



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 21, 2020 – 12:10 PM JST

PDB ID : 7CF6  
Title : Crystal structure of Beta-aspartyl dipeptidase from thermophilic keratin degrading *Fervidobacterium islandicum* AW-1 in complex with beta-Asp-Leu dipeptide  
Authors : Dhanasingh, I.; La, J.W.; Lee, D.W.; Lee, S.H.  
Deposited on : 2020-06-24  
Resolution : 2.75 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

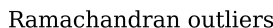
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.16  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.16

**i**

## X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.



R <sub>free</sub>
Clashscore
Ramachandran outliers
Sidechain outliers
BSBZ outliers

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.

1	A	391	<div> <div></div> <div>81%</div> <div>16%</div> <div>3%</div> <div>2%</div> </div>
1	B	391	<div> <div></div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
1	C	391	<div> <div></div> <div>73%</div> <div>21%</div> <div>5%</div> </div>
1	D	391	<div> <div></div> <div>69%</div> <div>21%</div> <div>5%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11800 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 Isoaspartyl dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	372	Total	C	N	O	S	0	0	0
			2865	1833	479	544	9			
1	A	384	Total	C	N	O	S	0	0	0
			2954	1886	496	562	10			
1	C	371	Total	C	N	O	S	0	0	0
			2857	1827	478	543	9			
1	D	370	Total	C	N	O	S	0	0	0
			2845	1819	477	540	9			

There are 16 discrepancies between the modelled and reference sequences:

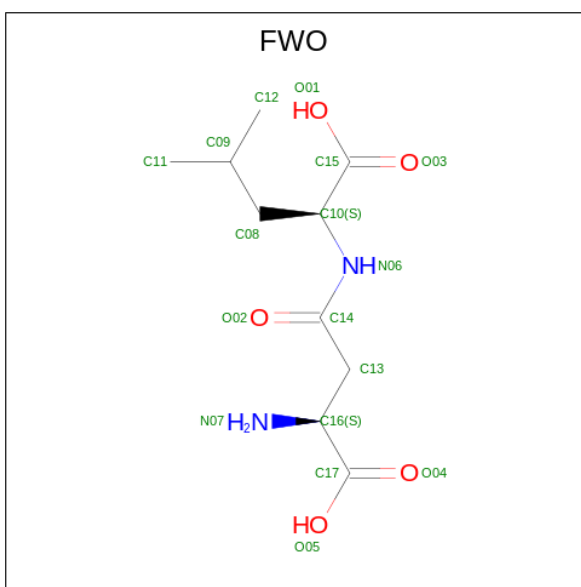
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	MET	-	initiating methionine	UNP A0A1B0VPV0
B	-2	ARG	-	expression tag	UNP A0A1B0VPV0
B	-1	GLY	-	expression tag	UNP A0A1B0VPV0
B	0	SER	-	expression tag	UNP A0A1B0VPV0
A	-3	MET	-	initiating methionine	UNP A0A1B0VPV0
A	-2	ARG	-	expression tag	UNP A0A1B0VPV0
A	-1	GLY	-	expression tag	UNP A0A1B0VPV0
A	0	SER	-	expression tag	UNP A0A1B0VPV0
C	-3	MET	-	initiating methionine	UNP A0A1B0VPV0
C	-2	ARG	-	expression tag	UNP A0A1B0VPV0
C	-1	GLY	-	expression tag	UNP A0A1B0VPV0
C	0	SER	-	expression tag	UNP A0A1B0VPV0
D	-3	MET	-	initiating methionine	UNP A0A1B0VPV0
D	-2	ARG	-	expression tag	UNP A0A1B0VPV0
D	-1	GLY	-	expression tag	UNP A0A1B0VPV0
D	0	SER	-	expression tag	UNP A0A1B0VPV0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 3 is (2S)-2-[[[(3S)-3-azanyl-4-oxidanyl-4-oxidanylidene-butanoyl]amino]-4-methyl-pentanoic acid (three-letter code: FWO) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>2</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			17	10	2	5		
3	A	1	Total	C	N	O	0	0
			17	10	2	5		
3	C	1	Total	C	N	O	0	0
			17	10	2	5		
3	D	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Zn	0	0
			2	2		
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

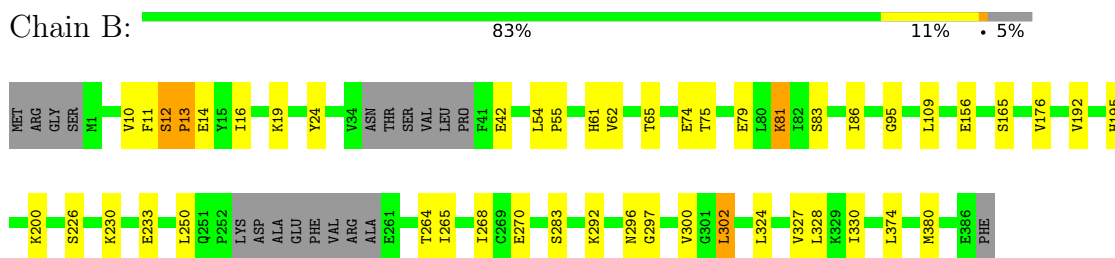
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	34	Total	O	0	0
			34	34		
6	A	27	Total	O	0	0
			27	27		
6	C	41	Total	O	0	0
			41	41		
6	D	21	Total	O	0	0
			21	21		

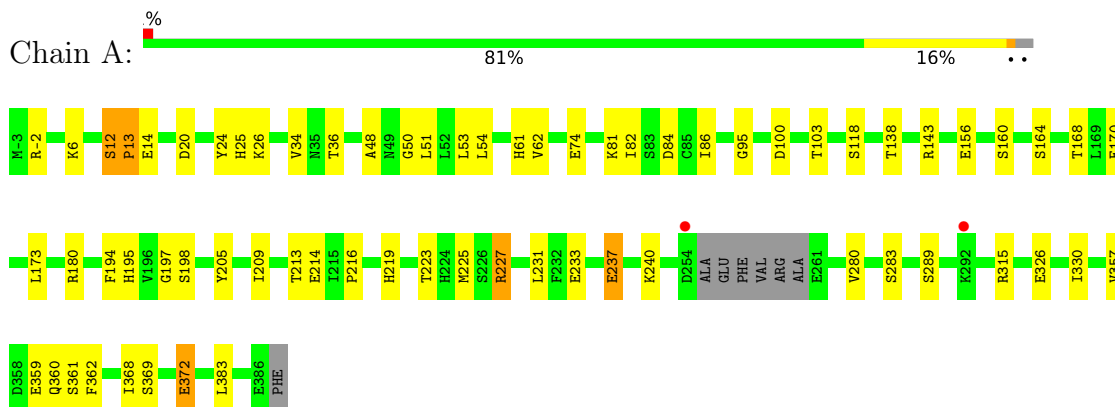
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

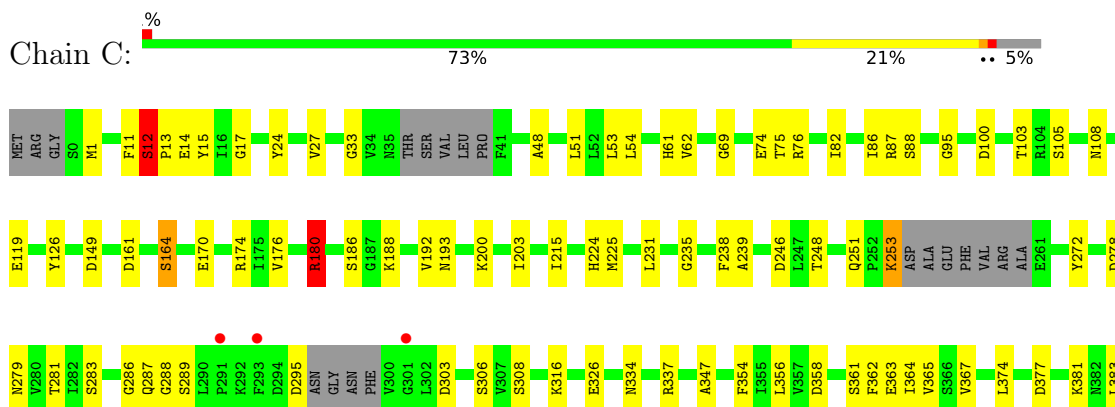
- Molecule 1: Isoaspartyl dipeptidase

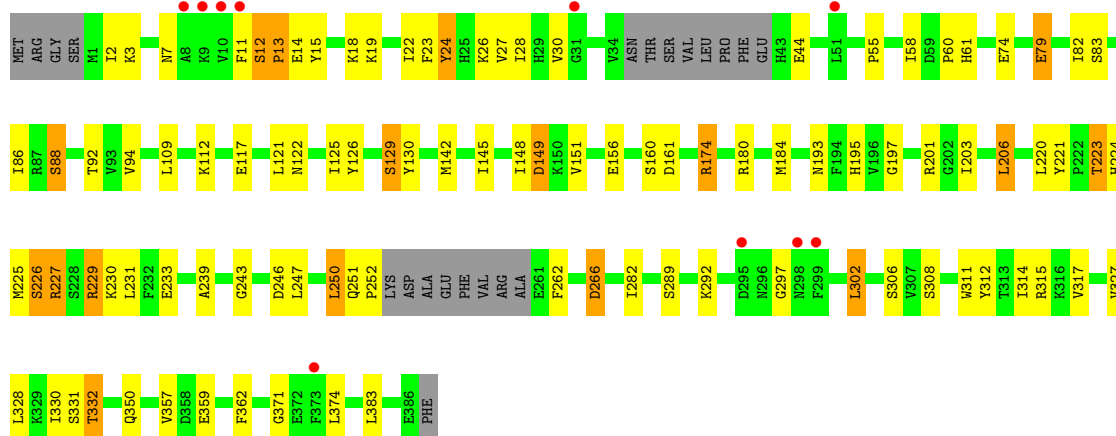


- Molecule 1: Isoaspartyl dipeptidase



- Molecule 1: Isoaspartyl dipeptidase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.61Å 150.43Å 152.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.66 – 2.75 47.62 – 2.75	Depositor EDS
% Data completeness (in resolution range)	77.5 (47.66-2.75) 77.5 (47.62-2.75)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.196 , 0.278 0.197 , 0.275	Depositor DCC
$R_{free}$ test set	1994 reflections (5.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: FWO, GOL, ZN, PEG

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	0.75	0/3005	0.86	0/4055
1	B	0.76	0/2914	0.85	0/3931
1	C	0.77	0/2904	0.88	1/3915 (0.0%)
1	D	0.77	0/2893	0.90	0/3903
All	All	0.76	0/11716	0.87	1/15804 (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	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	ARG	NE-CZ-NH1	6.19	123.40	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	SER	Peptide
1	B	12	SER	Peptide

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Mol	Chain	Res	Type	Group
1	C	12	SER	Peptide

## 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	2954	0	3005	40	0
1	B	2865	0	2912	26	0
1	C	2857	0	2912	46	0
1	D	2845	0	2896	62	0
2	A	18	0	24	0	0
2	B	24	0	32	0	0
2	C	18	0	24	0	0
2	D	6	0	8	0	0
3	A	17	0	0	1	0
3	B	17	0	0	0	0
3	C	17	0	0	0	0
3	D	17	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	7	0	10	0	0
5	C	7	0	10	0	0
6	A	27	0	0	0	0
6	B	34	0	0	1	0
6	C	41	0	0	2	0
6	D	21	0	0	0	0
All	All	11800	0	11833	172	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 7.

The worst 5 of 172 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:12:SER:O	1:A:14:GLU:N	1.96	0.97
1:D:282:ILE:HD11	1:D:331:SER:OG	1.70	0.90
1:D:328:LEU:O	1:D:332:THR:OG1	1.91	0.86
1:D:180:ARG:NH1	1:D:184:MET:SD	2.51	0.84
1:D:55:PRO:HG2	1:D:332:THR:HG21	1.57	0.84

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/391 (97%)	359 (94%)	20 (5%)	1 (0%)	41	60
1	B	366/391 (94%)	342 (93%)	20 (6%)	4 (1%)	14	25
1	C	363/391 (93%)	336 (93%)	22 (6%)	5 (1%)	11	19
1	D	364/391 (93%)	329 (90%)	30 (8%)	5 (1%)	11	19
All	All	1473/1564 (94%)	1366 (93%)	92 (6%)	15 (1%)	15	27

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	PRO
1	B	42	GLU
1	B	296	ASN
1	A	13	PRO
1	C	13	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	326/331 (98%)	312 (96%)	14 (4%)	29	48
1	B	315/331 (95%)	308 (98%)	7 (2%)	52	70
1	C	315/331 (95%)	296 (94%)	19 (6%)	19	33
1	D	313/331 (95%)	288 (92%)	25 (8%)	12	21
All	All	1269/1324 (96%)	1204 (95%)	65 (5%)	24	41

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	180	ARG
1	C	306	SER
1	D	266	ASP
1	C	200	LYS
1	C	253	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	C	334	ASN
1	D	193	ASN
1	D	382	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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 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	GOL	C	403	-	5,5,5	0.13	0	5,5,5	0.32	0
3	FWO	B	405	4	10,16,16	2.64	3 (30%)	12,21,21	1.34	2 (16%)
3	FWO	A	405	-	10,16,16	2.06	1 (10%)	12,21,21	0.84	0
3	FWO	D	402	4	10,16,16	2.61	2 (20%)	12,21,21	2.32	3 (25%)
2	GOL	B	402	-	5,5,5	0.13	0	5,5,5	0.38	0
2	GOL	A	404	-	5,5,5	0.16	0	5,5,5	0.50	0
2	GOL	C	404	-	5,5,5	0.17	0	5,5,5	0.42	0
5	PEG	A	402	-	6,6,6	0.61	0	5,5,5	0.77	0
5	PEG	C	402	-	6,6,6	0.68	0	5,5,5	0.73	0
2	GOL	A	401	-	5,5,5	0.32	0	5,5,5	0.68	0
2	GOL	D	401	-	5,5,5	0.13	0	5,5,5	0.35	0
2	GOL	C	401	-	5,5,5	0.15	0	5,5,5	0.39	0
3	FWO	C	405	-	10,16,16	2.62	4 (40%)	12,21,21	1.75	3 (25%)
2	GOL	B	401	-	5,5,5	0.16	0	5,5,5	0.40	0
2	GOL	A	403	-	5,5,5	0.16	0	5,5,5	0.35	0
2	GOL	B	403	-	5,5,5	0.21	0	5,5,5	0.42	0
2	GOL	B	404	-	5,5,5	0.08	0	5,5,5	0.25	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	GOL	C	403	-	-	2/4/4/4	-
3	FWO	B	405	4	-	2/12/20/20	-
3	FWO	A	405	-	-	6/12/20/20	-
3	FWO	D	402	4	-	4/12/20/20	-
2	GOL	B	402	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	404	-	-	1/4/4/4	-
2	GOL	C	404	-	-	2/4/4/4	-
5	PEG	A	402	-	-	2/4/4/4	-
5	PEG	C	402	-	-	4/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	D	401	-	-	2/4/4/4	-
2	GOL	C	401	-	-	4/4/4/4	-
3	FWO	C	405	-	-	2/12/20/20	-
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	A	403	-	-	3/4/4/4	-
2	GOL	B	403	-	-	0/4/4/4	-
2	GOL	B	404	-	-	4/4/4/4	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	FWO	C14-N06	7.16	1.49	1.34
3	B	405	FWO	C14-N06	6.68	1.48	1.34
3	C	405	FWO	C14-N06	6.65	1.48	1.34
3	A	405	FWO	C14-N06	6.10	1.47	1.34
3	B	405	FWO	C08-C10	3.74	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	FWO	C13-C14-N06	6.19	124.43	116.33
3	C	405	FWO	C13-C14-N06	4.60	122.35	116.33
3	D	402	FWO	O02-C14-C13	-3.44	116.45	121.50
3	B	405	FWO	C10-N06-C14	2.82	127.82	123.33
3	B	405	FWO	C08-C10-N06	2.63	114.49	109.80

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	403	GOL	C1-C2-C3-O3
3	B	405	FWO	C09-C08-C10-C15
3	D	402	FWO	C14-C13-C16-N07
2	C	401	GOL	O1-C1-C2-C3

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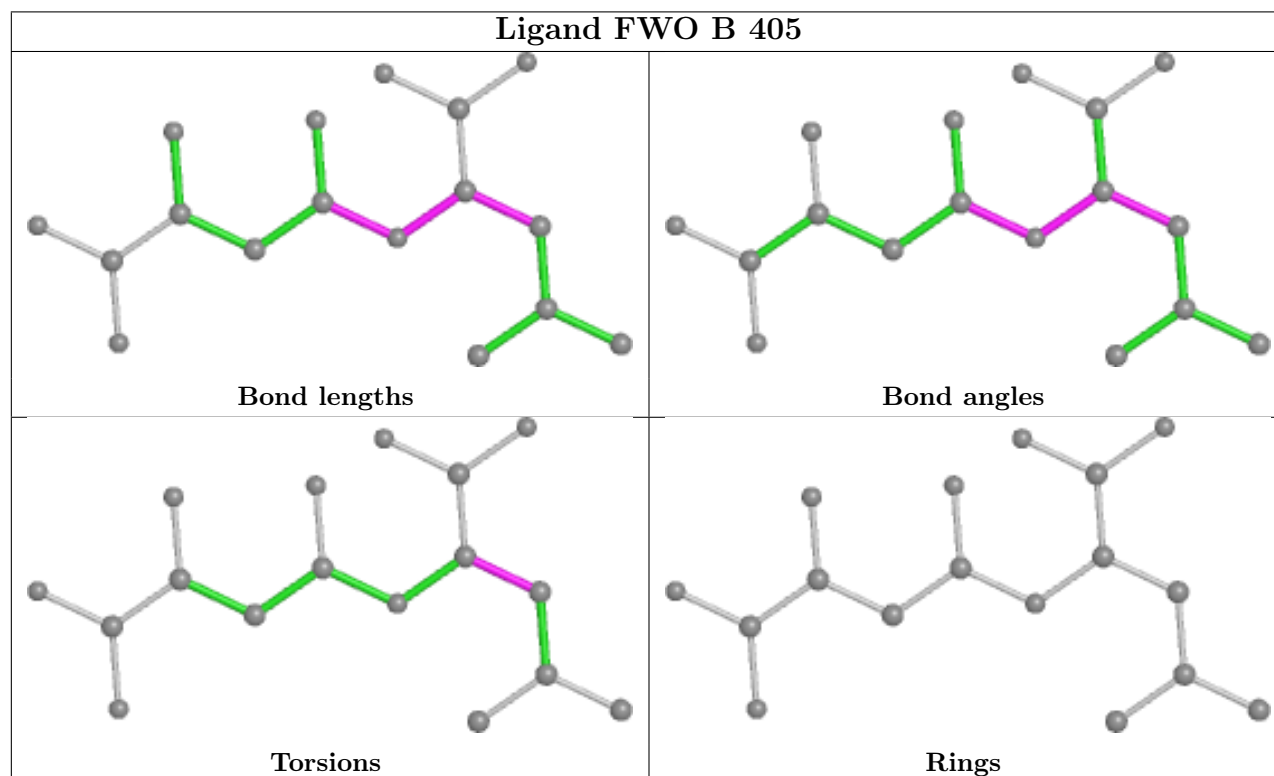
Mol	Chain	Res	Type	Atoms
3	C	405	FWO	C09-C08-C10-C15

There are no ring outliers.

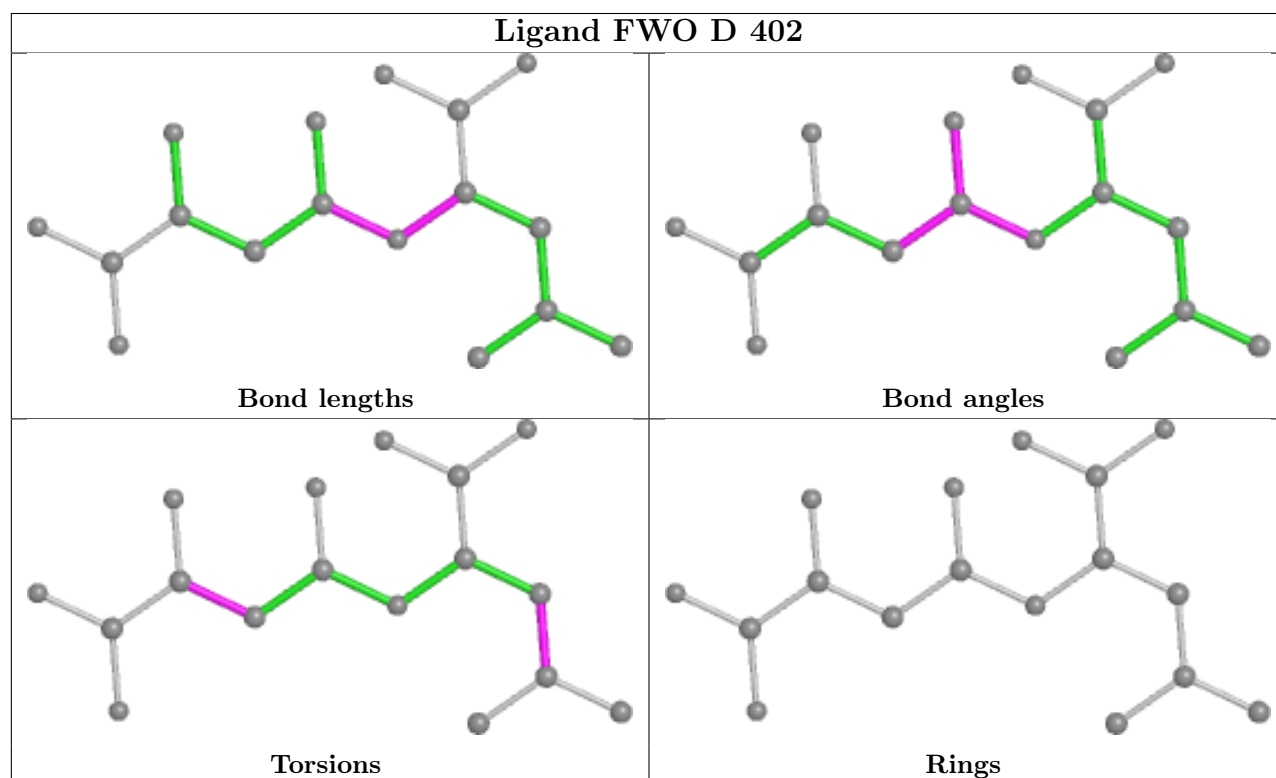
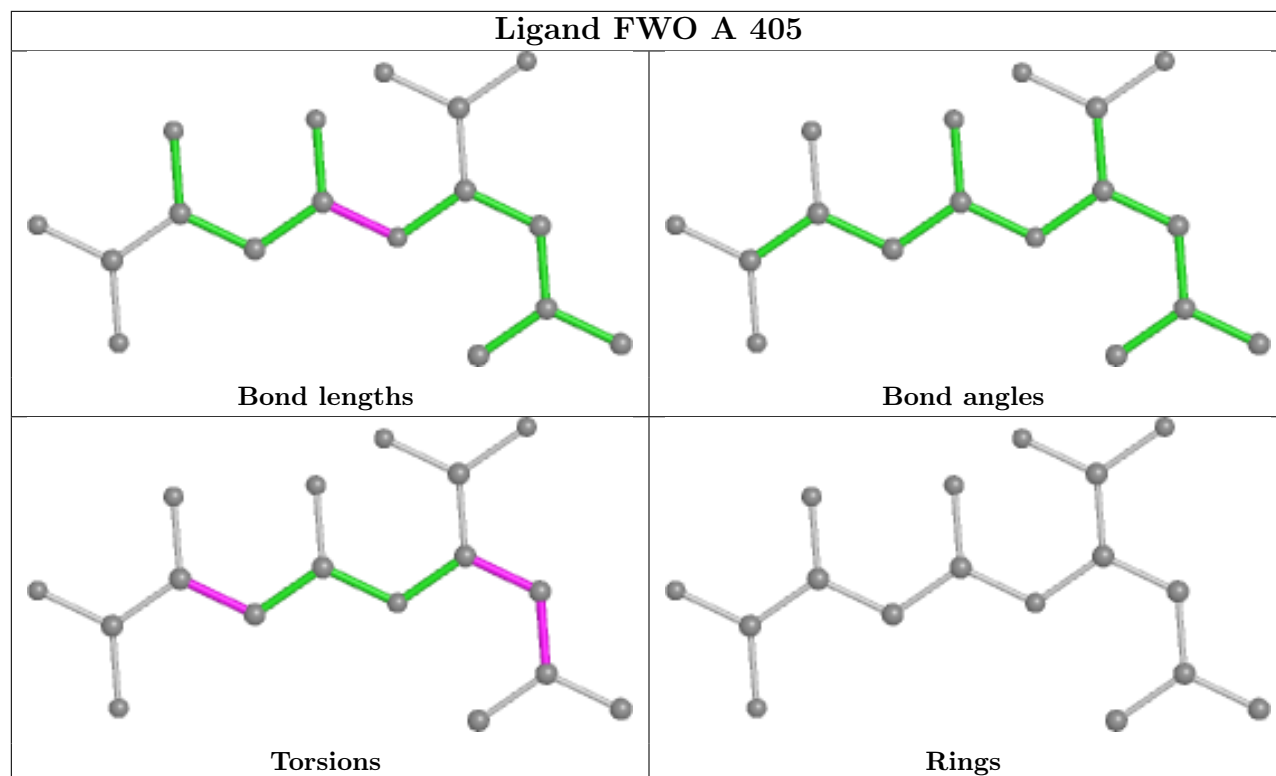
2 monomers are involved in 2 short contacts:

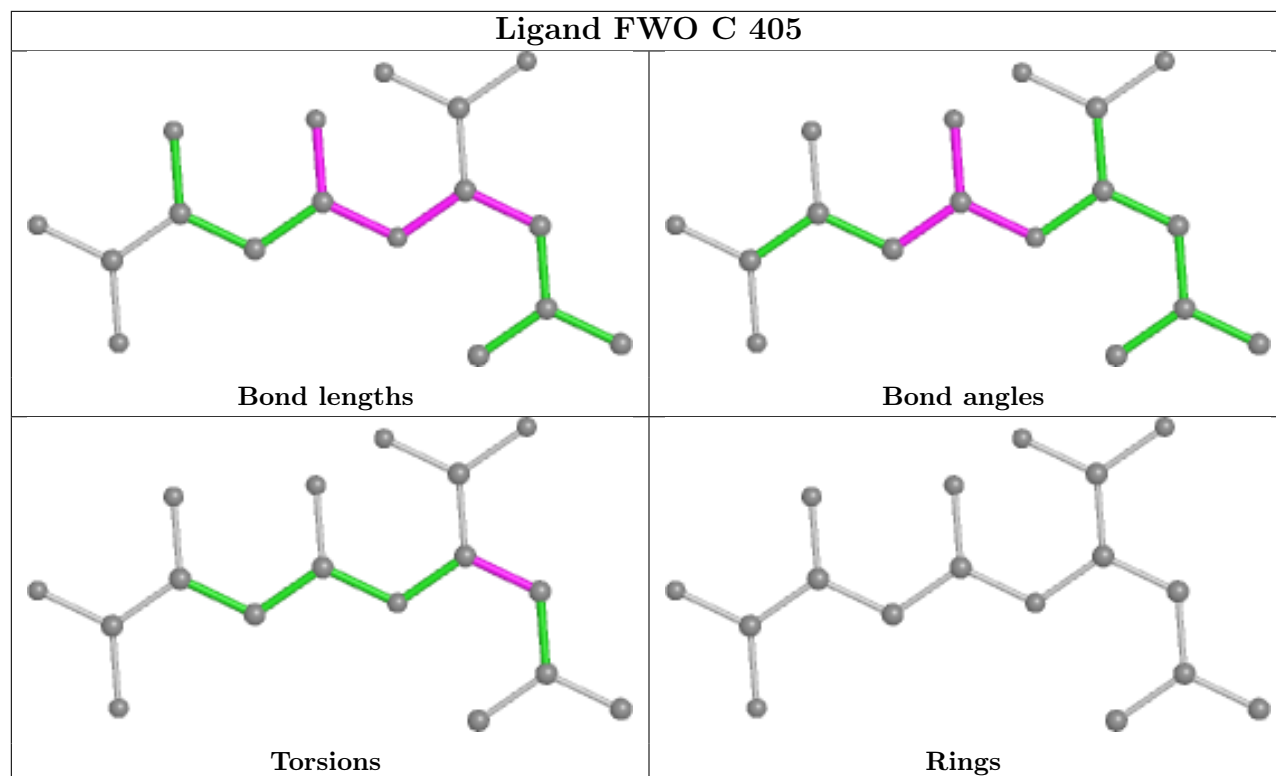
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	FWO	1	0
3	D	402	FWO	1	0

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	A	384/391 (98%)	-0.48	2 (0%) 91 94	26, 43, 76, 102	0
1	B	372/391 (95%)	-0.60	0 100 100	25, 39, 67, 91	0
1	C	371/391 (94%)	-0.38	3 (0%) 86 90	27, 48, 79, 128	0
1	D	370/391 (94%)	-0.08	10 (2%) 54 63	34, 61, 89, 119	0
All	All	1497/1564 (95%)	-0.39	15 (1%) 82 87	25, 46, 81, 128	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	301	GLY	4.1
1	D	299	PHE	3.3
1	C	293	PHE	3.3
1	D	31	GLY	3.3
1	D	10	VAL	3.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

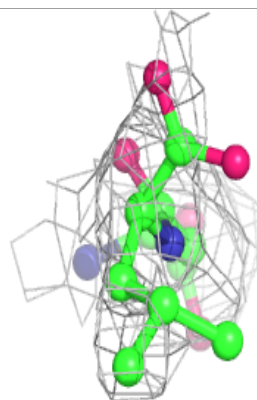
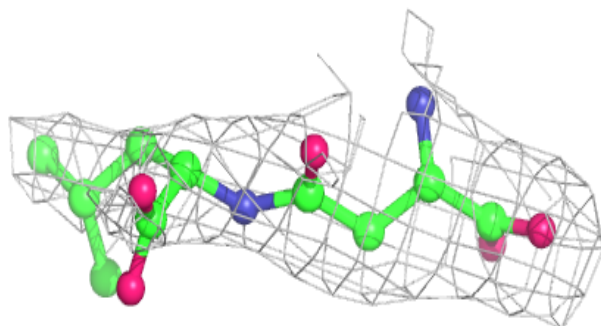
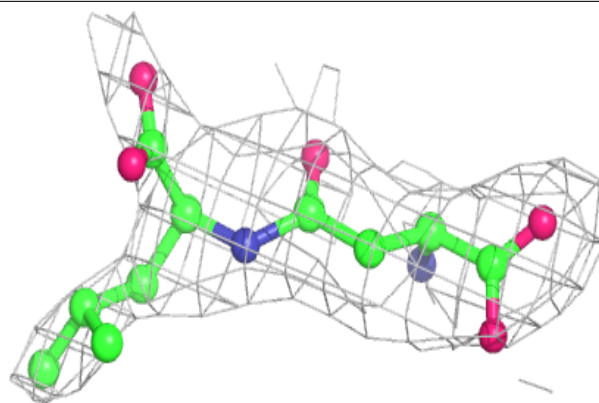
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	D	401	6/6	0.68	0.30	66,79,82,83	0
2	GOL	B	402	6/6	0.74	0.36	63,73,78,86	0
2	GOL	B	404	6/6	0.74	0.36	85,91,96,107	0
2	GOL	B	403	6/6	0.75	0.22	60,79,80,83	0
2	GOL	B	401	6/6	0.80	0.38	74,77,79,82	0
2	GOL	C	404	6/6	0.82	0.21	63,68,73,76	0
2	GOL	C	401	6/6	0.83	0.27	67,74,76,76	0
3	FWO	C	405	17/17	0.84	0.24	66,82,101,112	0
3	FWO	D	402	17/17	0.86	0.22	70,88,113,118	0
4	ZN	B	407	1/1	0.86	0.06	105,105,105,105	0
2	GOL	A	403	6/6	0.87	0.22	60,72,73,75	0
5	PEG	C	402	7/7	0.88	0.22	47,55,66,67	0
3	FWO	B	405	17/17	0.90	0.18	38,66,86,93	0
3	FWO	A	405	17/17	0.92	0.22	49,85,116,119	0
2	GOL	A	404	6/6	0.92	0.26	56,61,64,70	0
2	GOL	C	403	6/6	0.92	0.15	58,61,65,70	0
5	PEG	A	402	7/7	0.93	0.18	44,45,47,48	0
2	GOL	A	401	6/6	0.93	0.25	47,55,56,60	0
4	ZN	D	403	1/1	0.94	0.10	123,123,123,123	0
4	ZN	A	407	1/1	0.95	0.07	74,74,74,74	0
4	ZN	D	404	1/1	0.97	0.10	66,66,66,66	0
4	ZN	C	406	1/1	0.98	0.05	88,88,88,88	0
4	ZN	B	406	1/1	0.99	0.08	49,49,49,49	0
4	ZN	A	406	1/1	0.99	0.11	48,48,48,48	0
4	ZN	C	407	1/1	1.00	0.07	52,52,52,52	0

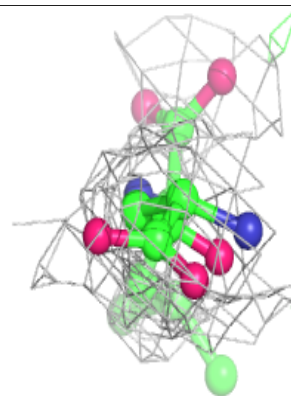
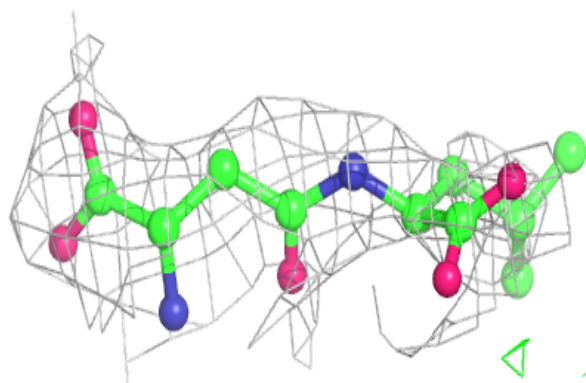
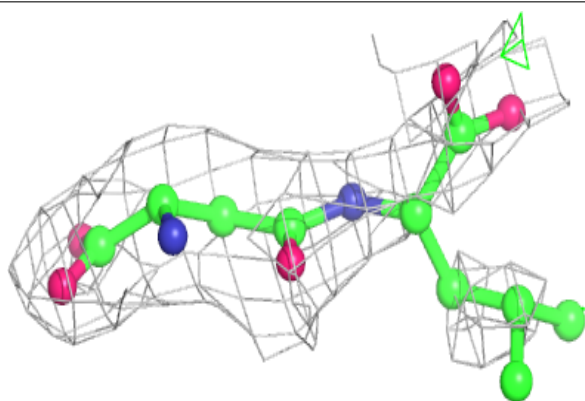
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FWO C 405:**

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

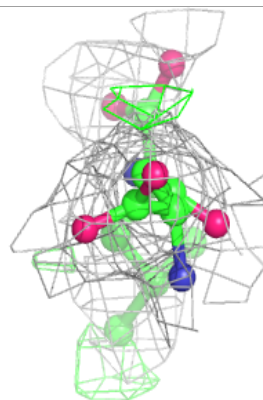
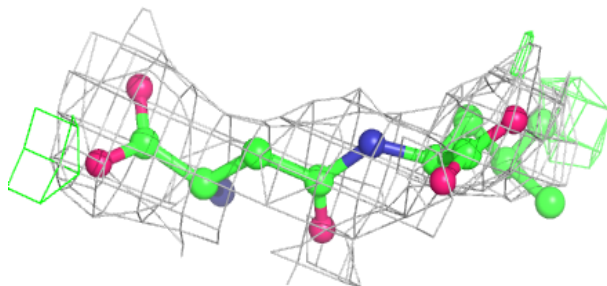
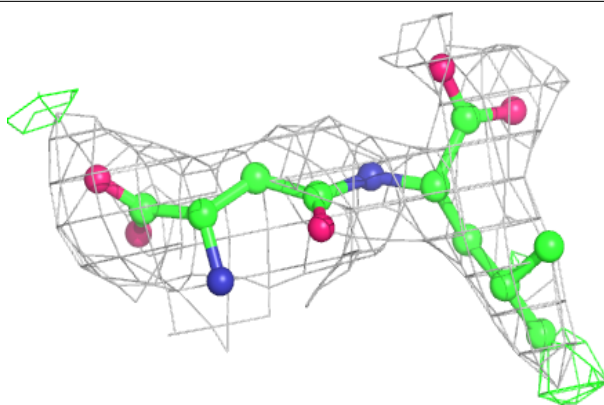
**Electron density around FWO D 402:**

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

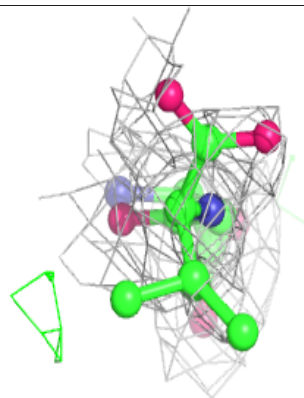
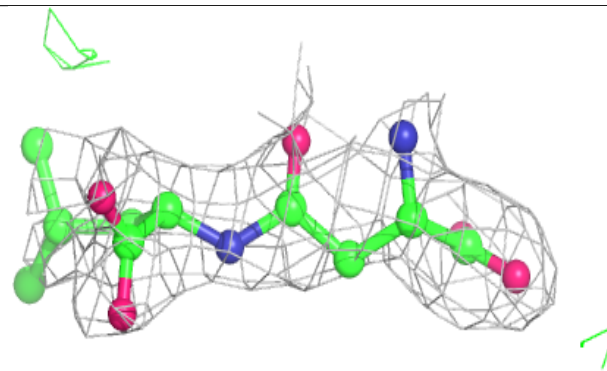
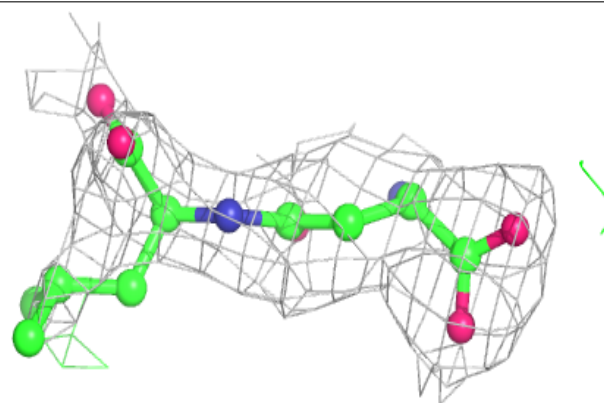


**Electron density around FWO B 405:**

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

**Electron density around FWO A 405:**

$2mF_o-DF_c$  (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.