



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 21, 2024 – 01:22 pm GMT

PDB ID : 7NBH  
Title : Crystal structure of human serine racemase in complex with DSiP fragment Z26781964, XChem fragment screen.  
Authors : Koulouris, C.R.; Roe, S.M.  
Deposited on : 2021-01-26  
Resolution : 1.77 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

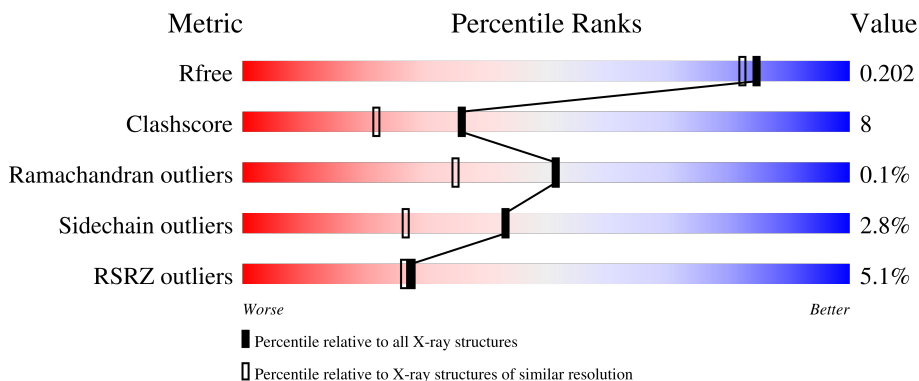
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	AAA	346	 4% 79% 12% 8%
1	BBB	346	 7% 81% 8% 11%
1	CCC	346	 3% 77% 14% 8%
1	DDD	346	 4% 76% 13% 9%

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
2	EDO	CCC	403	-	-	X	-
5	GOL	AAA	412[A]	-	-	X	-

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 11560 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 Serine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	AAA	320	Total 2710	C 1717	N 458	O 521	P 2	S 12	0	33	0
1	BBB	309	Total 2437	C 1551	N 407	O 467	P 1	S 11	0	18	1
1	CCC	317	Total 2587	C 1650	N 427	O 497	P 1	S 12	0	25	0
1	DDD	315	Total 2572	C 1638	N 428	O 491	P 1	S 14	0	25	0

There are 32 discrepancies between the modelled and reference sequences:

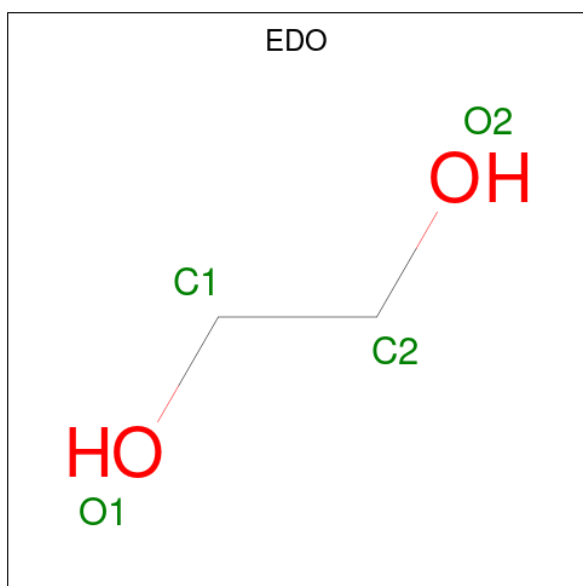
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	6	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	341	HIS	-	expression tag	UNP Q9GZT4
AAA	342	HIS	-	expression tag	UNP Q9GZT4
AAA	343	HIS	-	expression tag	UNP Q9GZT4
AAA	344	HIS	-	expression tag	UNP Q9GZT4
AAA	345	HIS	-	expression tag	UNP Q9GZT4
AAA	346	HIS	-	expression tag	UNP Q9GZT4
BBB	2	ASP	CYS	engineered mutation	UNP Q9GZT4
BBB	6	ASP	CYS	engineered mutation	UNP Q9GZT4
BBB	341	HIS	-	expression tag	UNP Q9GZT4
BBB	342	HIS	-	expression tag	UNP Q9GZT4
BBB	343	HIS	-	expression tag	UNP Q9GZT4
BBB	344	HIS	-	expression tag	UNP Q9GZT4
BBB	345	HIS	-	expression tag	UNP Q9GZT4
BBB	346	HIS	-	expression tag	UNP Q9GZT4
CCC	2	ASP	CYS	engineered mutation	UNP Q9GZT4
CCC	6	ASP	CYS	engineered mutation	UNP Q9GZT4
CCC	341	HIS	-	expression tag	UNP Q9GZT4
CCC	342	HIS	-	expression tag	UNP Q9GZT4
CCC	343	HIS	-	expression tag	UNP Q9GZT4

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	344	HIS	-	expression tag	UNP Q9GZT4
CCC	345	HIS	-	expression tag	UNP Q9GZT4
CCC	346	HIS	-	expression tag	UNP Q9GZT4
DDD	2	ASP	CYS	engineered mutation	UNP Q9GZT4
DDD	6	ASP	CYS	engineered mutation	UNP Q9GZT4
DDD	341	HIS	-	expression tag	UNP Q9GZT4
DDD	342	HIS	-	expression tag	UNP Q9GZT4
DDD	343	HIS	-	expression tag	UNP Q9GZT4
DDD	344	HIS	-	expression tag	UNP Q9GZT4
DDD	345	HIS	-	expression tag	UNP Q9GZT4
DDD	346	HIS	-	expression tag	UNP Q9GZT4

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 8 4 4	0	1
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	1
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 8 4 4	0	1
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	4	Total Na 5 5	0	1
3	BBB	1	Total Na 1 1	0	0
3	CCC	2	Total Na 2 2	0	0
3	DDD	2	Total Na 2 2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

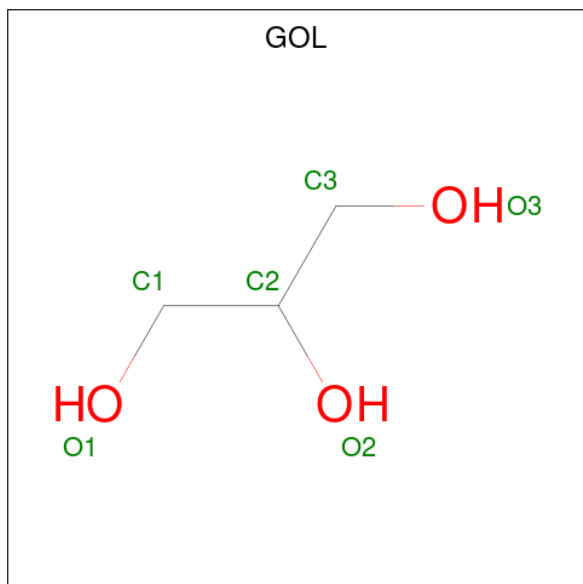
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total Ca 1 1	0	0
4	BBB	1	Total Ca 1 1	0	0
4	CCC	1	Total Ca 2 2	0	1

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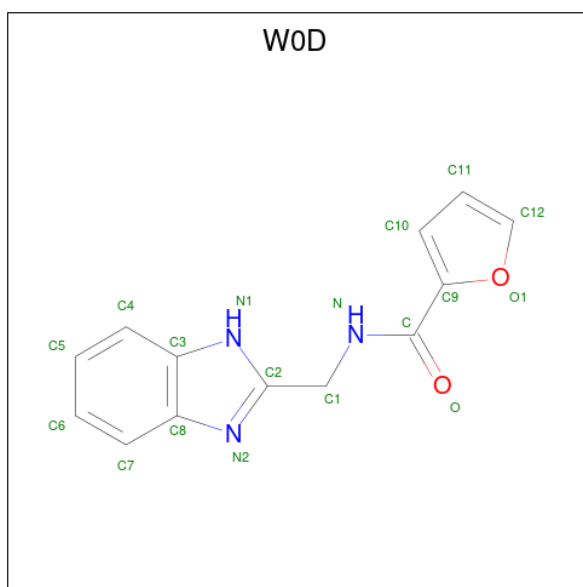
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	DDD	1	Total Ca 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 6 3 3	0	0
5	AAA	1	Total C O 6 3 3	0	0
5	AAA	1	Total C O 6 3 3	0	1
5	CCC	1	Total C O 6 3 3	0	0
5	CCC	1	Total C O 6 3 3	0	0
5	CCC	1	Total C O 12 6 6	0	1
5	DDD	1	Total C O 6 3 3	0	0

- Molecule 6 is N-[(1H-benzimidazol-2-yl)methyl]furan-2-carboxamide (three-letter code: W0D) (formula:  $C_{13}H_{11}N_3O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	N	O	0	0
			18	13	3	2		
6	AAA	1	Total	C	N	O	0	0
			18	13	3	2		
6	BBB	1	Total	C	N	O	0	0
			18	13	3	2		
6	BBB	1	Total	C	N	O	0	0
			18	13	3	2		
6	DDD	1	Total	C	N	O	0	1
			18	13	3	2		
6	DDD	1	Total	C	N	O	0	1
			18	13	3	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

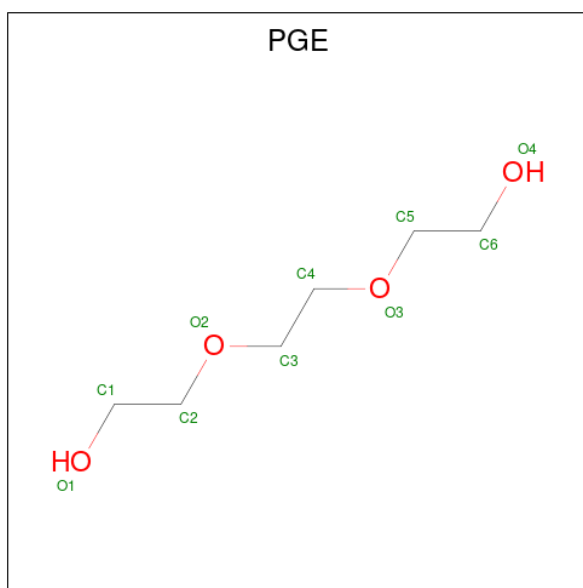
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	CCC	1	Total	Mg	0	0
			1	1		
7	DDD	1	Total	Mg	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	CCC	1	Total	Cl	0	0
			1	1		



- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	DDD	1	Total C O 10 6 4	0	0
9	DDD	1	Total C O 10 6 4	0	0

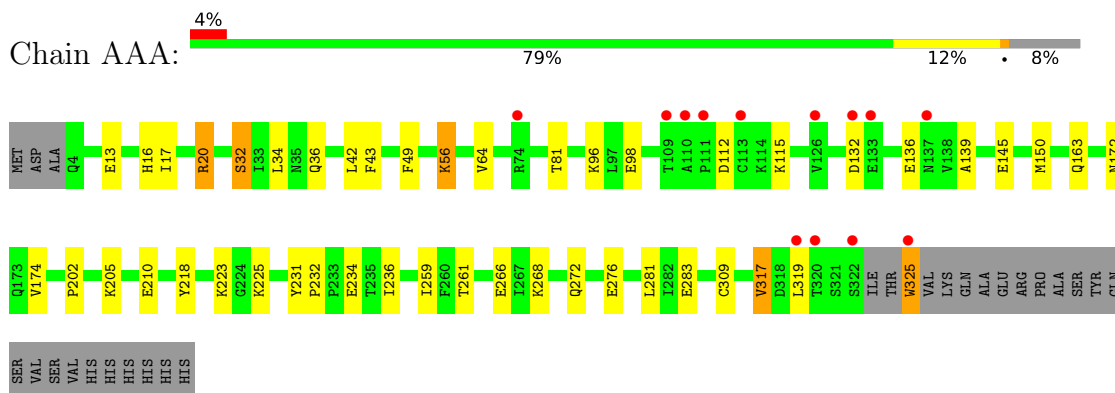
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	AAA	306	Total O 312 312	0	8
10	BBB	162	Total O 163 163	0	1
10	CCC	241	Total O 244 244	0	4
10	DDD	266	Total O 269 269	0	4

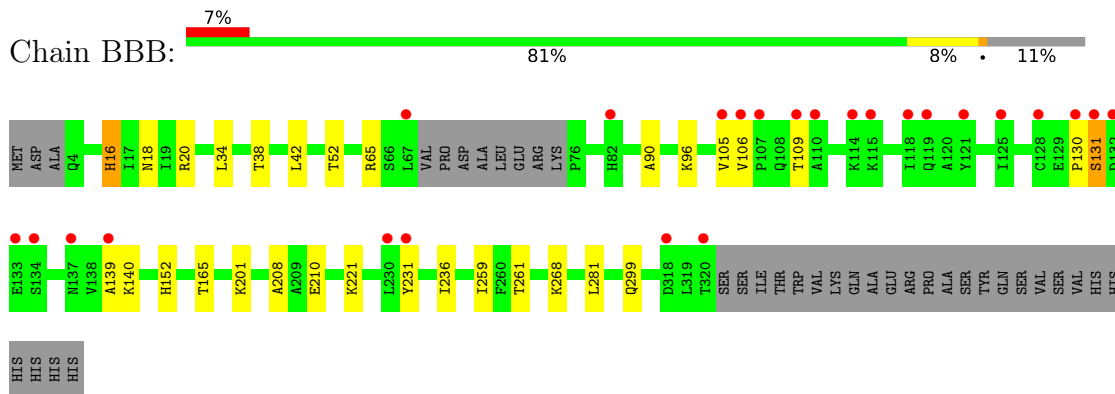
### 3 Residue-property plots [i](#)

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.

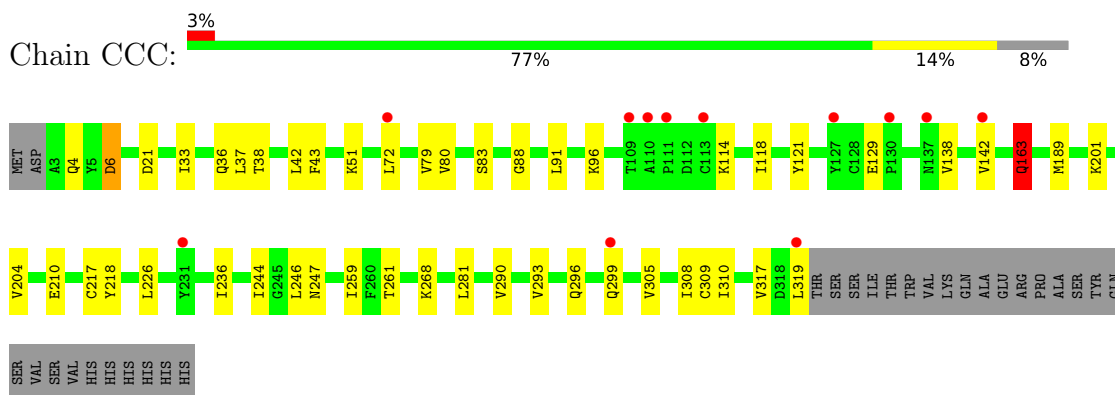
- Molecule 1: Serine racemase



- Molecule 1: Serine racemase



- Molecule 1: Serine racemase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.18Å 154.88Å 85.48Å 90.00° 98.04° 90.00°	Depositor
Resolution (Å)	47.75 – 1.77 47.71 – 1.77	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.75-1.77) 97.0 (47.71-1.77)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 1.77Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.169 , 0.202 0.170 , 0.202	Depositor DCC
$R_{free}$ test set	5859 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11560	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.52% 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: PGE, CA, W0D, GOL, LLP, EDO, CL, NA, MG

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	AAA	0.71	1/2709 (0.0%)	0.89	1/3686 (0.0%)
1	BBB	0.60	0/2454	0.84	1/3346 (0.0%)
1	CCC	0.60	0/2607	0.82	1/3562 (0.0%)
1	DDD	0.66	1/2591 (0.0%)	0.89	3/3527 (0.1%)
All	All	0.64	2/10361 (0.0%)	0.86	6/14121 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	DDD	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	266	GLU	CD-OE2	-6.12	1.19	1.25
1	DDD	283	GLU	CD-OE2	-5.20	1.20	1.25

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	114	LYS	N-CA-CB	-14.28	84.89	110.60
1	BBB	65	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	DDD	163	GLN	CB-CG-CD	5.78	126.61	111.60
1	AAA	283	GLU	CB-CA-C	5.56	121.52	110.40
1	CCC	163	GLN	CB-CG-CD	5.30	125.38	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DDD	113[A]	CYS	Peptide
1	DDD	113[B]	CYS	Peptide

## 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	AAA	2710	0	2698	58	0
1	BBB	2437	0	2412	20	1
1	CCC	2587	0	2570	38	1
1	DDD	2572	0	2549	54	0
2	AAA	28	0	41	2	0
2	BBB	8	0	12	1	0
2	CCC	20	0	30	4	0
2	DDD	16	0	24	1	0
3	AAA	5	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	2	0	0	0	0
3	DDD	2	0	0	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
4	CCC	2	0	0	0	0
4	DDD	1	0	0	0	0
5	AAA	18	0	24	9	0
5	CCC	24	0	32	3	0
5	DDD	6	0	8	2	0
6	AAA	36	0	0	0	0
6	BBB	36	0	0	0	0
6	DDD	36	0	0	2	0
7	CCC	1	0	0	0	0
7	DDD	1	0	0	0	0
8	CCC	1	0	0	0	0
9	DDD	20	0	28	3	0
10	AAA	312	0	0	19	0
10	BBB	163	0	0	4	0
10	CCC	244	0	0	6	0
10	DDD	269	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11560	0	10428	169	1

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 8.

The worst 5 of 169 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:DDD:18[B]:ASN:OD1	1:DDD:67[B]:LEU:HB2	1.14	1.27
1:DDD:18[B]:ASN:OD1	1:DDD:67[B]:LEU:CB	1.95	1.13
1:AAA:16[A]:HIS:ND1	10:AAA:501[A]:HOH:O	1.84	1.11
1:AAA:281[B]:LEU:HD21	1:CCC:281[B]:LEU:CD1	1.80	1.11
1:AAA:281[B]:LEU:CD2	1:CCC:281[B]:LEU:HD13	1.83	1.08

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:231[B]:TYR:OH	1:CCC:129:GLU:OE2[1_556]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	349/346 (101%)	342 (98%)	7 (2%)	0	100	100
1	BBB	322/346 (93%)	315 (98%)	6 (2%)	1 (0%)	41	25
1	CCC	342/346 (99%)	336 (98%)	6 (2%)	0	100	100
1	DDD	332/346 (96%)	326 (98%)	6 (2%)	0	100	100
All	All	1345/1384 (97%)	1319 (98%)	25 (2%)	1 (0%)	51	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	131	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AAA	292/290 (101%)	283 (97%)	9 (3%)	40 22
1	BBB	257/290 (89%)	253 (98%)	4 (2%)	62 51
1	CCC	276/290 (95%)	265 (96%)	11 (4%)	31 14
1	DDD	276/290 (95%)	264 (96%)	12 (4%)	29 12
All	All	1101/1160 (95%)	1065 (97%)	36 (3%)	43 21

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	113[B]	CYS
1	DDD	163	GLN
1	DDD	114	LYS
1	DDD	131	SER
1	BBB	140	LYS

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](#)

5 non-standard protein/DNA/RNA residues 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
1	LLP	AAA	56[B]	1	23,24,25	0.56	0	25,32,34	0.87	1 (4%)
1	LLP	DDD	56	1	23,24,25	0.80	0	25,32,34	1.23	1 (4%)
1	LLP	AAA	56[A]	1	23,24,25	0.58	0	25,32,34	1.00	1 (4%)
1	LLP	CCC	56	1	23,24,25	0.77	0	25,32,34	0.77	0
1	LLP	BBB	56	1	23,24,25	0.64	0	25,32,34	0.78	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
1	LLP	AAA	56[B]	1	-	2/16/17/19	0/1/1/1
1	LLP	DDD	56	1	-	2/16/17/19	0/1/1/1
1	LLP	AAA	56[A]	1	-	3/16/17/19	0/1/1/1
1	LLP	CCC	56	1	-	2/16/17/19	0/1/1/1
1	LLP	BBB	56	1	-	1/16/17/19	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	56	LLP	OP4-C5'-C5	4.45	117.83	109.35
1	AAA	56[A]	LLP	OP4-C5'-C5	3.32	115.68	109.35
1	AAA	56[B]	LLP	OP4-C5'-C5	3.25	115.55	109.35

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	56[A]	LLP	C6-C5-C5'-OP4
1	CCC	56	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	BBB	56	LLP	C4-C4'-NZ-CE
1	AAA	56[B]	LLP	C4-C4'-NZ-CE
1	AAA	56[A]	LLP	C4-C4'-NZ-CE

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	56[B]	LLP	1	0
1	DDD	56	LLP	1	0
1	AAA	56[A]	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 18 are monoatomic - leaving 34 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
2	EDO	AAA	408	-	3,3,3	0.16	0	2,2,2	0.19	0
9	PGE	DDD	410	-	9,9,9	0.38	0	8,8,8	0.31	0
2	EDO	BBB	401	-	3,3,3	0.08	0	2,2,2	0.44	0
2	EDO	DDD	404	-	3,3,3	0.42	0	2,2,2	0.11	0
2	EDO	AAA	401	-	3,3,3	0.18	0	2,2,2	0.43	0
6	W0D	AAA	414	-	14,20,20	0.79	0	14,27,27	1.18	1 (7%)
6	W0D	AAA	413	-	14,20,20	0.87	0	14,27,27	1.26	2 (14%)
2	EDO	AAA	415	-	3,3,3	0.88	0	2,2,2	0.41	0
5	GOL	AAA	410	-	5,5,5	0.19	0	5,5,5	0.52	0
2	EDO	AAA	406	-	3,3,3	0.36	0	2,2,2	0.25	0
5	GOL	CCC	401	-	5,5,5	0.09	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	CCC	405	-	3,3,3	0.12	0	2,2,2	0.13	0
6	W0D	DDD	412[A]	-	14,20,20	0.86	0	14,27,27	1.26	2 (14%)
2	EDO	DDD	406	-	3,3,3	0.15	0	2,2,2	0.13	0
2	EDO	CCC	404[B]	-	3,3,3	0.15	0	2,2,2	0.50	0
5	GOL	CCC	408[B]	-	5,5,5	0.08	0	5,5,5	0.30	0
5	GOL	AAA	409	-	5,5,5	0.13	0	5,5,5	0.45	0
5	GOL	CCC	406	-	5,5,5	0.12	0	5,5,5	0.35	0
6	W0D	BBB	404	-	14,20,20	0.83	0	14,27,27	1.00	1 (7%)
2	EDO	AAA	405[B]	-	3,3,3	0.10	0	2,2,2	0.25	0
2	EDO	DDD	405	-	3,3,3	0.23	0	2,2,2	0.40	0
5	GOL	CCC	408[A]	-	5,5,5	0.05	0	5,5,5	0.25	0
6	W0D	DDD	411[A]	-	14,20,20	0.89	1 (7%)	14,27,27	1.03	1 (7%)
2	EDO	CCC	404[A]	-	3,3,3	0.15	0	2,2,2	0.24	0
5	GOL	AAA	412[A]	-	5,5,5	0.20	0	5,5,5	0.47	0
2	EDO	BBB	406	-	3,3,3	0.27	0	2,2,2	0.41	0
2	EDO	AAA	405[A]	-	3,3,3	0.16	0	2,2,2	0.15	0
6	W0D	BBB	405	-	14,20,20	0.80	0	14,27,27	1.18	1 (7%)
2	EDO	DDD	407	-	3,3,3	0.08	0	2,2,2	0.28	0
2	EDO	CCC	407	-	3,3,3	0.15	0	2,2,2	0.14	0
9	PGE	DDD	408	-	9,9,9	0.28	0	8,8,8	0.25	0
5	GOL	DDD	409	-	5,5,5	0.36	0	5,5,5	0.44	0
2	EDO	CCC	403	3	3,3,3	0.21	0	2,2,2	0.73	0
2	EDO	AAA	407[A]	-	3,3,3	0.05	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
2	EDO	AAA	408	-	-	1/1/1/1	-
9	PGE	DDD	410	-	-	2/7/7/7	-
2	EDO	BBB	401	-	-	1/1/1/1	-
2	EDO	DDD	404	-	-	1/1/1/1	-
2	EDO	AAA	401	-	-	1/1/1/1	-
6	W0D	AAA	414	-	-	0/4/9/9	0/3/3/3
6	W0D	AAA	413	-	-	1/4/9/9	0/3/3/3
2	EDO	AAA	415	-	-	0/1/1/1	-
5	GOL	AAA	410	-	-	2/4/4/4	-
2	EDO	AAA	406	-	-	1/1/1/1	-
5	GOL	CCC	401	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	CCC	405	-	-	0/1/1/1	-
6	W0D	DDD	412[A]	-	-	0/4/9/9	0/3/3/3
2	EDO	DDD	406	-	-	0/1/1/1	-
2	EDO	CCC	404[B]	-	-	0/1/1/1	-
5	GOL	CCC	408[B]	-	-	4/4/4/4	-
5	GOL	AAA	409	-	-	3/4/4/4	-
5	GOL	CCC	406	-	-	4/4/4/4	-
6	W0D	BBB	404	-	-	1/4/9/9	0/3/3/3
2	EDO	AAA	405[B]	-	-	1/1/1/1	-
2	EDO	DDD	405	-	-	1/1/1/1	-
5	GOL	CCC	408[A]	-	-	4/4/4/4	-
6	W0D	DDD	411[A]	-	-	0/4/9/9	0/3/3/3
2	EDO	CCC	404[A]	-	-	1/1/1/1	-
5	GOL	AAA	412[A]	-	-	0/4/4/4	-
2	EDO	BBB	406	-	-	1/1/1/1	-
2	EDO	AAA	405[A]	-	-	0/1/1/1	-
6	W0D	BBB	405	-	-	0/4/9/9	0/3/3/3
2	EDO	DDD	407	-	-	1/1/1/1	-
2	EDO	CCC	407	-	-	1/1/1/1	-
9	PGE	DDD	408	-	-	4/7/7/7	-
5	GOL	DDD	409	-	-	2/4/4/4	-
2	EDO	CCC	403	3	-	1/1/1/1	-
2	EDO	AAA	407[A]	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	DDD	411[A]	W0D	C9-C	-2.02	1.46	1.49

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AAA	413	W0D	C5-C4-C3	-2.89	115.93	120.08
6	AAA	414	W0D	C5-C4-C3	-2.61	116.33	120.08
6	DDD	412[A]	W0D	C5-C4-C3	-2.59	116.35	120.08
6	BBB	405	W0D	C5-C4-C3	-2.52	116.46	120.08
6	DDD	411[A]	W0D	C5-C4-C3	-2.16	116.97	120.08

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

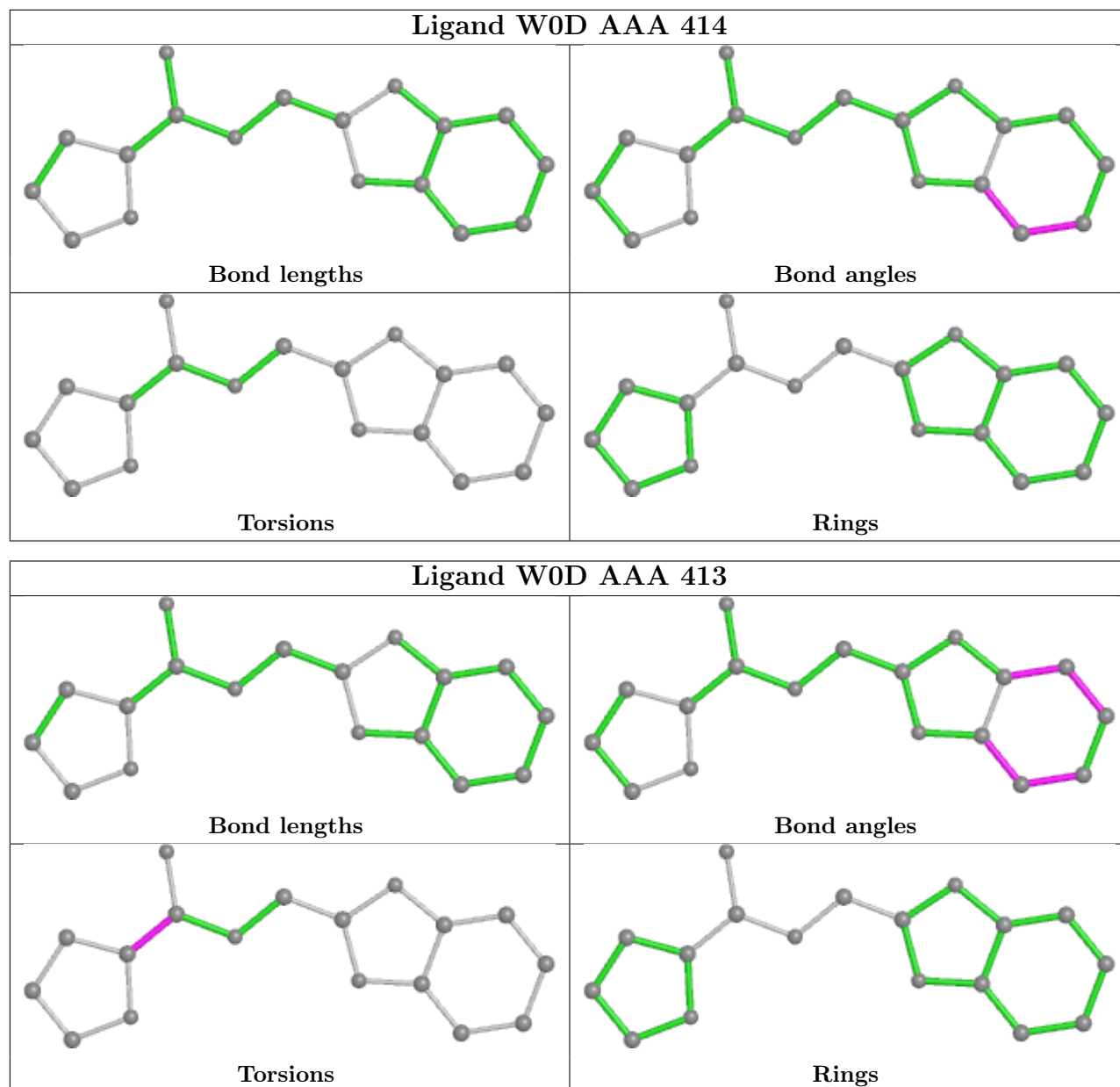
Mol	Chain	Res	Type	Atoms
5	AAA	409	GOL	C1-C2-C3-O3
5	CCC	401	GOL	O1-C1-C2-C3
5	CCC	406	GOL	O1-C1-C2-C3
5	CCC	406	GOL	C1-C2-C3-O3
5	CCC	408[B]	GOL	O2-C2-C3-O3

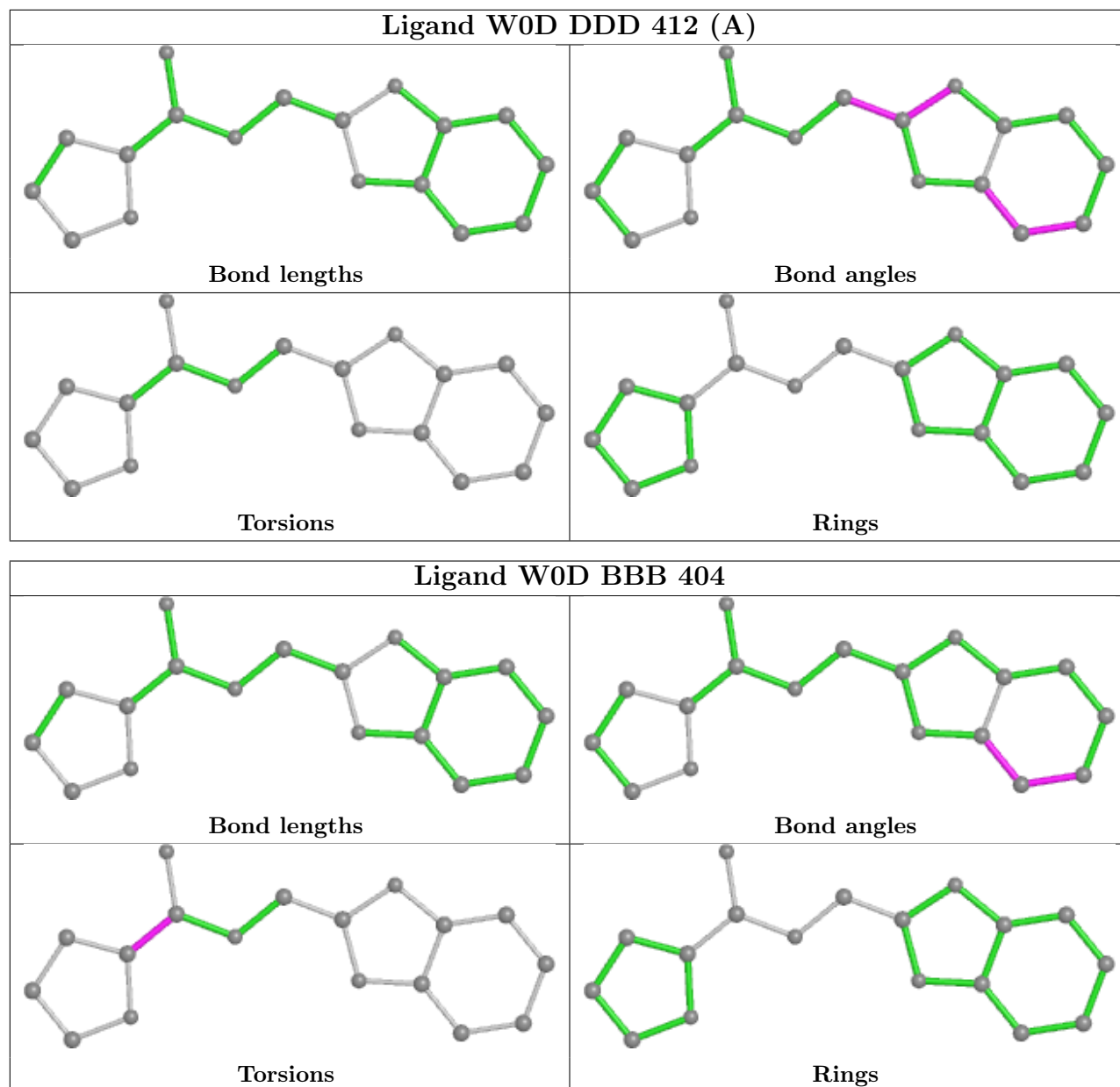
There are no ring outliers.

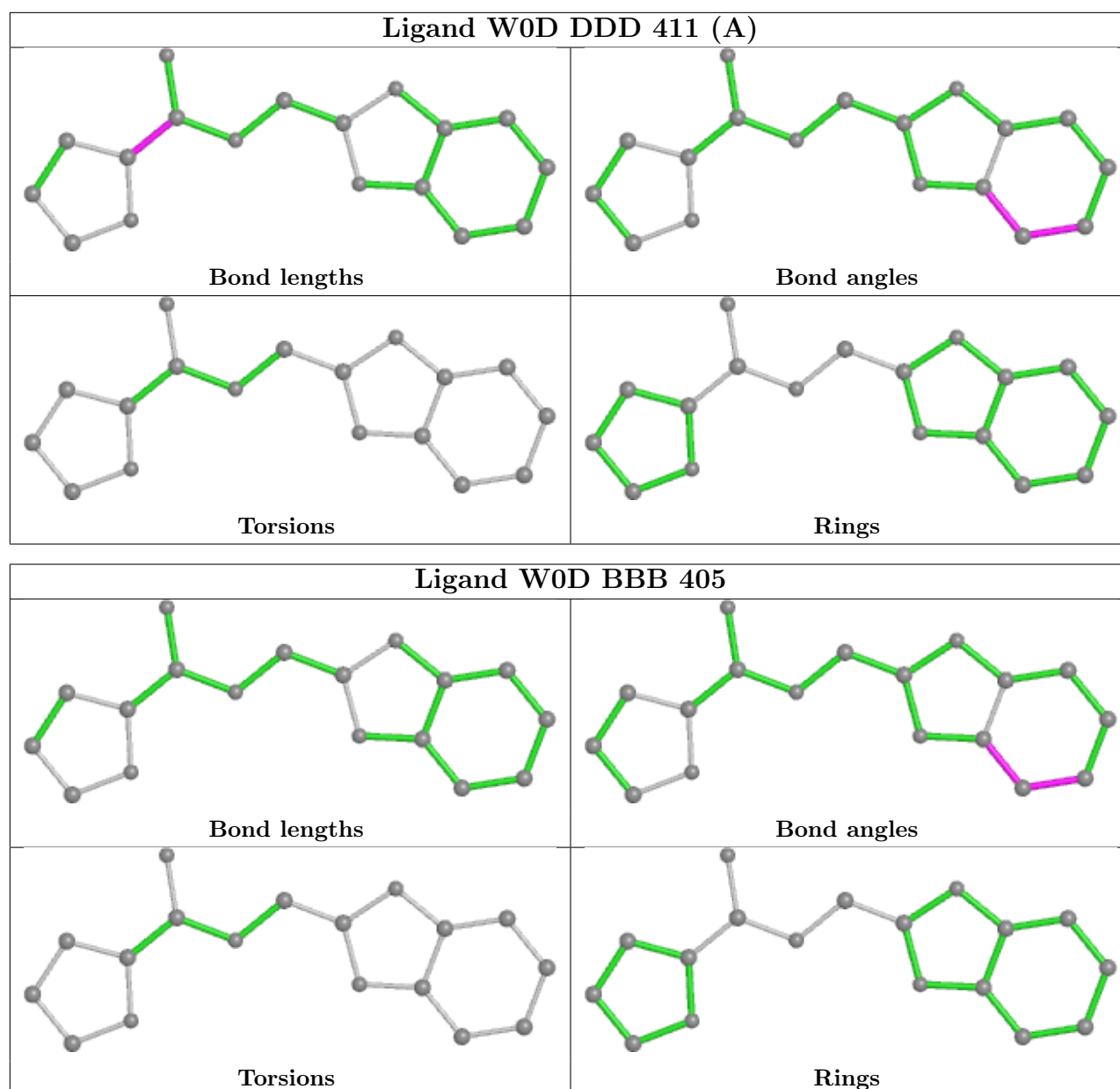
11 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	CCC	401	GOL	2	0
5	AAA	409	GOL	2	0
2	DDD	405	EDO	1	0
5	CCC	408[A]	GOL	1	0
6	DDD	411[A]	W0D	2	0
5	AAA	412[A]	GOL	7	0
2	BBB	406	EDO	1	0
2	AAA	405[A]	EDO	2	0
9	DDD	408	PGE	3	0
5	DDD	409	GOL	2	0
2	CCC	403	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.







## 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 [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	AAA	319/346 (92%)	-0.01	13 (4%) 37 35	16, 24, 66, 98	0
1	BBB	308/346 (89%)	0.08	25 (8%) 12 11	22, 34, 74, 113	0
1	CCC	316/346 (91%)	-0.03	12 (3%) 40 39	20, 32, 66, 76	0
1	DDD	314/346 (90%)	-0.04	14 (4%) 33 31	17, 26, 73, 122	0
All	All	1257/1384 (90%)	0.00	64 (5%) 28 26	16, 29, 69, 122	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	325	TRP	8.9
1	DDD	319	LEU	8.6
1	BBB	105	VAL	7.2
1	DDD	320	THR	7.2
1	BBB	106	VAL	7.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
1	LLP	AAA	56[A]	24/25	0.98	0.08	13,15,18,18	24
1	LLP	AAA	56[B]	24/25	0.98	0.08	16,18,21,23	24
1	LLP	CCC	56	24/25	0.98	0.08	21,23,27,31	0
1	LLP	BBB	56	24/25	0.99	0.06	22,24,27,28	0
1	LLP	DDD	56	24/25	0.99	0.08	16,18,20,22	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	NA	CCC	409	1/1	0.68	0.37	75,75,75,75	0
2	EDO	AAA	408	4/4	0.76	0.19	63,65,68,76	0
9	PGE	DDD	408	10/10	0.76	0.23	57,67,73,73	0
6	W0D	DDD	412[A]	18/18	0.78	0.20	38,44,53,57	18
7	MG	CCC	411	1/1	0.78	0.32	80,80,80,80	0
3	NA	AAA	402	1/1	0.78	0.12	71,71,71,71	0
6	W0D	BBB	405	18/18	0.79	0.24	50,63,69,71	0
5	GOL	CCC	401	6/6	0.79	0.16	39,56,59,62	0
5	GOL	AAA	410	6/6	0.80	0.16	46,54,64,68	0
2	EDO	BBB	406	4/4	0.81	0.30	49,61,64,65	0
5	GOL	AAA	409	6/6	0.81	0.16	43,54,59,61	0
2	EDO	CCC	404[B]	4/4	0.83	0.20	59,63,65,69	4
2	EDO	CCC	404[A]	4/4	0.83	0.20	43,44,47,55	4
6	W0D	AAA	413	18/18	0.83	0.19	38,59,74,84	0
6	W0D	AAA	414	18/18	0.83	0.27	57,65,75,76	0
2	EDO	CCC	405	4/4	0.84	0.20	57,63,67,79	0
5	GOL	CCC	406	6/6	0.85	0.13	51,58,63,65	0
5	GOL	CCC	408[A]	6/6	0.87	0.24	33,37,38,38	6
5	GOL	CCC	408[B]	6/6	0.87	0.24	112,114,115,118	6
2	EDO	AAA	406	4/4	0.87	0.20	41,48,54,60	0
2	EDO	CCC	407	4/4	0.87	0.24	56,60,62,71	0
2	EDO	CCC	403	4/4	0.88	0.16	56,57,65,82	0
6	W0D	BBB	404	18/18	0.88	0.18	52,61,70,78	0
6	W0D	DDD	411[A]	18/18	0.89	0.15	45,53,60,60	18
2	EDO	DDD	406	4/4	0.89	0.12	47,54,57,61	0
9	PGE	DDD	410	10/10	0.90	0.17	28,56,79,80	0
2	EDO	AAA	401	4/4	0.91	0.14	49,56,56,65	0
3	NA	DDD	401	1/1	0.91	0.08	59,59,59,59	0
5	GOL	DDD	409	6/6	0.91	0.21	30,38,47,54	0
2	EDO	DDD	405	4/4	0.91	0.14	41,52,53,55	0
3	NA	CCC	410	1/1	0.92	0.08	64,64,64,64	0
2	EDO	DDD	404	4/4	0.93	0.12	36,38,50,55	0

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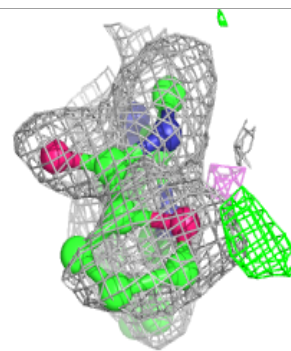
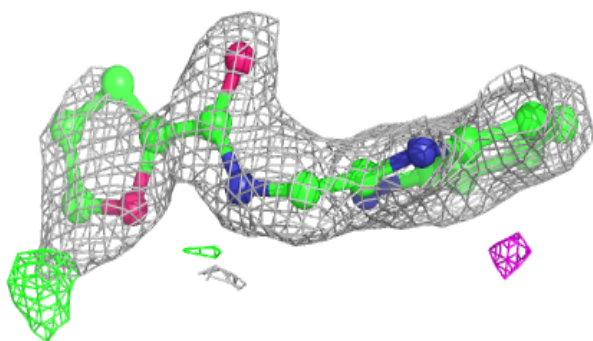
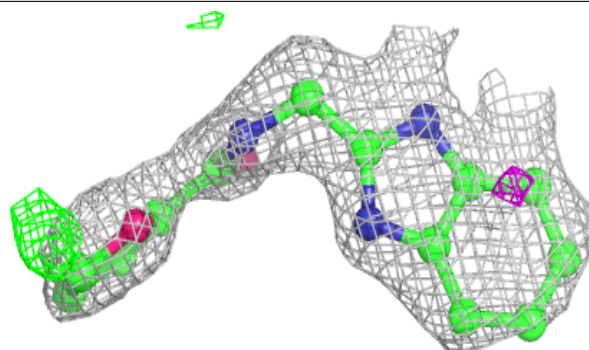
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	DDD	407	4/4	0.93	0.13	51,56,64,65	0
2	EDO	AAA	405[A]	4/4	0.94	0.20	34,51,52,52	4
5	GOL	AAA	412[A]	6/6	0.94	0.20	23,29,32,34	6
7	MG	DDD	413	1/1	0.94	0.20	54,54,54,54	0
2	EDO	AAA	405[B]	4/4	0.94	0.20	45,50,50,53	4
2	EDO	AAA	415	4/4	0.94	0.15	31,32,40,44	0
2	EDO	AAA	407[A]	4/4	0.95	0.22	44,48,50,57	4
2	EDO	BBB	401	4/4	0.95	0.14	58,60,63,65	0
3	NA	DDD	402	1/1	0.95	0.14	51,51,51,51	0
3	NA	AAA	416[A]	1/1	0.98	0.16	87,87,87,87	1
3	NA	AAA	416[B]	1/1	0.98	0.16	44,44,44,44	1
3	NA	AAA	404	1/1	0.98	0.07	28,28,28,28	0
3	NA	AAA	411	1/1	0.98	0.07	31,31,31,31	0
8	CL	CCC	412	1/1	0.99	0.06	41,41,41,41	0
3	NA	BBB	403	1/1	0.99	0.04	30,30,30,30	0
4	CA	BBB	402	1/1	0.99	0.05	32,32,32,32	0
4	CA	DDD	403	1/1	1.00	0.06	23,23,23,23	0
4	CA	AAA	403	1/1	1.00	0.09	19,19,19,19	0
4	CA	CCC	402[A]	1/1	1.00	0.06	22,22,22,22	1
4	CA	CCC	402[B]	1/1	1.00	0.06	21,21,21,21	1

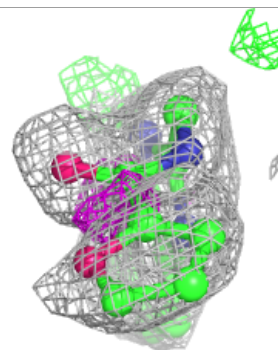
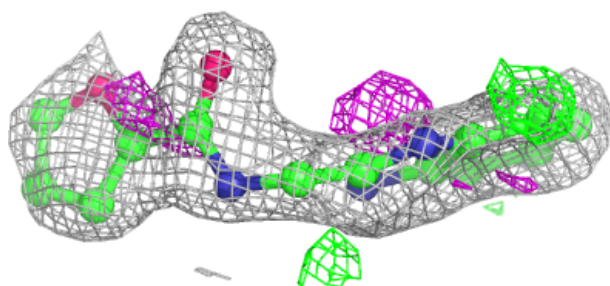
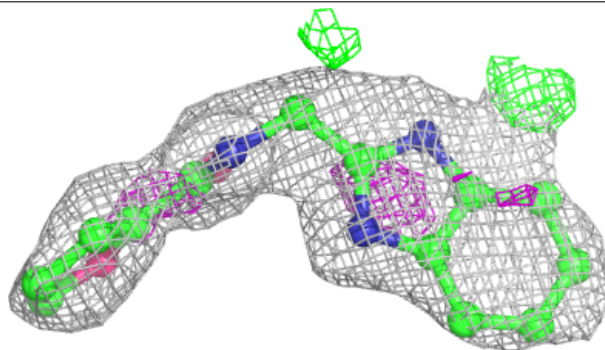
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around W0D DDD 412 (A):**

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

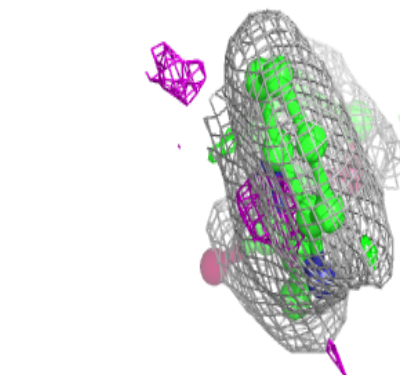
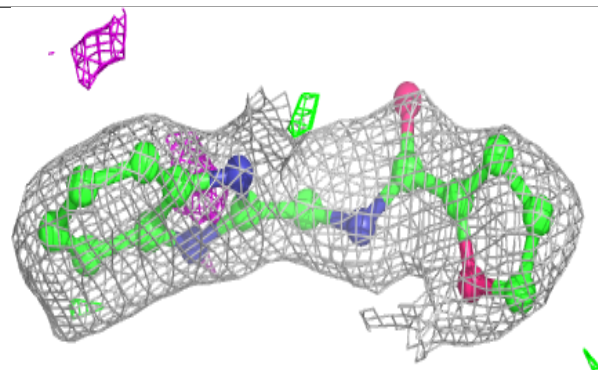
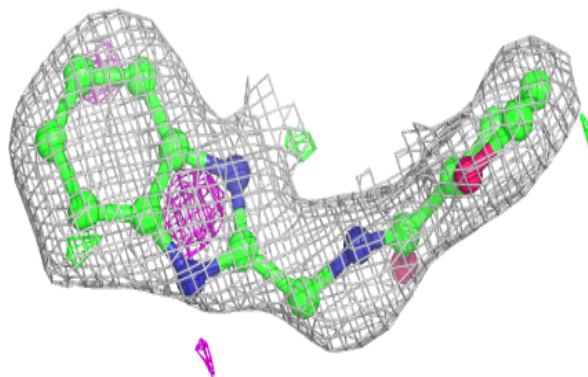
**Electron density around W0D BBB 405:**

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

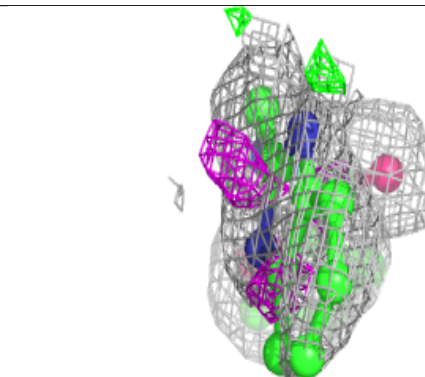
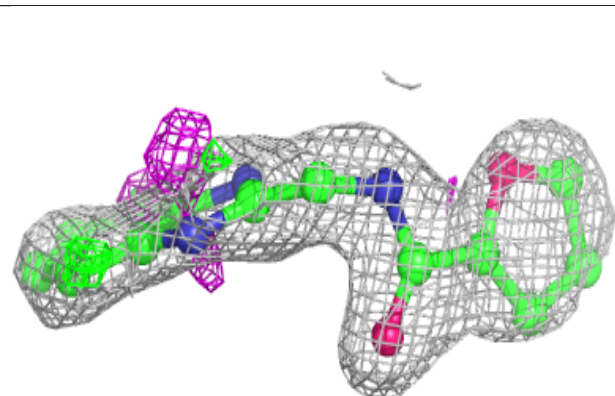
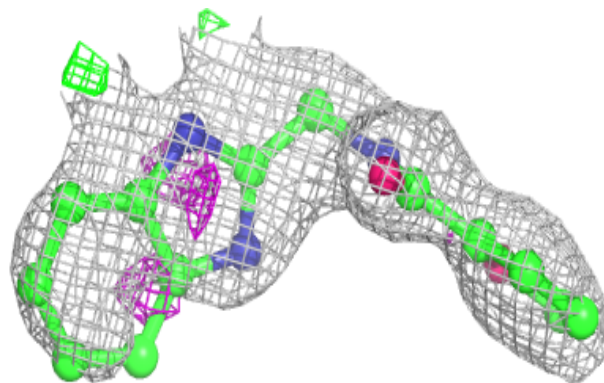


**Electron density around W0D AAA 413:**

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

**Electron density around W0D AAA 414:**

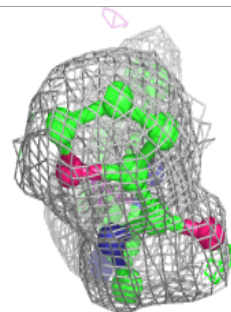
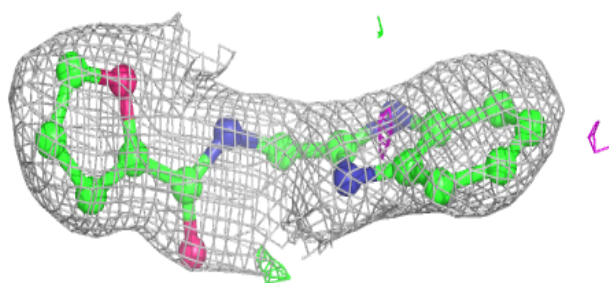
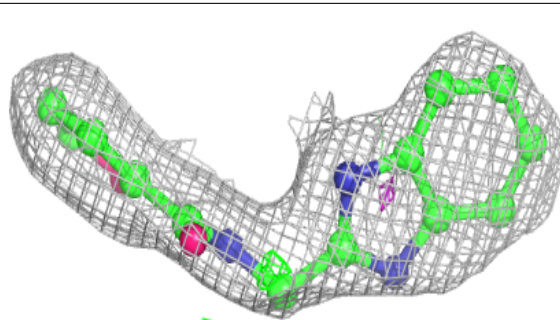
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



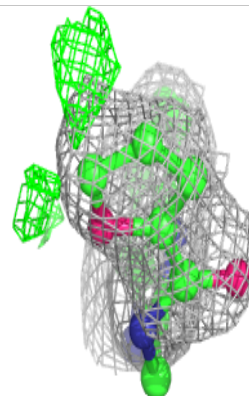
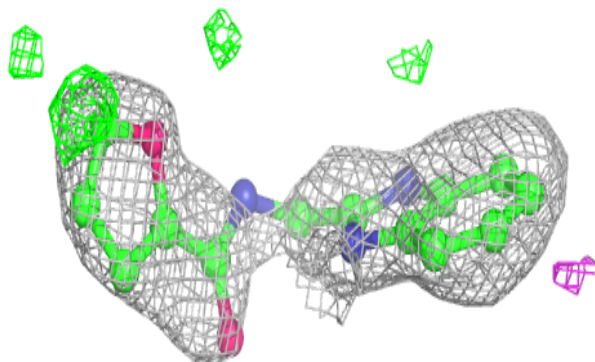
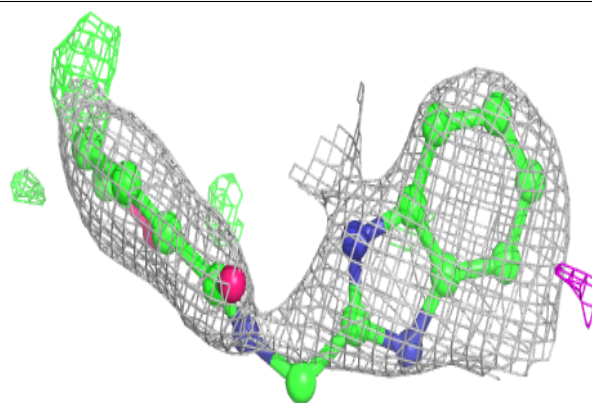


**Electron density around W0D BBB 404:**

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

**Electron density around W0D DDD 411 (A):**

$2mF_o-DF_c$  (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.