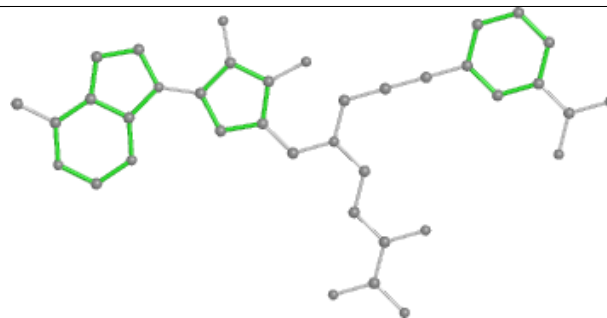
Bond lengths



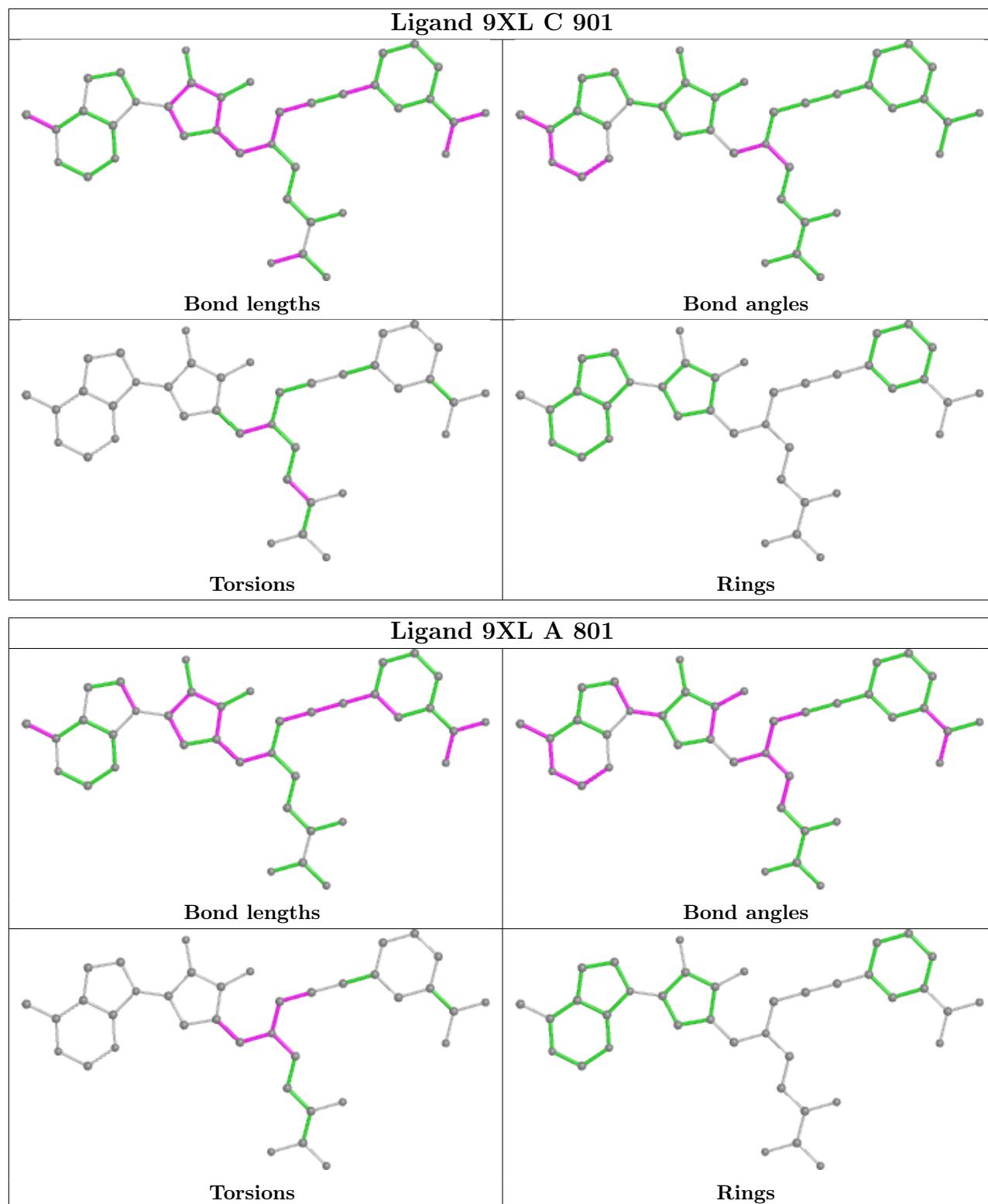
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	260:LEU	C	261:SER	N	3.18
1	A	260:LEU	C	261:SER	N	3.00



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	258/283 (91%)	-0.25	3 (1%) 79 81	16, 27, 43, 63	0
1	B	256/283 (90%)	-0.34	1 (0%) 92 93	17, 27, 39, 47	0
1	C	267/283 (94%)	-0.34	0 100 100	16, 25, 36, 45	0
1	D	257/283 (90%)	-0.07	7 (2%) 54 59	16, 33, 50, 58	0
All	All	1038/1132 (91%)	-0.25	11 (1%) 80 83	16, 27, 44, 63	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	HIS	3.9
1	D	5	PHE	3.2
1	D	151	ALA	2.6
1	D	7	SER	2.5
1	A	30	ARG	2.4
1	D	13	SER	2.3
1	D	6	THR	2.2
1	B	147	GLN	2.1
1	D	207	GLY	2.0
1	A	261	SER	2.0
1	D	9	ASP	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

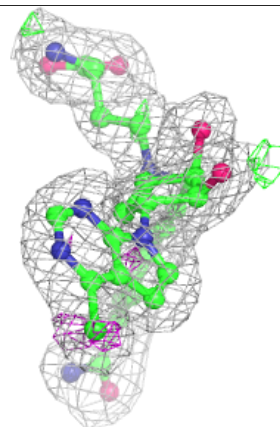
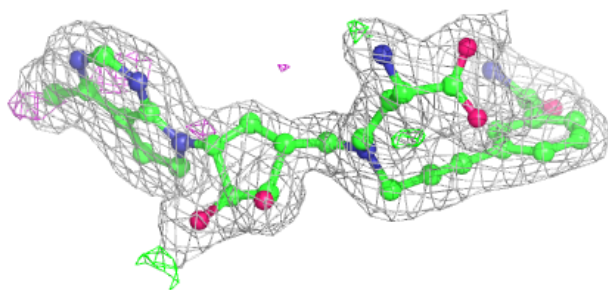
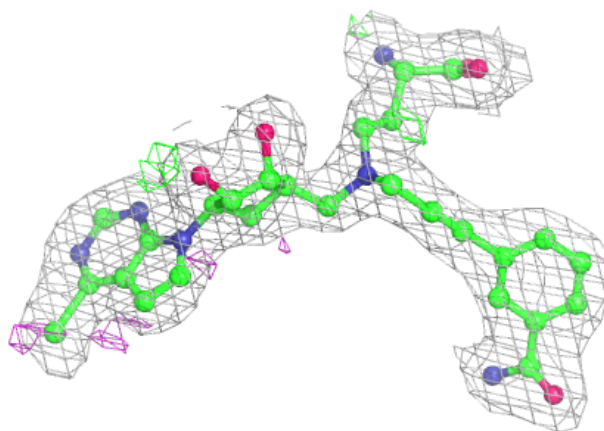
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PEG	B	502	7/7	0.77	0.26	48,53,56,61	0
3	PEG	C	904	7/7	0.79	0.18	39,41,47,57	0
3	PEG	C	905	7/7	0.80	0.26	30,35,35,41	0
3	PEG	A	802	7/7	0.83	0.34	52,56,61,65	0
3	PEG	C	902	7/7	0.84	0.40	47,47,49,55	0
3	PEG	C	903	7/7	0.84	0.23	30,34,39,41	0
3	PEG	C	906	7/7	0.88	0.22	37,42,48,48	0
3	PEG	A	803	7/7	0.89	0.20	29,32,41,43	0
2	9XL	B	501	38/38	0.92	0.11	19,23,30,40	0
2	9XL	A	801	38/38	0.93	0.10	19,25,29,50	0
2	9XL	C	901	38/38	0.93	0.10	14,21,26,44	0
2	9XL	D	301	38/38	0.94	0.11	22,32,37,54	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.

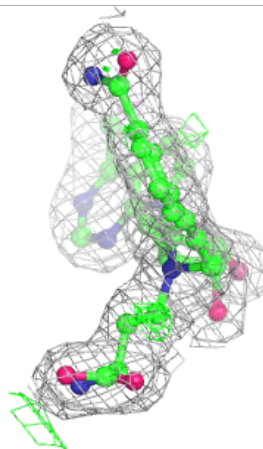
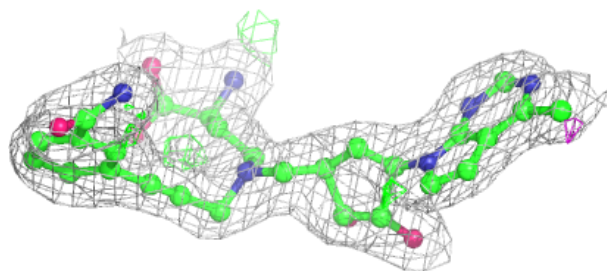
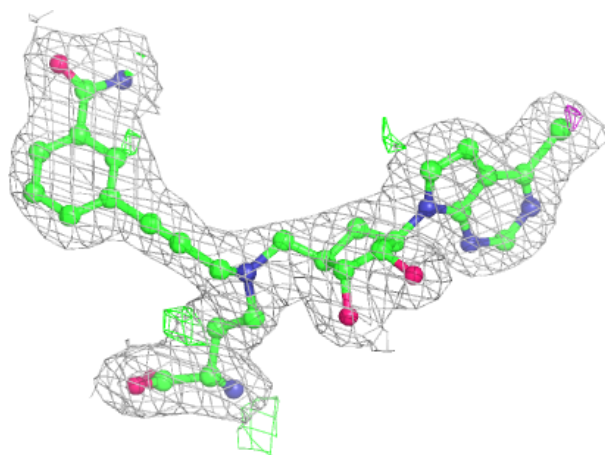
**Electron density around 9XL B 501:**

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



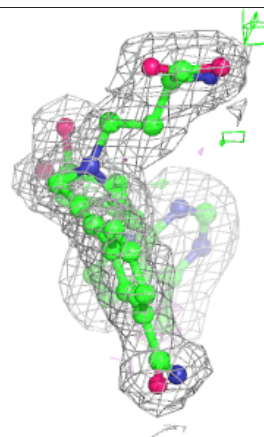
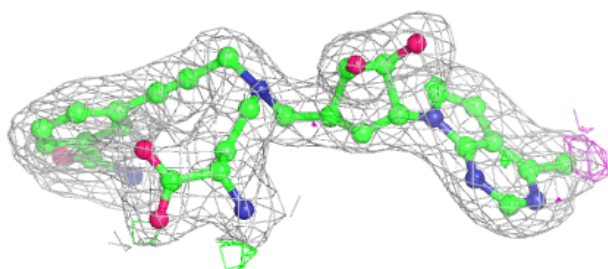
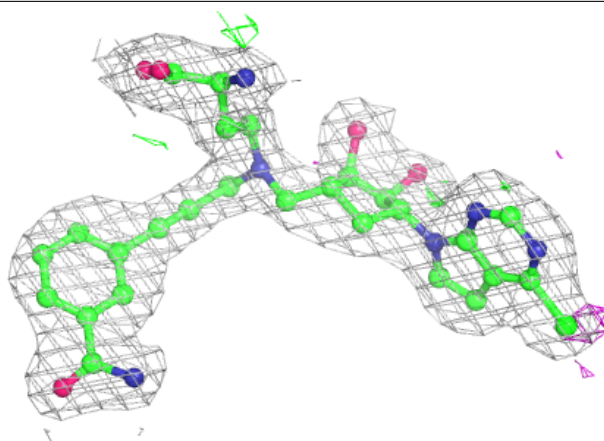
**Electron density around 9XL A 801:**

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



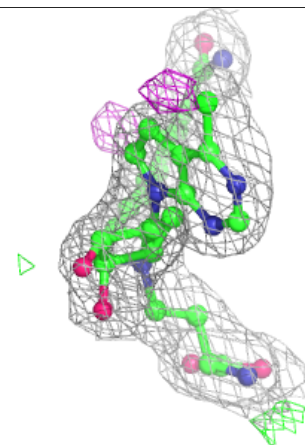
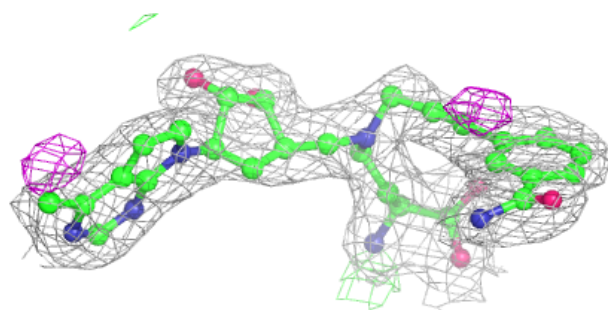
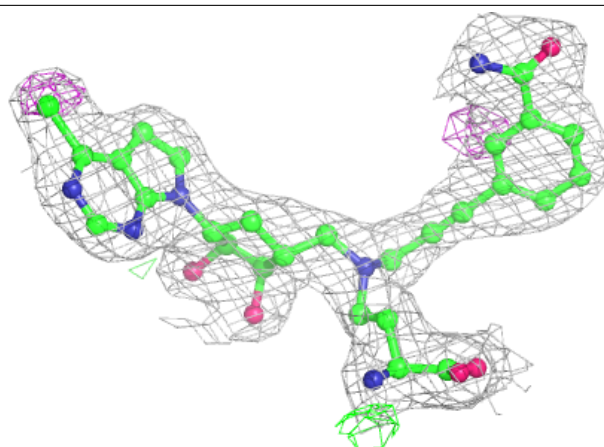
**Electron density around 9XL C 901:**

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



**Electron density around 9XL D 301:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.