



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:33 AM UTC

PDB ID : 9OK4 / pdb\_00009ok4  
Title : GID4 in complex with CLEO4-88 and ACAA1  
Authors : Chana, C.K.; Sicheri, F.  
Deposited on : 2025-05-09  
Resolution : 2.28 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

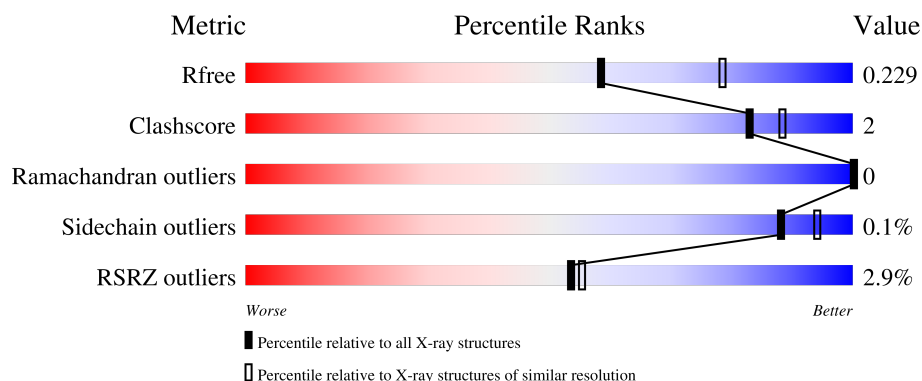
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	418	<div> <div>4%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div>
1	B	418	<div> <div>3%</div> <div>85%</div> <div>6%</div> <div>10%</div> </div>
2	C	167	<div> <div>%</div> <div>97%</div> <div>.</div> </div>
2	D	167	<div> <div>3%</div> <div>95%</div> <div>5%</div> <div>.</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8102 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 3-ketoacyl-CoA thiolase, peroxisomal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2595	1621	456	500	18			
1	B	377	Total	C	N	O	S	0	0	0
			2605	1637	450	501	17			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP P09110
A	8	HIS	-	expression tag	UNP P09110
A	9	HIS	-	expression tag	UNP P09110
A	10	HIS	-	expression tag	UNP P09110
A	11	HIS	-	expression tag	UNP P09110
A	12	HIS	-	expression tag	UNP P09110
A	13	HIS	-	expression tag	UNP P09110
A	14	SER	-	expression tag	UNP P09110
A	15	SER	-	expression tag	UNP P09110
A	16	GLY	-	expression tag	UNP P09110
A	17	VAL	-	expression tag	UNP P09110
A	18	ASP	-	expression tag	UNP P09110
A	19	LEU	-	expression tag	UNP P09110
A	20	GLY	-	expression tag	UNP P09110
A	21	THR	-	expression tag	UNP P09110
A	22	GLU	-	expression tag	UNP P09110
A	23	ASN	-	expression tag	UNP P09110
A	24	LEU	-	expression tag	UNP P09110
A	25	TYR	-	expression tag	UNP P09110
A	26	PHE	-	expression tag	UNP P09110
A	27	GLN	-	expression tag	UNP P09110
A	28	SER	-	expression tag	UNP P09110
A	29	MET	-	expression tag	UNP P09110
B	7	MET	-	initiating methionine	UNP P09110
B	8	HIS	-	expression tag	UNP P09110

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	HIS	-	expression tag	UNP P09110
B	10	HIS	-	expression tag	UNP P09110
B	11	HIS	-	expression tag	UNP P09110
B	12	HIS	-	expression tag	UNP P09110
B	13	HIS	-	expression tag	UNP P09110
B	14	SER	-	expression tag	UNP P09110
B	15	SER	-	expression tag	UNP P09110
B	16	GLY	-	expression tag	UNP P09110
B	17	VAL	-	expression tag	UNP P09110
B	18	ASP	-	expression tag	UNP P09110
B	19	LEU	-	expression tag	UNP P09110
B	20	GLY	-	expression tag	UNP P09110
B	21	THR	-	expression tag	UNP P09110
B	22	GLU	-	expression tag	UNP P09110
B	23	ASN	-	expression tag	UNP P09110
B	24	LEU	-	expression tag	UNP P09110
B	25	TYR	-	expression tag	UNP P09110
B	26	PHE	-	expression tag	UNP P09110
B	27	GLN	-	expression tag	UNP P09110
B	28	SER	-	expression tag	UNP P09110
B	29	MET	-	expression tag	UNP P09110

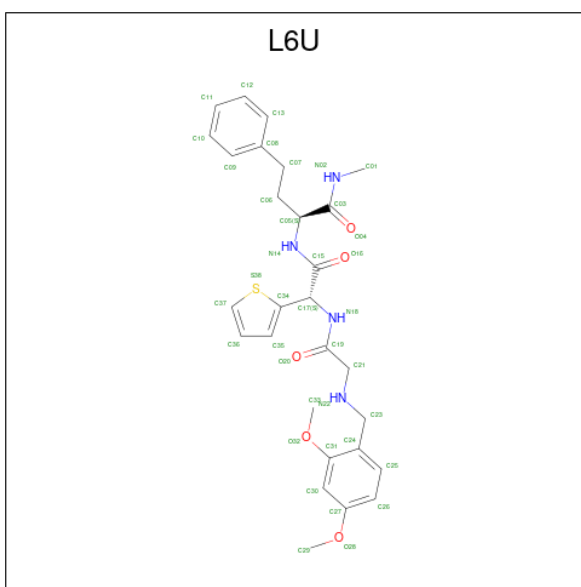
- Molecule 2 is a protein called Glucose-induced degradation protein 4 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	167	Total	C	N	O	S	0	0	0
			1333	870	214	246	3			
2	D	166	Total	C	N	O	S	0	0	0
			1302	853	205	241	3			

There are 2 discrepancies between the modelled and reference sequences:

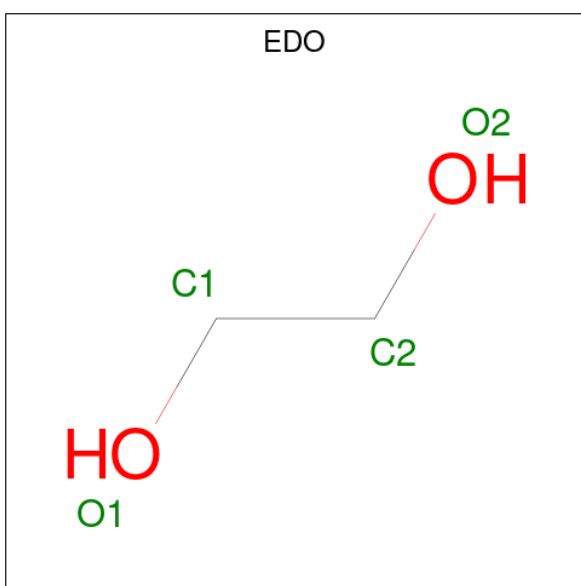
Chain	Residue	Modelled	Actual	Comment	Reference
C	123	GLY	-	expression tag	UNP Q8IVV7
D	123	GLY	-	expression tag	UNP Q8IVV7

- Molecule 3 is (2S)-2-[(2S)-2-({N-[(2,4-dimethoxyphenyl)methyl]glycyl}amino)-2-(thiophen-2-yl)acetyl]amino}-N-methyl-4-phenylbutanamide (CCD ID: L6U) (formula: C<sub>28</sub>H<sub>34</sub>N<sub>4</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total 38	C 28	N 4	O 5	S 1	0	0
3	D	1	Total 38	C 28	N 4	O 5	S 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



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

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

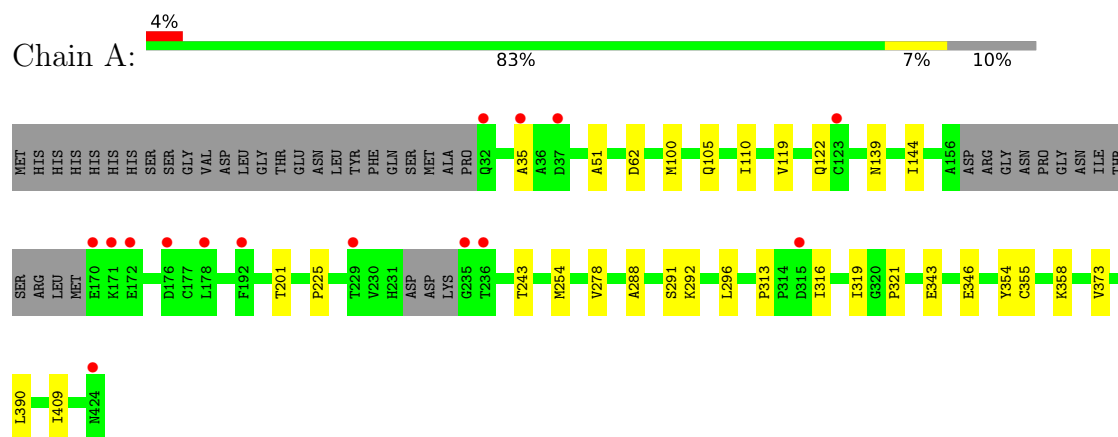
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total	O	0	0
			37	37		
5	C	49	Total	O	0	0
			49	49		
5	D	23	Total	O	0	0
			23	23		
5	B	66	Total	O	0	0
			66	66		

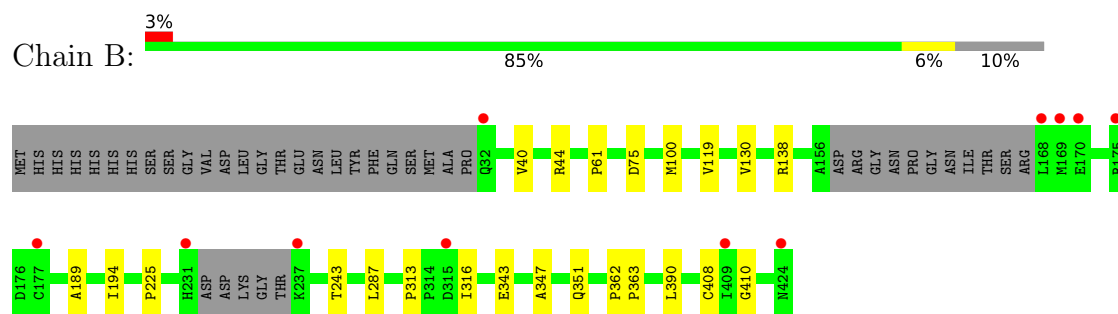
### 3 Residue-property plots [i](#)

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.

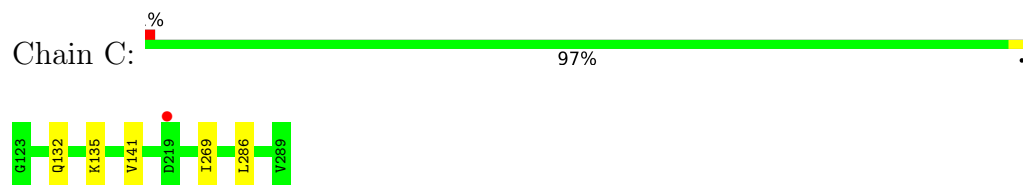
- Molecule 1: 3-ketoacyl-CoA thiolase, peroxisomal



- Molecule 1: 3-ketoacyl-CoA thiolase, peroxisomal



- Molecule 2: Glucose-induced degradation protein 4 homolog



- Molecule 2: Glucose-induced degradation protein 4 homolog







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.94Å 92.99Å 202.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 2.28 49.43 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.43-2.28) 99.9 (49.43-2.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.190 , 0.230 0.190 , 0.229	Depositor DCC
$R_{free}$ test set	2673 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.8	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: EDO, L6U

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	0.15	0/2629	0.32	0/3583
1	B	0.17	0/2639	0.33	0/3594
2	C	0.17	0/1377	0.33	0/1867
2	D	0.15	0/1345	0.33	0/1825
All	All	0.16	0/7990	0.33	0/10869

There are no bond length outliers.

There are no bond angle outliers.

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	2595	0	2499	17	0
1	B	2605	0	2536	14	0
2	C	1333	0	1186	3	0
2	D	1302	0	1137	4	0
3	C	38	0	0	1	0
3	D	38	0	0	0	0
4	B	4	0	6	0	0
4	C	12	0	18	0	0
5	A	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	66	0	0	0	0
5	C	49	0	0	0	0
5	D	23	0	0	0	0
All	All	8102	0	7382	36	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 2.

All (36) 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:119:VAL:HG12	1:B:119:VAL:HG12	1.68	0.74
2:D:196:ASP:OD1	2:D:199:ARG:NH1	2.31	0.64
1:B:313:PRO:HG2	1:B:316:ILE:HD12	1.84	0.59
1:B:189:ALA:HB1	1:B:194:ILE:HB	1.85	0.59
2:C:135:LYS:HD2	3:C:301:L6U:C08	2.34	0.57
1:B:225:PRO:HB3	1:B:243:THR:HG22	1.86	0.57
1:A:201:THR:HA	1:A:254:MET:HE1	1.87	0.56
1:A:139:ASN:OD1	1:B:138:ARG:NH1	2.37	0.53
1:A:225:PRO:HB3	1:A:243:THR:HG22	1.91	0.51
1:A:62:ASP:HB3	1:A:100:MET:HG2	1.93	0.51
1:A:292:LYS:HE3	1:A:296:LEU:HD11	1.94	0.50
2:C:269:ILE:HB	2:C:286:LEU:HB2	1.94	0.50
1:B:130:VAL:HG13	1:B:287:LEU:HD11	1.94	0.49
1:A:122:GLN:HB2	1:A:409:ILE:HG23	1.94	0.49
1:A:105:GLN:HG3	1:A:110:ILE:HB	1.94	0.49
1:A:346:GLU:HB3	1:A:373:VAL:HG23	1.95	0.48
1:A:319:ILE:HG22	1:A:321:PRO:HD2	1.95	0.48
1:B:343:GLU:HG3	1:B:390:LEU:HB2	1.96	0.47
1:B:347:ALA:HB3	1:B:351:GLN:NE2	2.31	0.45
1:A:35:ALA:HB1	1:A:291:SER:HB3	1.99	0.45
1:B:408:CYS:HB3	1:B:410:GLY:O	2.17	0.45
1:A:313:PRO:HB2	1:A:316:ILE:HD12	1.99	0.45
1:A:354:TYR:OH	1:A:358:LYS:NZ	2.49	0.44
1:B:40:VAL:HA	1:B:287:LEU:HD23	1.99	0.44
2:D:132:GLN:HG3	2:D:141:VAL:HG21	2.00	0.44
2:D:128:PHE:HB3	2:D:286:LEU:HB3	2.00	0.44
1:A:343:GLU:HG3	1:A:390:LEU:HB2	1.99	0.43
1:B:44:ARG:NH1	1:B:75:ASP:OD2	2.40	0.43
1:A:51:ALA:HB3	1:A:278:VAL:HG23	1.99	0.43
1:A:144:ILE:HG23	1:A:288:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:PRO:HA	1:B:363:PRO:HD3	1.92	0.42
2:C:132:GLN:HG3	2:C:141:VAL:HG21	2.01	0.42
1:A:321:PRO:HB2	1:A:355:CYS:SG	2.60	0.41
1:B:100:MET:HE3	1:B:100:MET:HB3	1.99	0.41
1:B:61:PRO:HG2	1:B:100:MET:HG3	2.01	0.41
2:D:164:LEU:HD12	2:D:164:LEU:HA	1.92	0.40

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	371/418 (89%)	366 (99%)	5 (1%)	0	100	100
1	B	371/418 (89%)	368 (99%)	3 (1%)	0	100	100
2	C	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
2	D	164/167 (98%)	163 (99%)	1 (1%)	0	100	100
All	All	1071/1170 (92%)	1060 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	244/325 (75%)	244 (100%)	0	100	100
1	B	248/325 (76%)	248 (100%)	0	100	100
2	C	128/147 (87%)	128 (100%)	0	100	100
2	D	121/147 (82%)	120 (99%)	1 (1%)	73	84
All	All	741/944 (78%)	740 (100%)	1 (0%)	88	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	147	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 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
4	EDO	C	304	-	3,3,3	0.45	0	2,2,2	0.30	0
4	EDO	C	303	-	3,3,3	0.37	0	2,2,2	0.67	0
4	EDO	C	302	-	3,3,3	0.48	0	2,2,2	0.40	0
3	L6U	D	300	-	39,40,40	2.50	19 (48%)	47,52,52	1.87	11 (23%)
3	L6U	C	301	-	39,40,40	2.42	17 (43%)	47,52,52	1.81	11 (23%)
4	EDO	B	501	-	3,3,3	0.51	0	2,2,2	0.26	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
4	EDO	C	304	-	-	0/1/1/1	-
4	EDO	C	303	-	-	0/1/1/1	-
4	EDO	C	302	-	-	0/1/1/1	-
3	L6U	D	300	-	-	3/37/37/37	0/3/3/3
3	L6U	C	301	-	-	3/37/37/37	0/3/3/3
4	EDO	B	501	-	-	0/1/1/1	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	300	L6U	C03-N02	6.75	1.42	1.33
3	C	301	L6U	C03-N02	6.42	1.42	1.33
3	C	301	L6U	C19-N18	4.80	1.44	1.34
3	D	300	L6U	C19-N18	4.34	1.43	1.34
3	D	300	L6U	C17-N18	3.93	1.50	1.45
3	D	300	L6U	C17-C15	3.77	1.62	1.54
3	C	301	L6U	C15-N14	3.75	1.42	1.34
3	C	301	L6U	C26-C25	3.72	1.44	1.38
3	D	300	L6U	C26-C25	3.57	1.44	1.38
3	D	300	L6U	O32-C31	3.50	1.42	1.37
3	D	300	L6U	C15-N14	3.46	1.41	1.34
3	C	301	L6U	C17-C15	3.39	1.61	1.54
3	C	301	L6U	O32-C31	3.20	1.42	1.37
3	D	300	L6U	C30-C27	3.10	1.44	1.39
3	C	301	L6U	C17-N18	3.07	1.49	1.45
3	C	301	L6U	C30-C27	2.97	1.43	1.39
3	D	300	L6U	C25-C24	2.96	1.44	1.39
3	D	300	L6U	C30-C31	2.90	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	L6U	C25-C24	2.74	1.44	1.39
3	C	301	L6U	C30-C31	2.66	1.43	1.38
3	C	301	L6U	O28-C27	2.64	1.42	1.37
3	D	300	L6U	C10-C09	2.56	1.43	1.38
3	C	301	L6U	C10-C09	2.48	1.43	1.38
3	D	300	L6U	C12-C13	2.40	1.43	1.38
3	D	300	L6U	O28-C27	2.35	1.42	1.37
3	D	300	L6U	C07-C08	2.34	1.58	1.51
3	C	301	L6U	C12-C13	2.34	1.42	1.38
3	C	301	L6U	C31-C24	2.26	1.43	1.39
3	D	300	L6U	C31-C24	2.21	1.43	1.39
3	D	300	L6U	C23-C24	2.19	1.57	1.51
3	D	300	L6U	C05-N14	2.19	1.50	1.45
3	D	300	L6U	C13-C08	2.19	1.43	1.38
3	C	301	L6U	C23-C24	2.16	1.57	1.51
3	C	301	L6U	C05-N14	2.11	1.50	1.45
3	C	301	L6U	C07-C08	2.04	1.57	1.51
3	D	300	L6U	C01-N02	2.00	1.49	1.45

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	300	L6U	C05-C03-N02	6.51	126.81	116.99
3	C	301	L6U	C05-C03-N02	6.07	126.15	116.99
3	D	300	L6U	C21-C19-N18	3.92	125.50	116.16
3	C	301	L6U	C21-C19-N18	3.89	125.42	116.16
3	D	300	L6U	C17-N18-C19	3.80	125.37	121.29
3	D	300	L6U	C17-C15-N14	3.68	126.55	116.67
3	D	300	L6U	O16-C15-N14	-3.11	117.39	122.96
3	C	301	L6U	C17-C15-N14	3.05	124.86	116.67
3	C	301	L6U	O04-C03-C05	-3.02	114.16	120.48
3	C	301	L6U	C17-N18-C19	2.95	124.45	121.29
3	C	301	L6U	O20-C19-N18	-2.86	118.11	122.95
3	D	300	L6U	O04-C03-N02	-2.82	118.43	123.13
3	D	300	L6U	O04-C03-C05	-2.73	114.75	120.48
3	D	300	L6U	O20-C19-N18	-2.73	118.32	122.95
3	C	301	L6U	C05-N14-C15	2.71	127.46	121.65
3	D	300	L6U	O16-C15-C17	-2.66	116.06	120.66
3	C	301	L6U	O16-C15-C17	-2.57	116.22	120.66
3	C	301	L6U	C37-S38-C34	2.54	98.01	92.87
3	C	301	L6U	O16-C15-N14	-2.26	118.92	122.96
3	D	300	L6U	C37-S38-C34	2.11	97.15	92.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	L6U	O04-C03-N02	-2.06	119.69	123.13
3	D	300	L6U	O20-C19-C21	-2.06	116.16	120.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	L6U	C05-C06-C07-C08
3	D	300	L6U	N18-C19-C21-N22
3	D	300	L6U	O20-C19-C21-N22
3	C	301	L6U	N18-C19-C21-N22
3	C	301	L6U	O20-C19-C21-N22
3	D	300	L6U	C05-C06-C07-C08

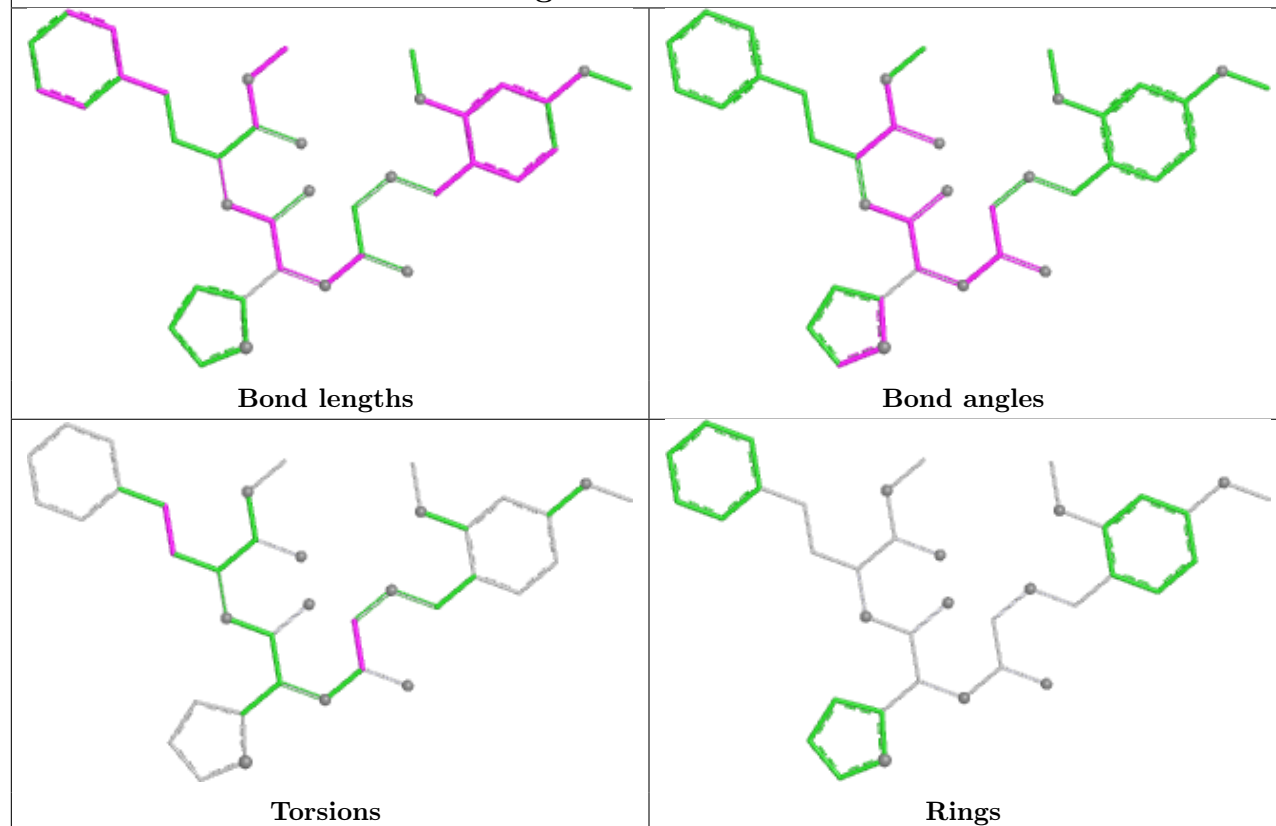
There are no ring outliers.

1 monomer is involved in 1 short contact:

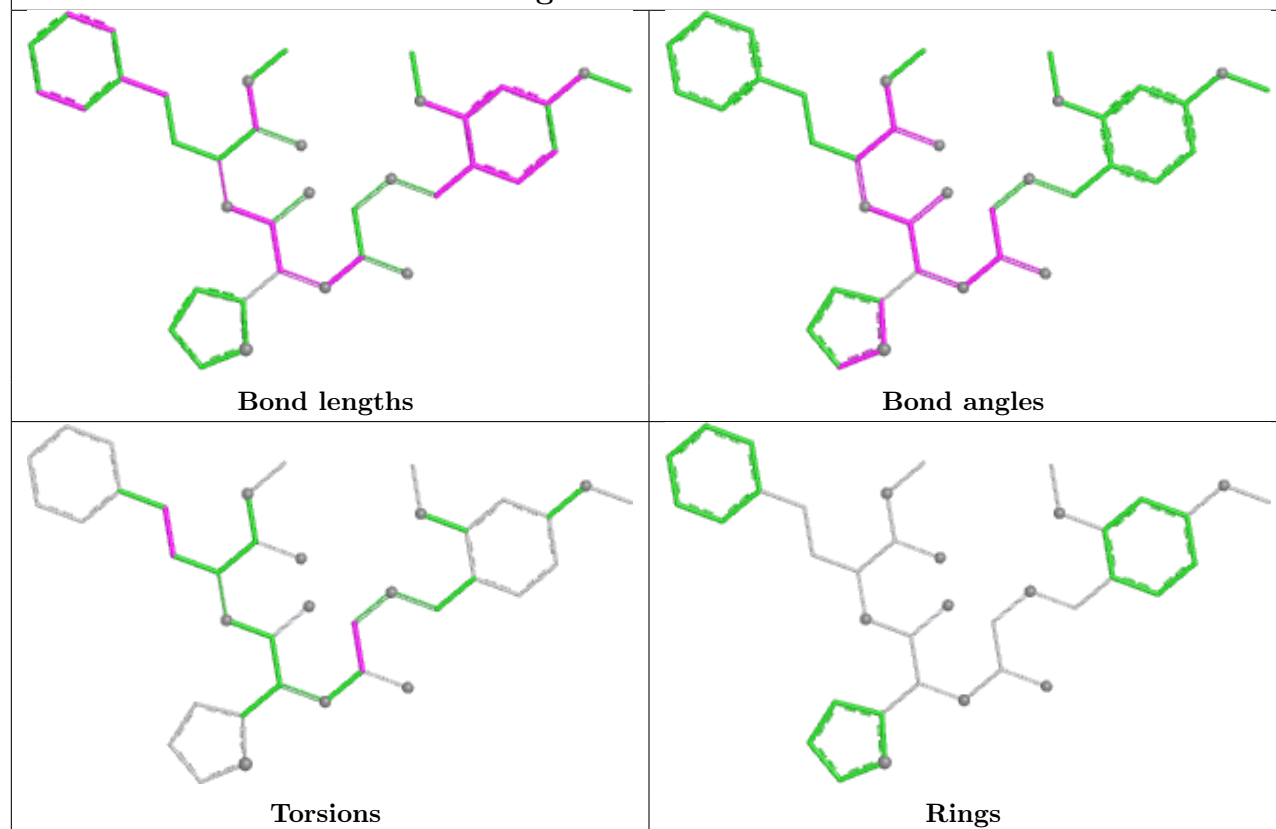
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	L6U	1	0

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.

## Ligand L6U D 300



## Ligand L6U C 301



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	377/418 (90%)	0.22	15 (3%) 42 44	41, 56, 83, 110	0
1	B	377/418 (90%)	0.10	11 (2%) 53 55	37, 50, 79, 123	0
2	C	167/167 (100%)	-0.08	1 (0%) 85 86	36, 48, 68, 80	0
2	D	166/167 (99%)	0.22	5 (3%) 52 54	39, 56, 102, 121	0
All	All	1087/1170 (92%)	0.13	32 (2%) 53 55	36, 53, 83, 123	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	GLY	4.0
1	A	424	ASN	3.6
1	A	32	GLN	3.2
1	B	32	GLN	3.1
2	D	225	LEU	3.1
1	A	176	ASP	3.0
1	B	168	LEU	3.0
1	A	123	CYS	2.8
1	B	231	HIS	2.8
2	C	219	ASP	2.7
1	A	170	GLU	2.6
2	D	219	ASP	2.6
1	A	178	LEU	2.5
1	A	172	GLU	2.5
1	B	169	MET	2.5
1	A	171	LYS	2.4
1	B	177	CYS	2.4
1	B	409	ILE	2.4
1	A	37	ASP	2.3
1	B	315	ASP	2.2
1	A	192	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	229	THR	2.2
2	D	289	VAL	2.2
1	B	170	GLU	2.2
1	B	237	LYS	2.2
1	A	236	THR	2.2
1	B	175	ARG	2.1
2	D	152	ASN	2.1
1	A	315	ASP	2.1
1	B	424	ASN	2.1
2	D	124	SER	2.0
1	A	35	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

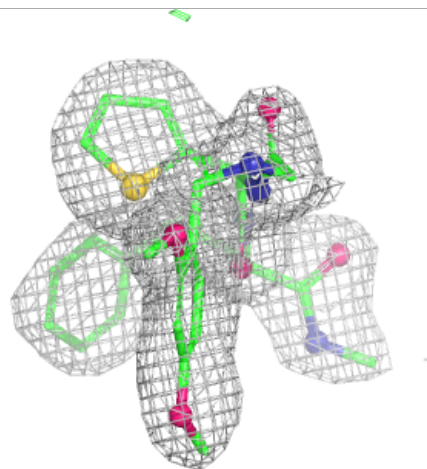
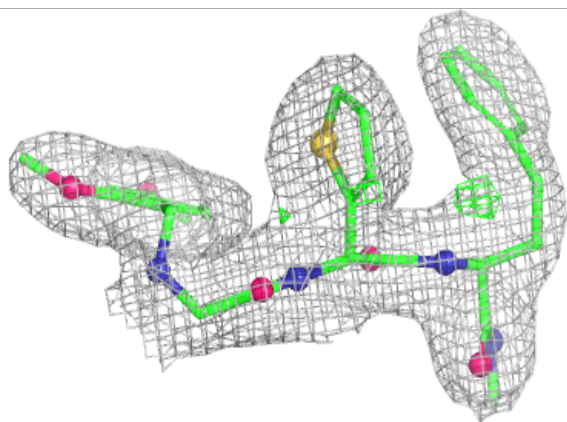
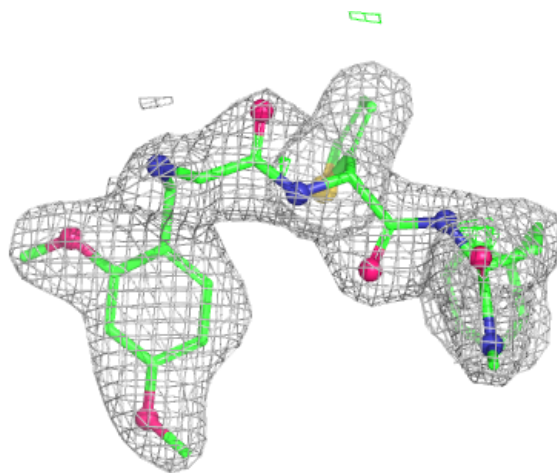
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
4	EDO	B	501	4/4	0.78	0.18	50,51,53,55	0
4	EDO	C	303	4/4	0.92	0.10	44,47,47,57	0
3	L6U	D	300	38/38	0.94	0.09	38,44,47,49	0
4	EDO	C	304	4/4	0.95	0.09	47,48,49,49	0
3	L6U	C	301	38/38	0.95	0.08	37,40,43,45	0
4	EDO	C	302	4/4	0.96	0.07	42,46,50,52	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.

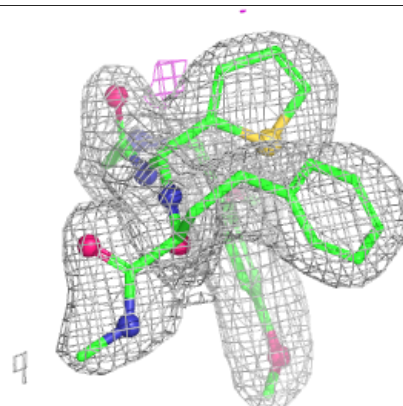
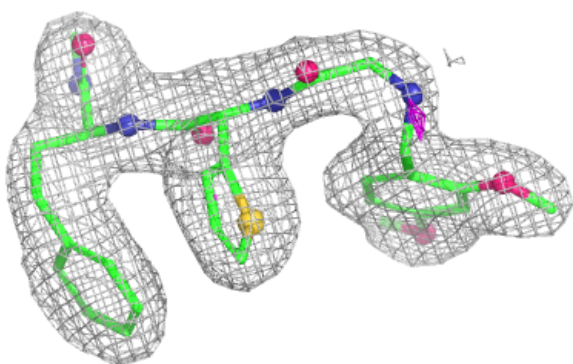
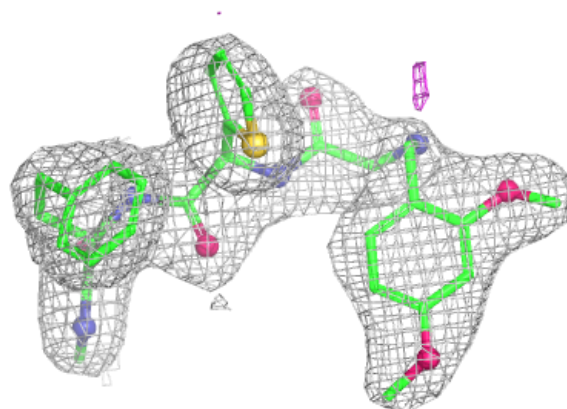
**Electron density around L6U D 300:**

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



**Electron density around L6U C 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 [i](#)

There are no such residues in this entry.