



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 08:34 PM EDT

PDB ID : 2NWL  
Title : Crystal structure of GltPh in complex with L-Asp  
Authors : Gouaux, E.; Boudker, O.; Ryan, R.; Yernool, D.; Shimamoto, K.  
Deposited on : 2006-11-15  
Resolution : 2.96 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.

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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 : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

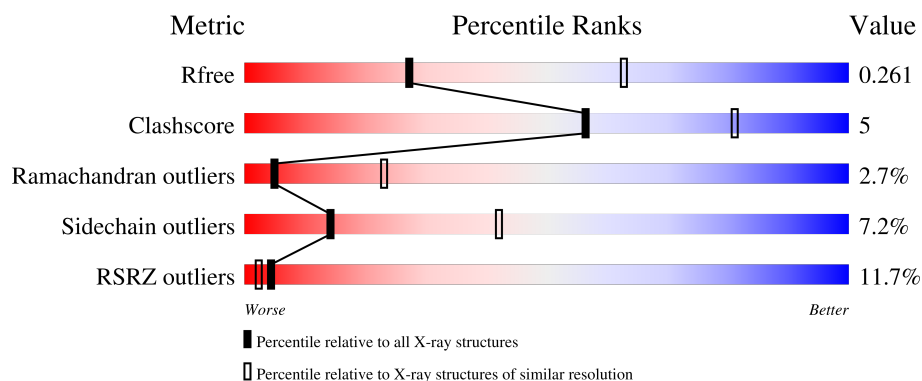
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	422	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	B	422	<div> <div>14%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>• 6%</div> </div> </div>
1	C	422	<div> <div>13%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• 5%</div> </div> </div>

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	PLM	A	801	-	-	-	X
2	PLM	B	901	-	-	-	X
2	PLM	C	1001	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8656 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 glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			2868	1888	458	505	17			
1	B	398	Total	C	N	O	S	0	0	0
			2838	1870	452	499	17			
1	C	403	Total	C	N	O	S	0	0	0
			2869	1889	458	505	17			

There are 36 discrepancies between the modelled and reference sequences:

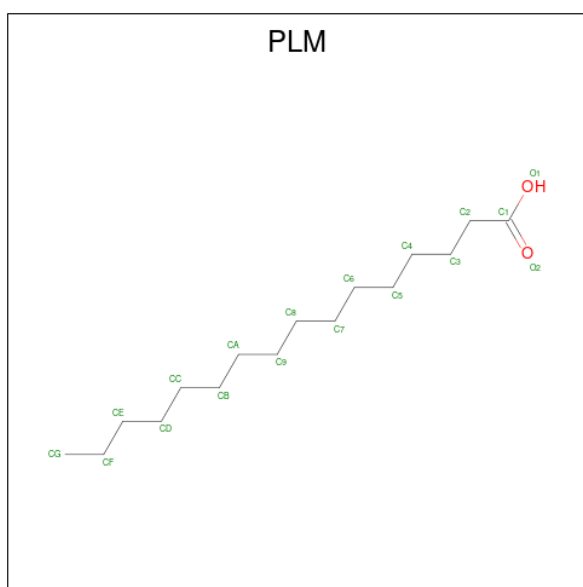
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	418	THR	-	cloning artifact	UNP O59010
A	419	LEU	-	cloning artifact	UNP O59010
A	420	VAL	-	cloning artifact	UNP O59010
A	421	PRO	-	cloning artifact	UNP O59010
A	422	ARG	-	cloning artifact	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	125	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	368	HIS	GLU	engineered mutation	UNP O59010
B	418	THR	-	cloning artifact	UNP O59010
B	419	LEU	-	cloning artifact	UNP O59010
B	420	VAL	-	cloning artifact	UNP O59010
B	421	PRO	-	cloning artifact	UNP O59010

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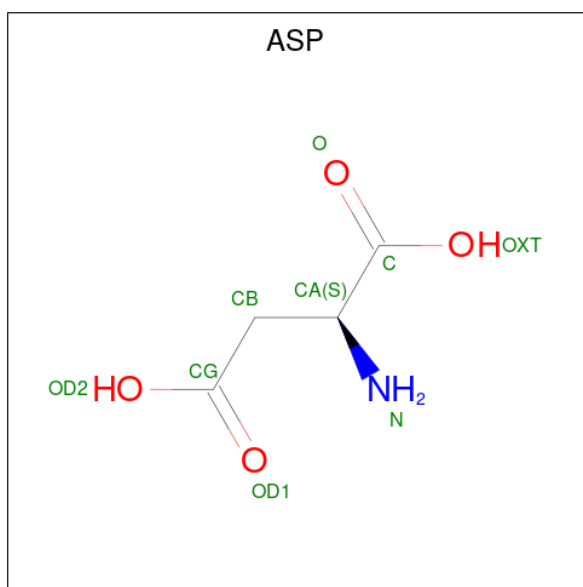
Chain	Residue	Modelled	Actual	Comment	Reference
B	422	ARG	-	cloning artifact	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	125	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	418	THR	-	cloning artifact	UNP O59010
C	419	LEU	-	cloning artifact	UNP O59010
C	420	VAL	-	cloning artifact	UNP O59010
C	421	PRO	-	cloning artifact	UNP O59010
C	422	ARG	-	cloning artifact	UNP O59010

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula:  $C_{16}H_{32}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	16	1		
2	B	1	Total	C	O	0	0
			17	16	1		
2	C	1	Total	C	O	0	0
			17	16	1		

- Molecule 3 is ASPARTIC ACID (three-letter code: ASP) (formula:  $C_4H_7NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			9	4	1	4		
3	C	1	Total	C	N	O	0	0
			9	4	1	4		
3	C	1	Total	C	N	O	0	0
			9	4	1	4		

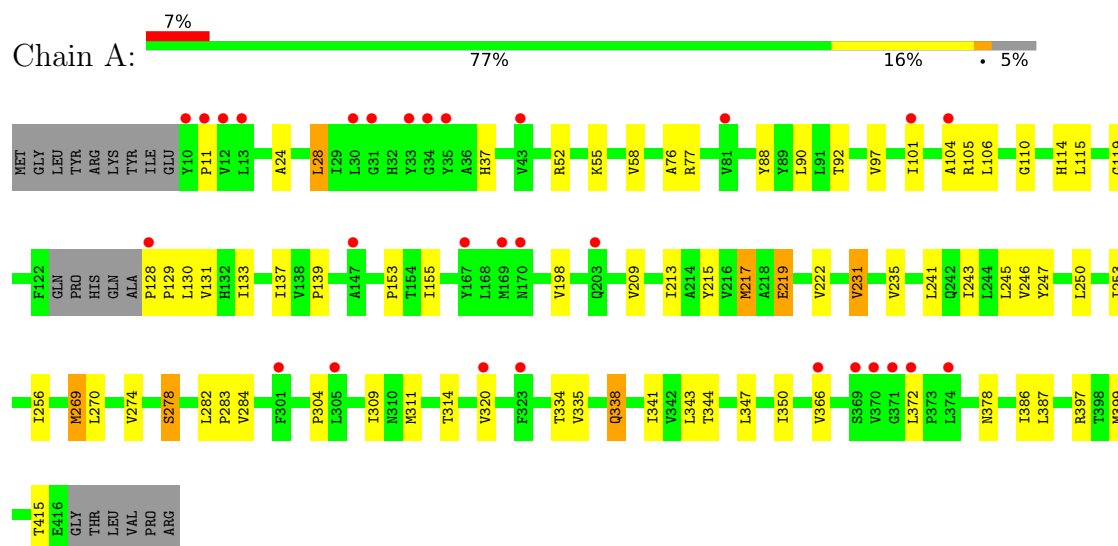
- Molecule 4 is water.

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

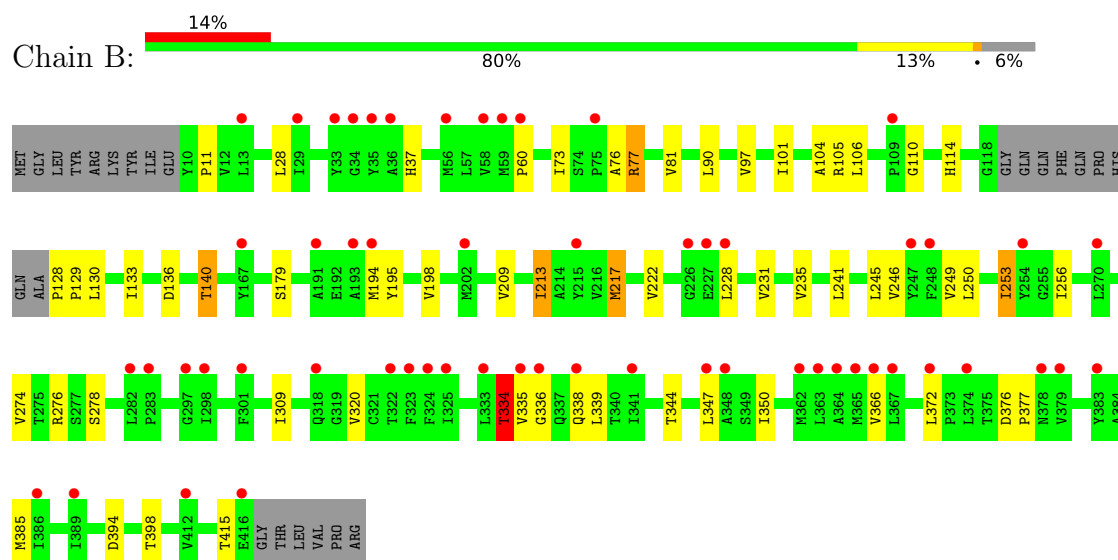
### 3 Residue-property plots

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.

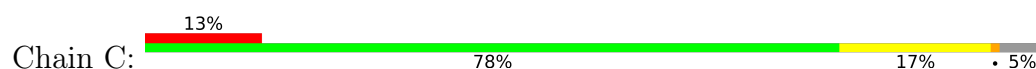
- Molecule 1: glutamate symport protein

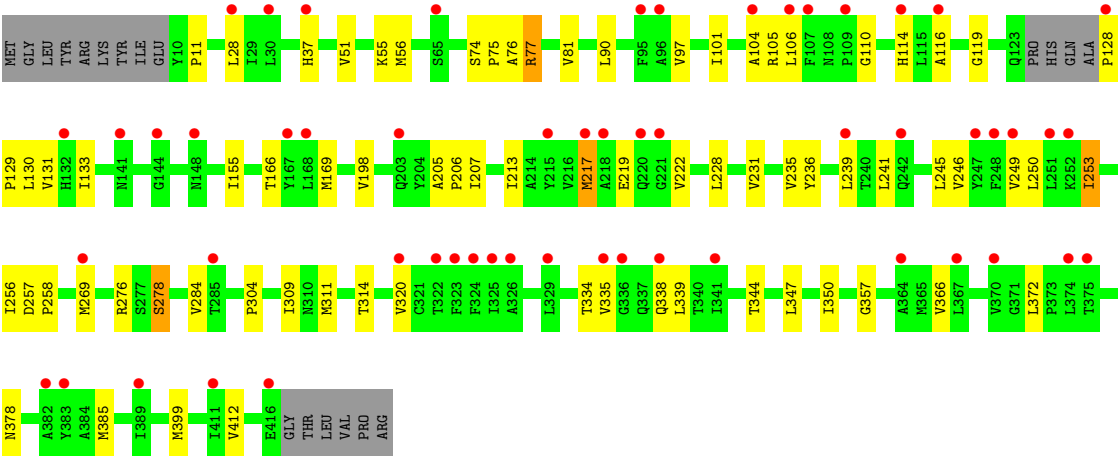


- Molecule 1: glutamate symport protein



- Molecule 1: glutamate symport protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.30Å 115.30Å 323.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.96 49.34 – 2.96	Depositor EDS
% Data completeness (in resolution range)	69.3 (100.00-2.96) 69.3 (49.34-2.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.236 , 0.265 0.235 , 0.261	Depositor DCC
$R_{free}$ test set	1728 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	111.3	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 134.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.062 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLM

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	0.34	0/2920	0.54	0/3994
1	B	0.32	0/2890	0.51	0/3954
1	C	0.32	0/2921	0.50	0/3996
All	All	0.33	0/8731	0.52	0/11944

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

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	2868	0	2927	33	0
1	B	2838	0	2897	30	0
1	C	2869	0	2923	30	0
2	A	17	0	31	1	0
2	B	17	0	31	2	0
2	C	17	0	31	0	0
3	C	27	0	9	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	8656	0	8849	88	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 5.

All (88) 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:B:350:ILE:HG21	2:B:901:PLM:HE1	1.74	0.70
1:A:235:VAL:HG22	1:A:320:VAL:HG11	1.80	0.64
1:B:235:VAL:HG22	1:B:320:VAL:HG11	1.79	0.64
1:A:155:ILE:HD11	1:A:304:PRO:HB2	1.78	0.63
1:C:235:VAL:HG22	1:C:320:VAL:HG11	1.82	0.61
1:A:52:ARG:HH11	1:B:140:THR:HG23	1.65	0.61
1:C:311:MET:HB3	1:C:314:THR:HB	1.83	0.59
1:B:398:THR:HG1	3:C:601:ASP:N	2.00	0.59
1:B:309:ILE:HG13	1:B:350:ILE:HG23	1.83	0.59
1:C:155:ILE:HD11	1:C:304:PRO:HB2	1.87	0.56
1:B:249:VAL:O	1:B:253:ILE:HG22	2.05	0.56
1:B:309:ILE:HD11	2:B:901:PLM:HA1	1.86	0.56
1:B:344:THR:HB	1:B:366:VAL:HG23	1.87	0.56
1:B:246:VAL:O	1:B:250:LEU:HB2	2.05	0.56
1:A:314:THR:OG1	3:C:501:ASP:OD2	2.25	0.55
1:A:209:VAL:HA	1:A:274:VAL:HG11	1.89	0.55
1:B:241:LEU:O	1:B:245:LEU:HB2	2.07	0.54
1:A:344:THR:HB	1:A:366:VAL:HG23	1.88	0.54
1:A:246:VAL:O	1:A:250:LEU:HB2	2.09	0.53
1:C:344:THR:HB	1:C:366:VAL:HG23	1.89	0.53
1:B:77:ARG:O	1:B:81:VAL:N	2.34	0.52
1:C:309:ILE:HG13	1:C:350:ILE:HG23	1.92	0.52
1:A:24:ALA:O	1:A:28:LEU:HB2	2.09	0.52
1:B:128:PRO:HB2	1:B:133:ILE:HD11	1.92	0.52
1:C:228:LEU:HD21	1:C:385:MET:HG2	1.91	0.52
1:A:55:LYS:HB2	1:B:140:THR:HG22	1.91	0.51
1:A:241:LEU:O	1:A:245:LEU:HB2	2.11	0.51
1:C:231:VAL:O	1:C:235:VAL:HG23	2.11	0.50
1:B:209:VAL:HA	1:B:274:VAL:HG11	1.94	0.50
1:A:311:MET:HB3	1:A:314:THR:HB	1.94	0.50
1:C:97:VAL:O	1:C:101:ILE:HG12	2.10	0.50
1:A:231:VAL:O	1:A:235:VAL:HG23	2.12	0.50
1:B:28:LEU:HD13	1:B:217:MET:HG3	1.94	0.50
1:A:215:TYR:CE1	1:A:219:GLU:HG3	2.47	0.49
1:B:231:VAL:O	1:B:235:VAL:HG23	2.12	0.49
1:C:276:ARG:O	3:C:701:ASP:N	2.45	0.49
1:C:81:VAL:HG23	1:C:412:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ALA:HB2	1:C:320:VAL:HG23	1.95	0.48
1:C:241:LEU:O	1:C:245:LEU:HB2	2.13	0.48
1:A:97:VAL:O	1:A:101:ILE:HG12	2.13	0.48
1:B:104:ALA:HB2	1:B:320:VAL:HG23	1.96	0.48
1:A:350:ILE:HG22	2:A:801:PLM:H62	1.94	0.48
1:C:246:VAL:O	1:C:250:LEU:HB2	2.14	0.47
1:C:278:SER:HB2	3:C:701:ASP:OXT	2.13	0.47
1:C:51:VAL:O	1:C:55:LYS:HG2	2.14	0.47
1:A:137:ILE:O	1:A:153:PRO:HA	2.14	0.47
1:B:73:ILE:HB	1:B:77:ARG:HG2	1.97	0.47
1:A:52:ARG:NH2	1:B:136:ASP:HA	2.31	0.46
1:C:28:LEU:HD13	1:C:217:MET:HG3	1.98	0.46
1:B:97:VAL:O	1:B:101:ILE:HG12	2.16	0.45
1:C:129:PRO:O	1:C:131:VAL:N	2.50	0.45
1:C:249:VAL:O	1:C:253:ILE:HG22	2.17	0.45
1:A:58:VAL:HG22	1:A:283:PRO:HD3	1.99	0.45
1:A:270:LEU:O	1:A:274:VAL:HG23	2.16	0.44
1:B:376:ASP:HA	1:B:377:PRO:HD3	1.82	0.44
1:B:128:PRO:HA	1:B:129:PRO:HD3	1.76	0.44
1:B:228:LEU:HD21	1:B:385:MET:HG2	1.99	0.44
1:C:206:PRO:HG2	1:C:207:ILE:HD12	2.00	0.44
1:A:128:PRO:HA	1:A:129:PRO:HD3	1.74	0.44
1:C:128:PRO:HA	1:C:129:PRO:HD3	1.73	0.44
1:C:314:THR:OG1	3:C:701:ASP:OD2	2.34	0.44
1:A:28:LEU:HD13	1:A:217:MET:HG3	1.99	0.44
1:B:334:THR:O	1:B:336:GLY:N	2.50	0.44
1:C:128:PRO:HB2	1:C:133:ILE:HD11	1.99	0.44
1:C:257:ASP:HA	1:C:258:PRO:HD3	1.89	0.44
1:A:243:ILE:HA	1:A:247:TYR:CD1	2.53	0.43
1:C:77:ARG:O	1:C:81:VAL:N	2.35	0.43
1:B:60:PRO:HB2	1:B:194:MET:HG3	2.01	0.43
1:C:269:MET:O	1:C:399:MET:HG3	2.18	0.43
1:A:282:LEU:HD21	1:A:304:PRO:HA	1.99	0.43
1:C:236:TYR:HA	1:C:239:LEU:HD12	2.00	0.43
1:A:131:VAL:C	1:A:133:ILE:H	2.22	0.43
1:A:139:PRO:O	1:C:56:MET:HB2	2.18	0.42
1:A:52:ARG:NH1	1:B:140:THR:HG23	2.34	0.42
1:C:166:THR:HA	1:C:169:MET:HE2	2.00	0.42
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.55	0.42
1:A:269:MET:O	1:A:399:MET:HG3	2.20	0.42
1:C:205:ALA:N	1:C:206:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ILE:HD13	1:A:386:ILE:HA	1.86	0.41
1:B:213:ILE:H	1:B:213:ILE:HG13	1.69	0.41
1:B:394:ASP:OD1	3:C:601:ASP:N	2.52	0.41
1:A:309:ILE:HG13	1:A:350:ILE:HG23	2.02	0.41
1:B:276:ARG:O	3:C:601:ASP:N	2.53	0.41
1:A:278:SER:HB2	3:C:501:ASP:OXT	2.21	0.41
1:B:195:TYR:HA	1:B:198:VAL:HG12	2.02	0.40
1:A:104:ALA:HB2	1:A:320:VAL:HG23	2.04	0.40
1:A:338:GLN:HB2	1:A:341:ILE:HD12	2.04	0.40
1:C:74:SER:HB3	1:C:75:PRO:HD3	2.03	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	398/422 (94%)	363 (91%)	24 (6%)	11 (3%)	5	22
1	B	394/422 (93%)	360 (91%)	25 (6%)	9 (2%)	6	27
1	C	399/422 (94%)	362 (91%)	25 (6%)	12 (3%)	4	20
All	All	1191/1266 (94%)	1085 (91%)	74 (6%)	32 (3%)	5	23

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	334	THR
1	C	334	THR
1	A	114	HIS
1	A	335	VAL
1	B	114	HIS
1	B	334	THR

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Mol	Chain	Res	Type
1	B	335	VAL
1	C	335	VAL
1	A	77	ARG
1	A	222	VAL
1	B	11	PRO
1	B	77	ARG
1	C	11	PRO
1	C	77	ARG
1	C	114	HIS
1	C	130	LEU
1	B	110	GLY
1	C	76	ALA
1	C	222	VAL
1	A	11	PRO
1	A	76	ALA
1	A	130	LEU
1	B	76	ALA
1	B	130	LEU
1	C	116	ALA
1	A	110	GLY
1	B	222	VAL
1	C	110	GLY
1	C	119	GLY
1	A	119	GLY
1	C	357	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/330 (85%)	257 (92%)	23 (8%)	11	36
1	B	277/330 (84%)	260 (94%)	17 (6%)	18	49
1	C	279/330 (84%)	262 (94%)	17 (6%)	18	49
All	All	836/990 (84%)	779 (93%)	57 (7%)	14	45

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	37	HIS
1	A	90	LEU
1	A	105	ARG
1	A	106	LEU
1	A	198	VAL
1	A	213	ILE
1	A	217	MET
1	A	219	GLU
1	A	231	VAL
1	A	253	ILE
1	A	256	ILE
1	A	269	MET
1	A	278	SER
1	A	284	VAL
1	A	338	GLN
1	A	343	LEU
1	A	347	LEU
1	A	372	LEU
1	A	378	ASN
1	A	387	LEU
1	A	397	ARG
1	A	415	THR
1	B	37	HIS
1	B	90	LEU
1	B	105	ARG
1	B	106	LEU
1	B	140	THR
1	B	179	SER
1	B	213	ILE
1	B	217	MET
1	B	253	ILE
1	B	256	ILE
1	B	278	SER
1	B	334	THR
1	B	338	GLN
1	B	339	LEU
1	B	347	LEU
1	B	372	LEU
1	B	415	THR
1	C	37	HIS
1	C	90	LEU

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Mol	Chain	Res	Type
1	C	105	ARG
1	C	106	LEU
1	C	198	VAL
1	C	213	ILE
1	C	217	MET
1	C	219	GLU
1	C	253	ILE
1	C	256	ILE
1	C	278	SER
1	C	284	VAL
1	C	338	GLN
1	C	339	LEU
1	C	347	LEU
1	C	372	LEU
1	C	378	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	148	ASN
1	A	327	ASN
1	B	40	HIS
1	B	148	ASN
1	B	327	ASN
1	C	327	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

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	$\# Z  > 2$
3	ASP	C	701	-	2,8,8	0.74	0	1,10,10	0.15	0
2	PLM	A	801	-	16,16,17	0.46	0	15,15,17	0.58	0
3	ASP	C	501	-	2,8,8	0.71	0	1,10,10	0.64	0
2	PLM	C	1001	-	16,16,17	0.50	0	15,15,17	0.54	0
2	PLM	B	901	-	16,16,17	0.49	0	15,15,17	0.57	0
3	ASP	C	601	-	2,8,8	0.76	0	1,10,10	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ASP	C	701	-	-	0/2/8/8	-
2	PLM	A	801	-	-	9/13/14/15	-
3	ASP	C	501	-	-	0/2/8/8	-
2	PLM	C	1001	-	-	11/13/14/15	-
2	PLM	B	901	-	-	10/13/14/15	-
3	ASP	C	601	-	-	0/2/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	PLM	CB-CC-CD-CE
2	B	901	PLM	C3-C4-C5-C6
2	C	1001	PLM	C8-C9-CA-CB

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Mol	Chain	Res	Type	Atoms
2	A	801	PLM	C8-C9-CA-CB
2	A	801	PLM	CC-CD-CE-CF
2	B	901	PLM	CC-CD-CE-CF
2	A	801	PLM	C9-CA-CB-CC
2	B	901	PLM	C7-C8-C9-CA
2	B	901	PLM	CA-CB-CC-CD
2	A	801	PLM	C3-C4-C5-C6
2	C	1001	PLM	C3-C4-C5-C6
2	C	1001	PLM	CC-CD-CE-CF
2	B	901	PLM	C8-C9-CA-CB
2	C	1001	PLM	C4-C5-C6-C7
2	C	1001	PLM	CB-CC-CD-CE
2	C	1001	PLM	C7-C8-C9-CA
2	A	801	PLM	C7-C8-C9-CA
2	C	1001	PLM	C2-C3-C4-C5
2	C	1001	PLM	CA-CB-CC-CD
2	C	1001	PLM	C9-CA-CB-CC
2	A	801	PLM	CA-CB-CC-CD
2	B	901	PLM	C2-C3-C4-C5
2	A	801	PLM	C4-C5-C6-C7
2	B	901	PLM	CB-CC-CD-CE
2	B	901	PLM	C4-C5-C6-C7
2	C	1001	PLM	C5-C6-C7-C8
2	A	801	PLM	C5-C6-C7-C8
2	B	901	PLM	C6-C7-C8-C9
2	C	1001	PLM	CD-CE-CF-CG
2	B	901	PLM	C5-C6-C7-C8

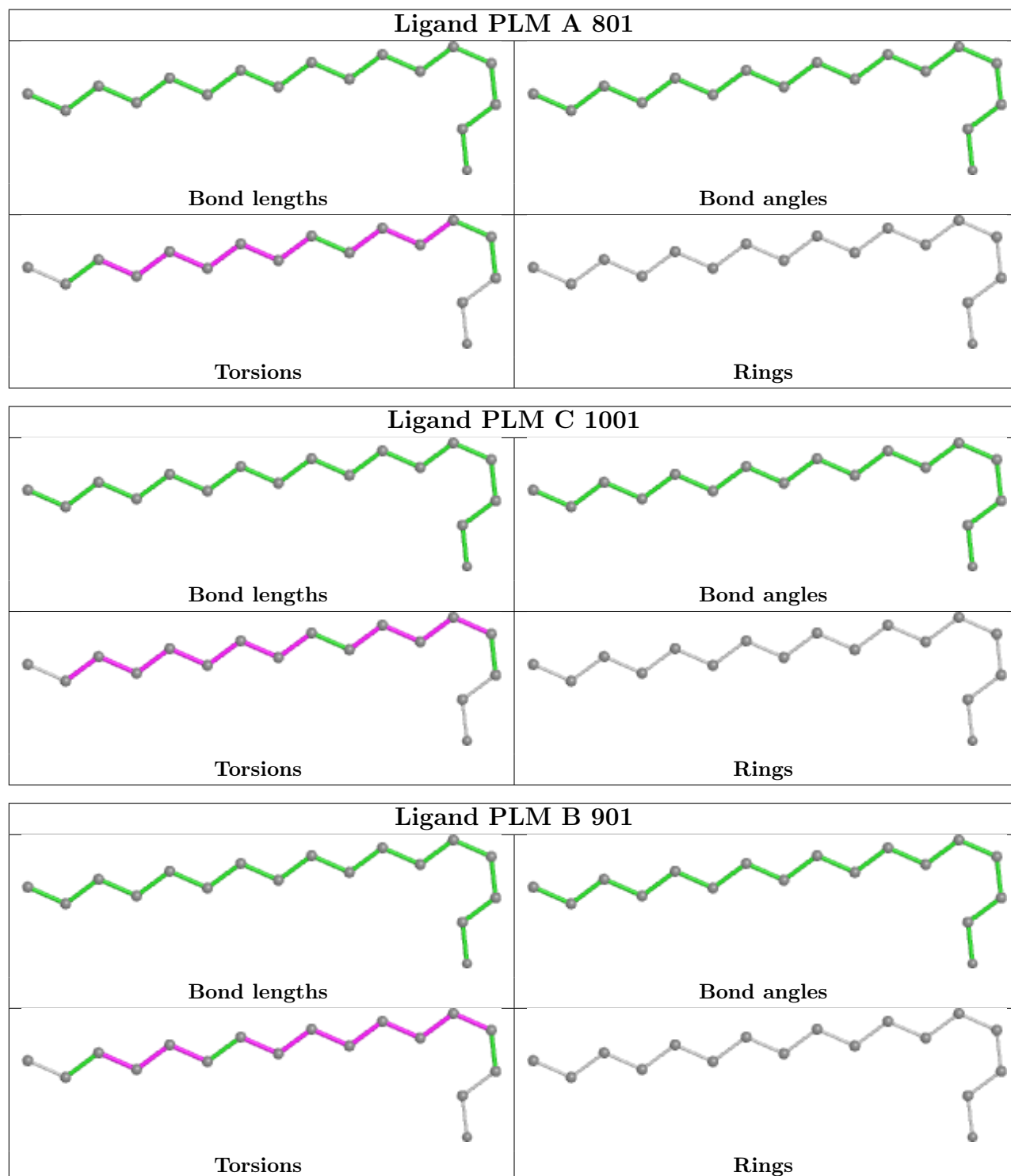
There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	ASP	3	0
2	A	801	PLM	1	0
3	C	501	ASP	2	0
2	B	901	PLM	2	0
3	C	601	ASP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	402/422 (95%)	0.37	29 (7%) 15 8	113, 137, 170, 199	0
1	B	398/422 (94%)	0.74	57 (14%) 2 1	114, 140, 164, 204	0
1	C	403/422 (95%)	0.64	55 (13%) 3 1	119, 140, 168, 214	0
All	All	1203/1266 (95%)	0.58	141 (11%) 4 2	113, 139, 168, 214	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	TYR	8.4
1	C	325	ILE	7.8
1	B	323	PHE	7.2
1	C	324	PHE	7.2
1	B	322	THR	6.8
1	C	374	LEU	6.6
1	B	374	LEU	6.2
1	C	247	TYR	5.9
1	B	227	GLU	5.9
1	C	323	PHE	5.7
1	B	325	ILE	5.3
1	C	106	LEU	5.1
1	B	35	TYR	5.0
1	C	383	TYR	4.8
1	C	336	GLY	4.8
1	B	324	PHE	4.8
1	A	320	VAL	4.5
1	C	322	THR	4.5
1	B	383	TYR	4.5
1	C	114	HIS	4.4
1	C	217	MET	4.4
1	A	370	VAL	4.4
1	B	318	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	338	GLN	4.1
1	C	203	GLN	4.1
1	A	35	TYR	4.0
1	C	218	ALA	4.0
1	A	33	TYR	4.0
1	B	336	GLY	4.0
1	C	221	GLY	4.0
1	A	372	LEU	3.9
1	C	104	ALA	3.9
1	B	347	LEU	3.9
1	B	298	ILE	3.8
1	C	370	VAL	3.8
1	A	13	LEU	3.8
1	B	215	TYR	3.8
1	C	107	PHE	3.7
1	C	252	LYS	3.7
1	B	365	MET	3.7
1	A	369	SER	3.6
1	A	128	PRO	3.6
1	A	11	PRO	3.6
1	C	320	VAL	3.5
1	B	372	LEU	3.5
1	B	379	VAL	3.5
1	B	378	ASN	3.5
1	B	335	VAL	3.5
1	B	228	LEU	3.3
1	B	29	ILE	3.3
1	C	335	VAL	3.3
1	B	75	PRO	3.2
1	C	251	LEU	3.1
1	B	341	ILE	3.1
1	A	12	VAL	3.1
1	C	109	PRO	3.0
1	B	364	ALA	3.0
1	A	31	GLY	3.0
1	C	95	PHE	3.0
1	A	170	ASN	2.9
1	C	367	LEU	2.9
1	B	254	TYR	2.9
1	B	362	MET	2.9
1	B	363	LEU	2.9
1	B	367	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	2.8
1	B	226	GLY	2.8
1	A	169	MET	2.8
1	C	116	ALA	2.7
1	B	109	PRO	2.7
1	C	269	MET	2.7
1	B	167	TYR	2.7
1	C	341	ILE	2.7
1	A	323	PHE	2.7
1	C	389	ILE	2.7
1	C	416	GLU	2.6
1	B	348	ALA	2.6
1	C	215	TYR	2.6
1	B	248	PHE	2.6
1	C	411	ILE	2.5
1	C	249	VAL	2.5
1	C	242	GLN	2.5
1	B	36	ALA	2.5
1	B	59	MET	2.5
1	C	132	HIS	2.5
1	B	191	ALA	2.5
1	B	13	LEU	2.5
1	B	416	GLU	2.5
1	B	412	VAL	2.4
1	C	37	HIS	2.4
1	C	239	LEU	2.4
1	B	60	PRO	2.4
1	B	297	GLY	2.4
1	A	101	ILE	2.4
1	C	220	GLN	2.4
1	C	148	ASN	2.4
1	A	167	TYR	2.3
1	C	168	LEU	2.3
1	A	104	ALA	2.3
1	C	326	ALA	2.3
1	C	167	TYR	2.3
1	C	30	LEU	2.3
1	A	371	GLY	2.3
1	C	144	GLY	2.3
1	B	301	PHE	2.3
1	C	128	PRO	2.3
1	B	333	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	386	ILE	2.2
1	C	248	PHE	2.2
1	C	28	LEU	2.2
1	B	389	ILE	2.2
1	B	247	TYR	2.2
1	C	65	SER	2.2
1	A	305	LEU	2.2
1	B	283	PRO	2.2
1	A	203	GLN	2.2
1	B	366	VAL	2.2
1	B	34	GLY	2.2
1	A	301	PHE	2.2
1	C	364	ALA	2.2
1	A	10	TYR	2.2
1	B	58	VAL	2.2
1	B	56	MET	2.1
1	A	81	VAL	2.1
1	C	141	ASN	2.1
1	C	338	GLN	2.1
1	A	374	LEU	2.1
1	B	270	LEU	2.1
1	B	282	LEU	2.1
1	A	147	ALA	2.1
1	B	193	ALA	2.1
1	C	329	LEU	2.1
1	B	194	MET	2.1
1	C	382	ALA	2.1
1	A	30	LEU	2.1
1	A	43	VAL	2.1
1	A	366	VAL	2.0
1	B	202	MET	2.0
1	C	96	ALA	2.0
1	C	285	THR	2.0
1	C	375	THR	2.0

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

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



## 6.3 Carbohydrates [i](#)

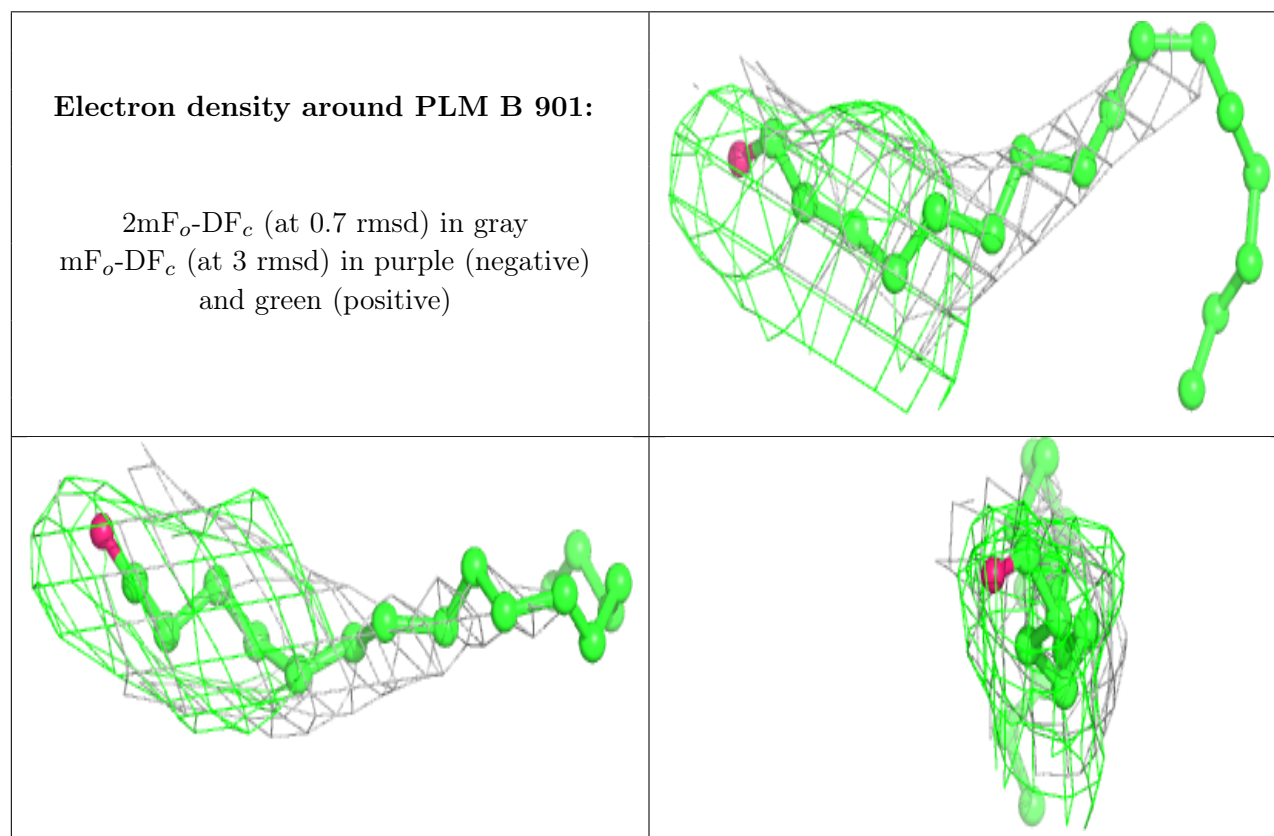
There are no monosaccharides in this entry.

## 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.

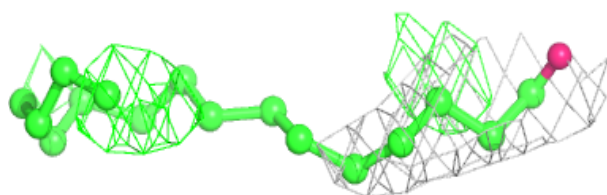
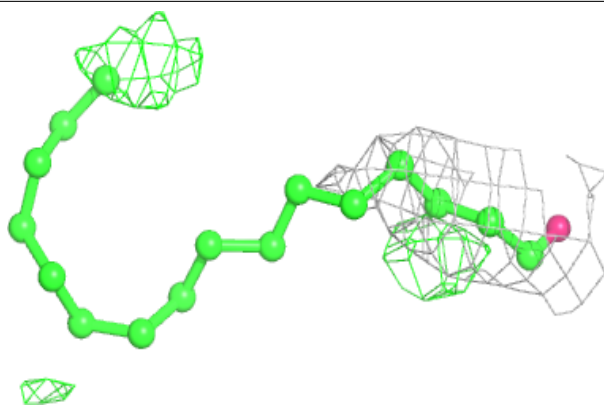
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PLM	B	901	17/18	0.10	0.90	126,138,155,156	0
2	PLM	C	1001	17/18	0.17	1.08	145,149,156,156	0
2	PLM	A	801	17/18	0.35	1.16	141,154,167,167	0
3	ASP	C	601	9/9	0.91	0.15	123,125,129,130	0
3	ASP	C	701	9/9	0.91	0.13	129,132,136,136	0
3	ASP	C	501	9/9	0.96	0.11	124,129,136,136	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.

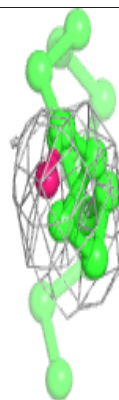
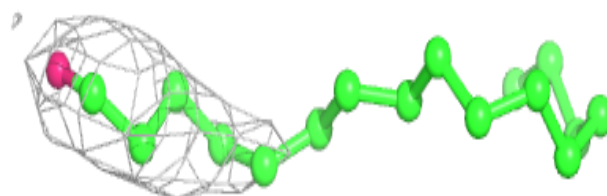
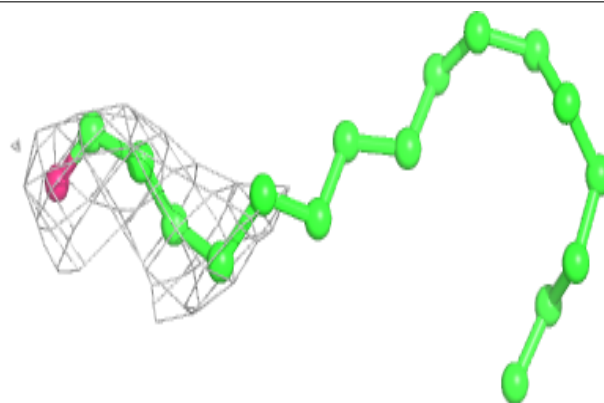


**Electron density around PLM C 1001:**

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

**Electron density around PLM A 801:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.