



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2026 – 10:09 AM JST

PDB ID : 26TP / pdb_000026tp
Title : Crystal structure of the Pseudomonas aeruginosa MlaC-MlaD complex in space group P1
Authors : Ozu, S.; Matsumoto, D.; Watanabe, Y.
Deposited on : 2026-05-14
Resolution : 2.56 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

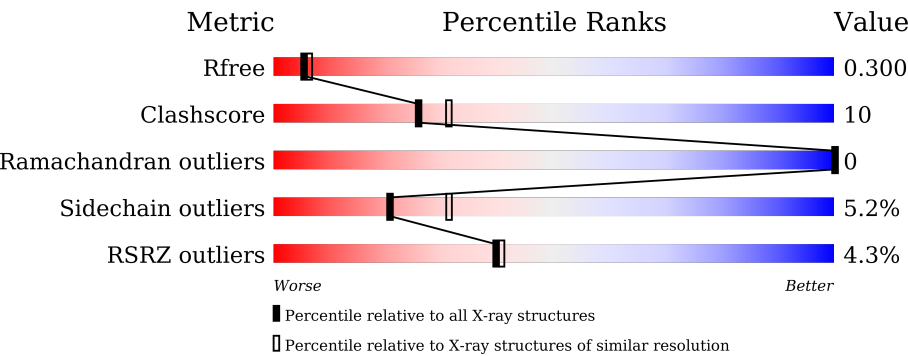
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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 ≥ 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	123	2% 69% 23% • 5%
1	B	123	% 67% 23% • 7%
1	C	123	2% 71% 19% • 10%
1	D	123	2% 71% 20% • 8%
1	E	123	3% 69% 22% • 7%
1	F	123	4% 69% 22% • 8%

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Mol	Chain	Length	Quality of chain
2	G	197	5% 80% 15% • 5%
2	H	197	5% 78% 18% •
2	I	197	8% 71% 22% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9211 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 Mce/MlaD domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	0	0
			839	527	138	173	1			
1	B	115	Total	C	N	O	S	0	0	0
			829	522	136	170	1			
1	C	111	Total	C	N	O	S	0	0	0
			797	503	128	165	1			
1	D	113	Total	C	N	O	S	0	0	0
			809	513	132	163	1			
1	E	114	Total	C	N	O	S	0	0	0
			801	506	126	168	1			
1	F	113	Total	C	N	O	S	0	0	0
			805	511	129	164	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	GLY	-	expression tag	UNP Q9HVVW3
A	36	PRO	-	expression tag	UNP Q9HVVW3
B	35	GLY	-	expression tag	UNP Q9HVVW3
B	36	PRO	-	expression tag	UNP Q9HVVW3
C	35	GLY	-	expression tag	UNP Q9HVVW3
C	36	PRO	-	expression tag	UNP Q9HVVW3
D	35	GLY	-	expression tag	UNP Q9HVVW3
D	36	PRO	-	expression tag	UNP Q9HVVW3
E	35	GLY	-	expression tag	UNP Q9HVVW3
E	36	PRO	-	expression tag	UNP Q9HVVW3
F	35	GLY	-	expression tag	UNP Q9HVVW3
F	36	PRO	-	expression tag	UNP Q9HVVW3

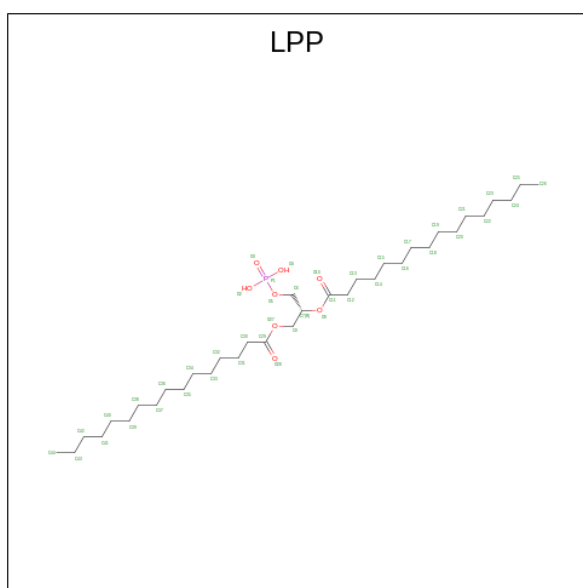
- Molecule 2 is a protein called Toluene tolerance protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	188	Total	C	N	O	S	0	0	0
			1357	858	229	265	5			
2	H	190	Total	C	N	O	S	0	0	0
			1380	865	236	274	5			
2	I	185	Total	C	N	O	S	0	0	0
			1347	845	230	267	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	19	GLY	-	expression tag	UNP Q9HVVW4
G	20	PRO	-	expression tag	UNP Q9HVVW4
G	21	HIS	-	expression tag	UNP Q9HVVW4
G	22	MET	-	expression tag	UNP Q9HVVW4
H	19	GLY	-	expression tag	UNP Q9HVVW4
H	20	PRO	-	expression tag	UNP Q9HVVW4
H	21	HIS	-	expression tag	UNP Q9HVVW4
H	22	MET	-	expression tag	UNP Q9HVVW4
I	19	GLY	-	expression tag	UNP Q9HVVW4
I	20	PRO	-	expression tag	UNP Q9HVVW4
I	21	HIS	-	expression tag	UNP Q9HVVW4
I	22	MET	-	expression tag	UNP Q9HVVW4

- Molecule 3 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	O	P	0	0
			44	35	8	1		
3	G	1	Total	C	O	P	0	0
			44	35	8	1		
3	H	1	Total	C	O	P	0	0
			44	35	8	1		
3	H	1	Total	C	O	P	0	0
			44	35	8	1		

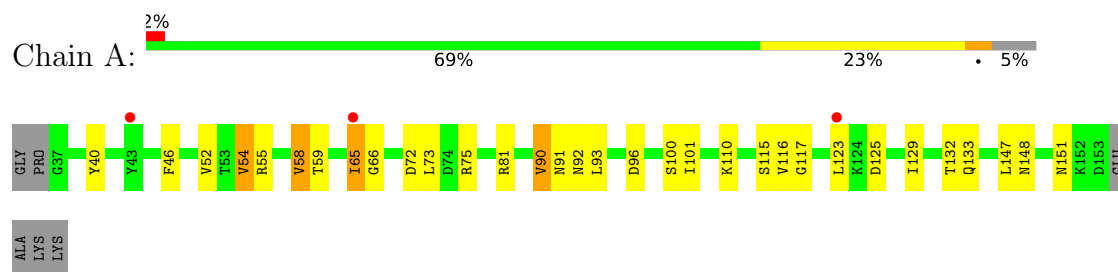
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	13	Total	O	0	0
			13	13		
4	C	8	Total	O	0	0
			8	8		
4	D	10	Total	O	0	0
			10	10		
4	E	5	Total	O	0	0
			5	5		
4	F	7	Total	O	0	0
			7	7		
4	G	4	Total	O	0	0
			4	4		
4	H	9	Total	O	0	0
			9	9		
4	I	8	Total	O	0	0
			8	8		

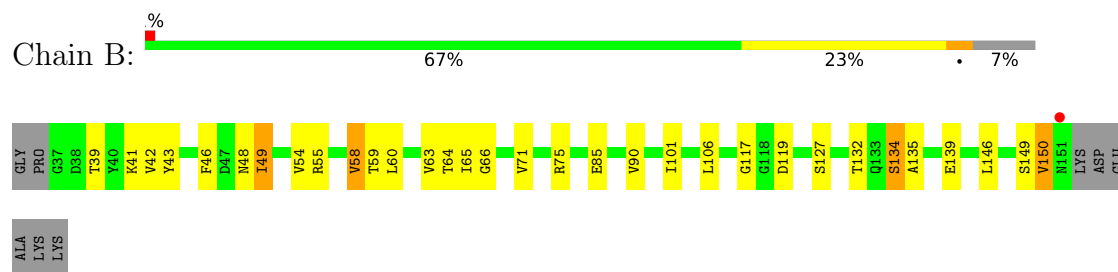
3 Residue-property plots [i](#)

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.

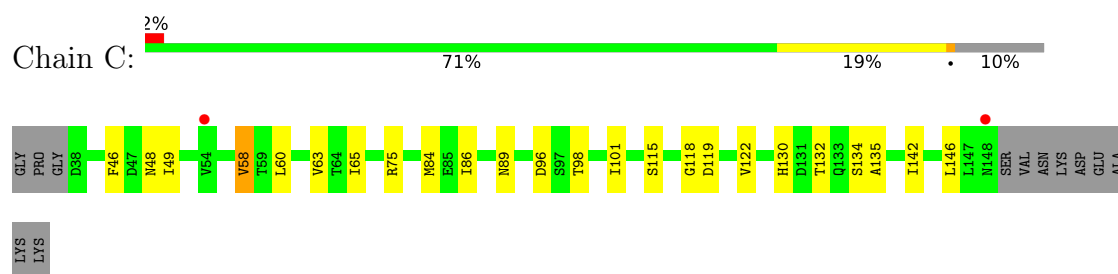
- Molecule 1: Mce/MlaD domain-containing protein



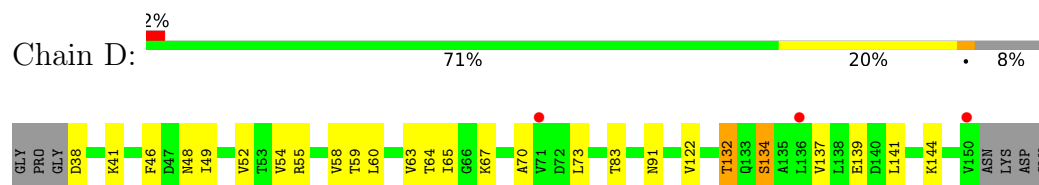
- Molecule 1: Mce/MlaD domain-containing protein



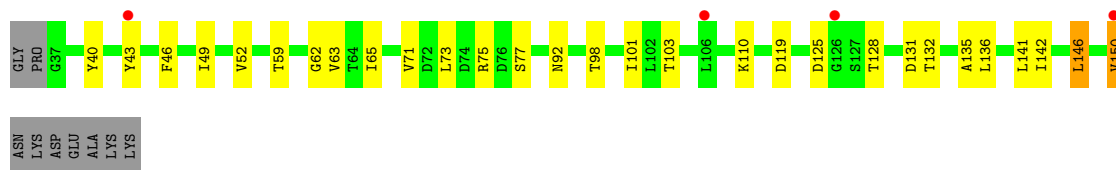
- Molecule 1: Mce/MlaD domain-containing protein



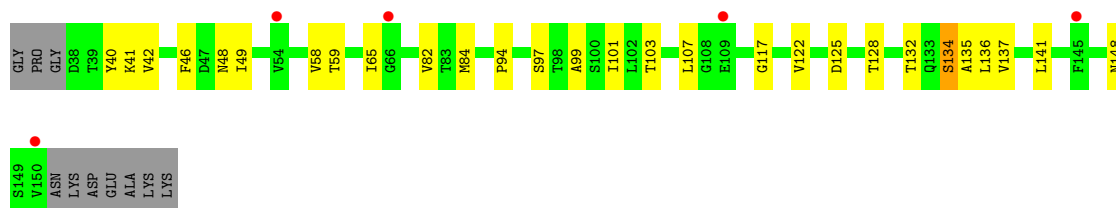
- Molecule 1: Mce/MlaD domain-containing protein



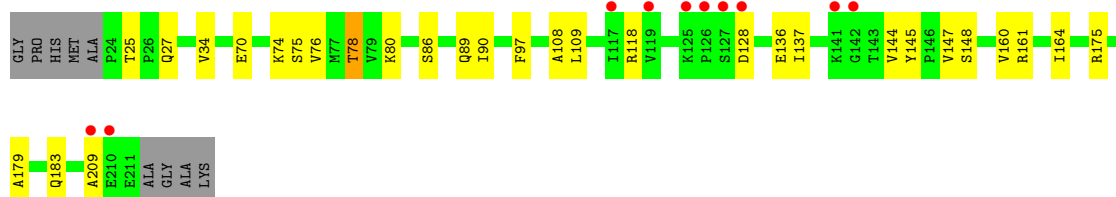
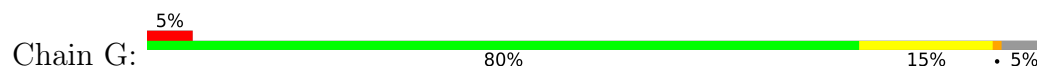
- Molecule 1: Mce/MlaD domain-containing protein



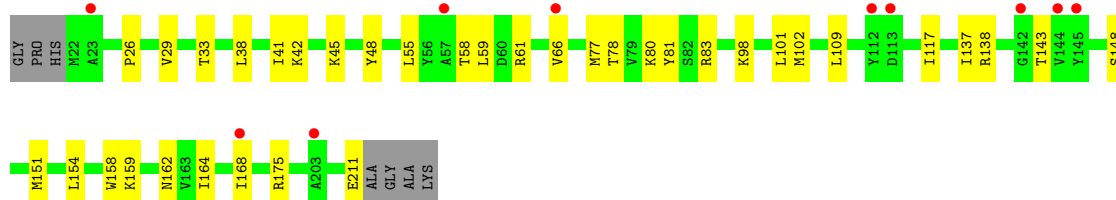
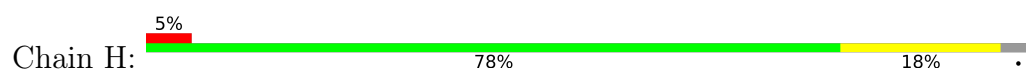
- Molecule 1: Mce/MlaD domain-containing protein



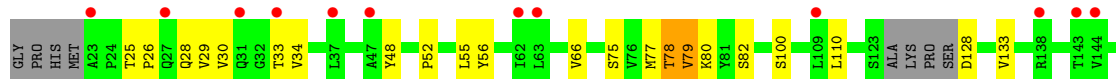
- Molecule 2: Toluene tolerance protein



- Molecule 2: Toluene tolerance protein



- Molecule 2: Toluene tolerance protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.71Å 88.64Å 88.81Å 64.65° 72.37° 72.28°	Depositor
Resolution (Å)	47.44 – 2.56 47.44 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.44-2.56) 98.7 (47.44-2.56)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.249 , 0.303 0.247 , 0.300	Depositor DCC
R_{free} test set	2662 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9211	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: LPP

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	0.14	0/846	0.35	0/1155
1	B	0.14	0/837	0.31	0/1141
1	C	0.14	0/805	0.31	0/1100
1	D	0.13	0/816	0.33	0/1112
1	E	0.12	0/809	0.31	0/1108
1	F	0.15	0/812	0.32	0/1109
2	G	0.13	0/1379	0.30	0/1881
2	H	0.15	0/1401	0.33	0/1910
2	I	0.13	0/1366	0.31	0/1860
All	All	0.14	0/9071	0.32	0/12376

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	839	0	818	18	0
1	B	829	0	811	20	0
1	C	797	0	770	15	0
1	D	809	0	802	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	801	0	765	18	0
1	F	805	0	793	15	0
2	G	1357	0	1272	22	0
2	H	1380	0	1296	24	0
2	I	1347	0	1260	34	0
3	G	88	0	134	8	0
3	H	88	0	134	5	0
4	A	7	0	0	0	0
4	B	13	0	0	1	0
4	C	8	0	0	1	0
4	D	10	0	0	1	0
4	E	5	0	0	0	0
4	F	7	0	0	0	0
4	G	4	0	0	0	0
4	H	9	0	0	2	0
4	I	8	0	0	1	0
All	All	9211	0	8855	171	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 10.

All (171) 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)
2:I:78:THR:HG22	2:I:80:LYS:H	1.48	0.78
1:D:60:LEU:HB2	1:D:65:ILE:HD11	1.66	0.78
1:E:136:LEU:HD13	1:E:141:LEU:HD21	1.66	0.77
2:I:30:VAL:HG21	2:I:133:VAL:HG11	1.66	0.76
2:G:86:SER:HB3	2:G:89:GLN:HG3	1.69	0.73
2:H:78:THR:HG22	2:H:80:LYS:H	1.53	0.73
1:E:49:ILE:HD13	1:E:71:VAL:HG21	1.70	0.73
2:H:38:LEU:HD21	2:H:117:ILE:HD12	1.73	0.69
1:C:60:LEU:HB2	1:C:65:ILE:HD13	1.75	0.68
1:C:75:ARG:NH1	1:D:91:ASN:OD1	2.27	0.68
2:G:78:THR:HG23	2:G:80:LYS:H	1.58	0.67
2:G:34:VAL:HG22	3:G:301:LPP:H411	1.75	0.67
2:I:25:THR:HG22	2:I:28:GLN:HG3	1.78	0.65
1:D:46:PHE:HA	1:D:132:THR:HG21	1.79	0.63
1:A:147:LEU:HA	2:G:209:ALA:HB1	1.80	0.63
2:H:33:THR:HG21	2:H:66:VAL:HG21	1.81	0.63
2:H:26:PRO:HD3	2:H:158:TRP:CE2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:THR:HG22	1:E:131:ASP:HB3	1.81	0.62
1:A:52:VAL:HG11	1:A:101:ILE:HD12	1.82	0.61
1:A:100:SER:OG	1:A:133:GLN:OE1	2.15	0.61
1:A:91:ASN:OD1	1:B:75:ARG:NH2	2.34	0.61
1:F:99:ALA:HB3	1:F:132:THR:HG22	1.82	0.61
1:A:58:VAL:HG22	1:A:65:ILE:HG23	1.82	0.61
2:I:79:VAL:HA	2:I:82:SER:HB3	1.83	0.61
1:D:144:LYS:NZ	4:D:201:HOH:O	2.32	0.60
1:A:96:ASP:HB3	1:A:117:GLY:HA3	1.85	0.59
1:E:150:VAL:HG23	1:F:148:ASN:HD21	1.68	0.59
1:C:142:ILE:HD12	1:D:141:LEU:HD11	1.86	0.58
1:A:54:VAL:O	1:A:55:ARG:HG2	2.05	0.57
1:C:119:ASP:OD1	2:G:161:ARG:NH2	2.37	0.57
1:B:117:GLY:HA2	2:H:175:ARG:HH12	1.70	0.57
2:I:176:ASP:O	2:I:180:ASP:N	2.36	0.56
2:I:133:VAL:HG13	2:I:149:TYR:HB2	1.88	0.56
1:A:75:ARG:NH1	1:C:89:ASN:O	2.39	0.55
1:F:101:ILE:HG21	1:F:135:ALA:HB2	1.89	0.55
1:B:54:VAL:HG12	1:B:55:ARG:HD2	1.88	0.55
1:A:92:ASN:OD1	1:A:92:ASN:N	2.39	0.55
2:H:162:ASN:ND2	4:H:402:HOH:O	2.40	0.54
2:I:177:GLN:O	2:I:181:THR:OG1	2.22	0.54
1:F:136:LEU:HD13	1:F:141:LEU:HD21	1.89	0.54
1:D:38:ASP:OD2	1:D:38:ASP:N	2.40	0.54
1:A:72:ASP:OD2	1:A:81:ARG:NH2	2.33	0.54
2:H:77:MET:O	2:H:78:THR:HB	2.07	0.53
2:I:29:VAL:O	2:I:33:THR:HG23	2.09	0.53
2:H:41:ILE:O	2:H:45:LYS:N	2.42	0.53
2:G:70:GLU:HG2	2:G:74:LYS:HE3	1.91	0.53
2:I:48:TYR:HB3	2:I:55:LEU:HB2	1.90	0.52
1:D:73:LEU:HD23	1:E:65:ILE:HD11	1.92	0.52
2:I:75:SER:HB2	2:I:161:ARG:HH21	1.74	0.52
1:E:40:TYR:HB2	1:E:125:ASP:HB2	1.92	0.52
1:E:142:ILE:O	1:E:146:LEU:HD22	2.10	0.52
2:G:179:ALA:O	2:G:183:GLN:HG3	2.11	0.51
2:H:29:VAL:O	2:H:33:THR:HG23	2.10	0.51
2:G:74:LYS:HE2	2:G:90:ILE:CG2	2.40	0.51
1:B:48:ASN:H	1:B:134:SER:HB3	1.76	0.51
1:B:59:THR:HG22	1:B:64:THR:HA	1.92	0.51
1:D:49:ILE:HG13	1:E:62:GLY:HA3	1.92	0.51
1:A:148:ASN:HD21	1:B:149:SER:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:TYR:HB3	2:H:55:LEU:HB2	1.93	0.50
2:G:148:SER:HB2	2:G:164:ILE:HB	1.91	0.50
1:B:41:LYS:NZ	1:B:43:TYR:OH	2.44	0.50
2:H:59:LEU:HD22	2:H:102:MET:HG2	1.93	0.50
1:C:49:ILE:HD11	1:D:63:VAL:HG22	1.93	0.50
1:E:119:ASP:OD1	2:I:161:ARG:NH2	2.45	0.49
1:C:84:MET:HE2	1:C:86:ILE:HD11	1.93	0.49
1:B:60:LEU:HB2	1:B:65:ILE:HD13	1.94	0.49
2:I:147:VAL:HG23	2:I:149:TYR:HE2	1.78	0.49
2:I:100:SER:HB3	2:I:200:VAL:HG11	1.94	0.49
1:C:98:THR:OG1	1:C:115:SER:HB3	2.12	0.49
2:I:48:TYR:HB2	2:I:110:LEU:HD21	1.95	0.49
1:B:46:PHE:CD1	1:B:132:THR:HB	2.48	0.49
2:I:169:ASN:HB3	2:I:172:LYS:HB3	1.94	0.49
1:D:48:ASN:N	1:D:134:SER:OG	2.45	0.48
2:G:75:SER:HB2	2:G:161:ARG:NH2	2.28	0.48
1:D:59:THR:HG22	1:D:64:THR:HA	1.94	0.48
1:E:101:ILE:HG21	1:E:135:ALA:HB2	1.96	0.48
1:F:94:PRO:HG2	1:F:117:GLY:H	1.79	0.48
1:D:55:ARG:HG2	1:D:67:LYS:HD2	1.96	0.47
1:B:146:LEU:O	1:B:150:VAL:HG12	2.15	0.47
2:I:128:ASP:HB3	2:I:158:TRP:HH2	1.79	0.47
1:A:123:LEU:HD21	1:A:129:ILE:HD11	1.96	0.47
1:F:42:VAL:HG23	1:F:84:MET:HE3	1.96	0.47
2:H:148:SER:HB3	2:H:164:ILE:HB	1.97	0.47
2:I:25:THR:N	2:I:28:GLN:HE21	2.13	0.47
1:B:119:ASP:O	4:B:201:HOH:O	2.20	0.46
2:I:179:ALA:O	2:I:183:GLN:HG3	2.15	0.46
1:F:46:PHE:HB2	1:F:49:ILE:HG23	1.96	0.46
2:I:147:VAL:HG12	2:I:165:ILE:HG23	1.97	0.46
2:G:147:VAL:HG21	3:G:302:LPP:H311	1.97	0.46
2:I:25:THR:HG22	2:I:28:GLN:CG	2.45	0.46
1:A:58:VAL:HG13	1:A:66:GLY:C	2.40	0.46
1:B:106:LEU:HD23	1:F:107:LEU:HD21	1.98	0.46
2:I:181:THR:HG22	2:I:185:ASN:OD1	2.16	0.46
1:D:70:ALA:HB3	1:D:83:THR:HB	1.98	0.46
3:G:302:LPP:H122	3:G:302:LPP:H152	1.52	0.46
1:D:60:LEU:HB2	1:D:65:ILE:CD1	2.39	0.45
1:B:46:PHE:CE1	1:B:132:THR:HB	2.51	0.45
2:G:109:LEU:HD21	3:G:301:LPP:H361	1.98	0.45
2:I:26:PRO:HD3	2:I:158:TRP:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HG13	1:A:90:VAL:HG21	1.98	0.45
2:I:206:THR:O	2:I:210:GLU:HG3	2.17	0.45
1:A:40:TYR:HB2	1:A:125:ASP:HB2	1.97	0.45
1:E:103:THR:OG1	1:E:110:LYS:NZ	2.50	0.45
2:I:172:LYS:NZ	2:I:175:ARG:HD2	2.31	0.45
2:H:80:LYS:HE2	2:H:81:TYR:CZ	2.52	0.44
1:E:52:VAL:HG21	1:E:101:ILE:HD12	1.98	0.44
2:I:77:MET:O	2:I:78:THR:HB	2.16	0.44
4:C:201:HOH:O	2:G:161:ARG:NH2	2.50	0.44
2:H:151:MET:HE3	2:H:151:MET:HB3	1.79	0.44
3:H:302:LPP:H151	3:H:302:LPP:H122	1.90	0.44
2:I:25:THR:OG1	2:I:26:PRO:HD2	2.18	0.44
1:B:117:GLY:HA2	2:H:175:ARG:NH1	2.33	0.44
1:F:48:ASN:N	1:F:134:SER:OG	2.49	0.44
2:H:101:LEU:HB3	3:H:302:LPP:H222	2.00	0.44
1:B:46:PHE:HB2	1:B:49:ILE:HG22	1.99	0.44
3:H:301:LPP:H382	3:H:302:LPP:H192	2.00	0.44
2:I:172:LYS:O	2:I:172:LYS:HD3	2.18	0.44
2:H:58:THR:HG23	2:H:61:ARG:NH2	2.33	0.43
1:F:58:VAL:HG21	1:F:84:MET:HB3	2.00	0.43
2:G:74:LYS:HE2	2:G:90:ILE:HG21	2.00	0.43
2:H:117:ILE:HG23	2:H:137:ILE:HG12	2.01	0.43
2:H:168:ILE:HD11	2:H:211:GLU:OE2	2.19	0.43
3:G:301:LPP:H151	3:G:302:LPP:H322	2.00	0.43
2:G:137:ILE:HB	2:G:145:TYR:HB2	2.01	0.43
3:G:301:LPP:HC61	3:G:302:LPP:O5	2.18	0.43
3:G:302:LPP:H191	3:G:302:LPP:H161	1.57	0.43
1:C:48:ASN:N	1:C:134:SER:OG	2.52	0.43
1:C:58:VAL:HG11	1:C:84:MET:HG2	2.01	0.43
1:C:101:ILE:HG21	1:C:135:ALA:HB2	2.01	0.43
1:E:65:ILE:HD13	1:E:65:ILE:HA	1.83	0.43
2:G:76:VAL:HG21	2:G:97:PHE:HE2	1.84	0.43
1:A:101:ILE:HG22	1:A:110:LYS:HD2	2.01	0.42
1:C:46:PHE:CE1	1:C:132:THR:HB	2.55	0.42
1:C:130:HIS:CE1	2:G:128:ASP:HA	2.55	0.42
1:F:40:TYR:HB2	1:F:125:ASP:HB2	2.01	0.42
2:G:25:THR:HG22	2:G:27:GLN:H	1.85	0.42
2:H:138:ARG:HA	2:H:143:THR:O	2.19	0.42
2:H:154:LEU:HD22	2:H:159:LYS:HD3	2.00	0.42
1:E:75:ARG:C	1:E:77:SER:H	2.27	0.42
1:C:146:LEU:HD23	1:C:146:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:108:ALA:HB1	3:G:301:LPP:HC82	2.01	0.42
2:G:118:ARG:O	2:G:136:GLU:N	2.39	0.42
1:C:96:ASP:CG	1:C:118:GLY:H	2.25	0.42
1:D:41:LYS:HB2	1:D:41:LYS:HE2	1.71	0.42
2:G:70:GLU:O	2:G:74:LYS:HD3	2.18	0.42
1:A:46:PHE:CE2	1:A:132:THR:HB	2.54	0.42
1:B:63:VAL:HG22	1:F:49:ILE:HD11	2.02	0.42
1:D:139:GLU:OE1	1:D:139:GLU:N	2.52	0.42
1:A:148:ASN:HA	1:A:151:ASN:HD21	1.84	0.41
2:H:109:LEU:HD21	3:H:302:LPP:H182	2.02	0.41
2:I:148:SER:HB3	2:I:164:ILE:HB	2.03	0.41
1:B:39:THR:OG1	1:B:85:GLU:OE2	2.35	0.41
1:E:92:ASN:OD1	1:E:92:ASN:N	2.51	0.41
2:I:162:ASN:ND2	2:I:169:ASN:OD1	2.51	0.41
1:E:43:TYR:HB2	1:E:128:THR:HG22	2.01	0.41
1:E:46:PHE:CE2	1:E:132:THR:HB	2.56	0.41
2:G:75:SER:O	2:G:175:ARG:NE	2.54	0.41
1:B:58:VAL:HG13	1:B:66:GLY:C	2.46	0.41
1:B:101:ILE:HG21	1:B:135:ALA:HB2	2.03	0.41
1:E:73:LEU:HD22	1:F:65:ILE:HD11	2.03	0.41
1:F:94:PRO:O	1:F:97:SER:HB2	2.21	0.41
2:H:101:LEU:HD23	2:H:101:LEU:HA	1.97	0.41
3:H:302:LPP:H172	3:H:302:LPP:H141	1.64	0.41
1:F:41:LYS:HA	1:F:84:MET:O	2.20	0.41
2:I:33:THR:HG21	2:I:66:VAL:HG21	2.03	0.41
1:B:139:GLU:N	1:B:139:GLU:OE2	2.54	0.40
2:H:83:ARG:NH1	4:H:404:HOH:O	2.47	0.40
2:I:30:VAL:O	2:I:34:VAL:HG12	2.22	0.40
2:I:166:ASN:O	2:I:168:ILE:HG13	2.21	0.40
2:I:52:PRO:HB2	2:I:56:TYR:CZ	2.56	0.40
2:I:162:ASN:ND2	4:I:303:HOH:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	115/123 (94%)	111 (96%)	4 (4%)	0	100	100
1	B	113/123 (92%)	109 (96%)	4 (4%)	0	100	100
1	C	109/123 (89%)	105 (96%)	4 (4%)	0	100	100
1	D	111/123 (90%)	103 (93%)	8 (7%)	0	100	100
1	E	112/123 (91%)	104 (93%)	8 (7%)	0	100	100
1	F	111/123 (90%)	106 (96%)	5 (4%)	0	100	100
2	G	186/197 (94%)	174 (94%)	12 (6%)	0	100	100
2	H	188/197 (95%)	178 (95%)	10 (5%)	0	100	100
2	I	181/197 (92%)	171 (94%)	10 (6%)	0	100	100
All	All	1226/1329 (92%)	1161 (95%)	65 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	88/101 (87%)	79 (90%)	9 (10%)	7	9
1	B	87/101 (86%)	79 (91%)	8 (9%)	8	11
1	C	83/101 (82%)	80 (96%)	3 (4%)	31	44
1	D	84/101 (83%)	77 (92%)	7 (8%)	10	15
1	E	83/101 (82%)	79 (95%)	4 (5%)	23	34
1	F	84/101 (83%)	77 (92%)	7 (8%)	10	15
2	G	130/163 (80%)	127 (98%)	3 (2%)	44	60
2	H	135/163 (83%)	133 (98%)	2 (2%)	57	71
2	I	131/163 (80%)	127 (97%)	4 (3%)	35	50
All	All	905/1095 (83%)	858 (95%)	47 (5%)	21	31

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	58	VAL
1	A	59	THR
1	A	65	ILE
1	A	73	LEU
1	A	90	VAL
1	A	93	LEU
1	A	115	SER
1	A	116	VAL
1	B	42	VAL
1	B	49	ILE
1	B	58	VAL
1	B	71	VAL
1	B	90	VAL
1	B	127	SER
1	B	134	SER
1	B	150	VAL
1	C	58	VAL
1	C	63	VAL
1	C	122	VAL
1	D	52	VAL
1	D	54	VAL
1	D	58	VAL
1	D	122	VAL
1	D	132	THR
1	D	134	SER
1	D	137	VAL
1	E	59	THR
1	E	63	VAL
1	E	146	LEU
1	E	150	VAL
1	F	59	THR
1	F	82	VAL
1	F	103	THR
1	F	122	VAL
1	F	128	THR
1	F	134	SER
1	F	137	VAL
2	G	78	THR
2	G	144	VAL
2	G	160	VAL
2	H	42	LYS

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Mol	Chain	Res	Type
2	H	98	LYS
2	I	78	THR
2	I	79	VAL
2	I	181	THR
2	I	199	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	ASN
1	B	130	HIS
1	C	133	GLN
2	G	31	GLN
2	G	44	ASN
2	G	103	GLN
2	G	183	GLN
2	G	185	ASN
2	H	28	GLN
2	I	28	GLN
2	I	99	ASN
2	I	177	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	LPP	G	301	-	43,43,43	1.04	2 (4%)	47,48,48	1.19	2 (4%)
3	LPP	H	302	-	43,43,43	1.04	2 (4%)	47,48,48	1.14	2 (4%)
3	LPP	H	301	-	43,43,43	1.06	2 (4%)	47,48,48	1.12	2 (4%)
3	LPP	G	302	-	43,43,43	1.05	2 (4%)	47,48,48	1.09	3 (6%)

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	LPP	G	301	-	-	28/45/45/45	-
3	LPP	H	302	-	-	25/45/45/45	-
3	LPP	H	301	-	-	20/45/45/45	-
3	LPP	G	302	-	-	22/45/45/45	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	302	LPP	O27-C29	3.18	1.42	1.33
3	H	301	LPP	O27-C29	3.17	1.42	1.33
3	G	302	LPP	O27-C29	3.14	1.42	1.33
3	G	301	LPP	O27-C29	3.09	1.42	1.33
3	G	302	LPP	O9-C11	3.04	1.42	1.34
3	H	301	LPP	O9-C11	3.01	1.42	1.34
3	G	301	LPP	O9-C11	3.00	1.42	1.34
3	H	302	LPP	O9-C11	2.94	1.42	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	301	LPP	O9-C11-C12	4.00	120.12	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	LPP	O9-C11-C12	3.95	120.02	111.50
3	H	302	LPP	O9-C11-C12	3.77	119.63	111.50
3	G	302	LPP	O9-C11-C12	3.64	119.35	111.50
3	H	301	LPP	O27-C29-C30	2.71	120.41	111.91
3	G	302	LPP	O27-C29-C30	2.63	120.17	111.91
3	G	301	LPP	O27-C29-C30	2.55	119.92	111.91
3	H	302	LPP	O27-C29-C30	2.47	119.67	111.91
3	G	302	LPP	C7-O9-C11	-2.10	112.62	117.79

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	301	LPP	O9-C7-C8-O27
3	G	301	LPP	C12-C11-O9-C7
3	G	302	LPP	C12-C11-O9-C7
3	H	301	LPP	O5-C6-C7-O9
3	H	301	LPP	C12-C11-O9-C7
3	H	302	LPP	O9-C7-C8-O27
3	G	301	LPP	O10-C11-O9-C7
3	G	302	LPP	O10-C11-O9-C7
3	H	301	LPP	O10-C11-O9-C7
3	G	302	LPP	C30-C29-O27-C8
3	G	302	LPP	O28-C29-O27-C8
3	G	302	LPP	C16-C17-C18-C19
3	H	302	LPP	C30-C29-O27-C8
3	H	302	LPP	O28-C29-O27-C8
3	G	302	LPP	C12-C13-C14-C15
3	H	301	LPP	C37-C38-C39-C40
3	G	302	LPP	C11-C12-C13-C14
3	H	301	LPP	C29-C30-C31-C32
3	G	301	LPP	C11-C12-C13-C14
3	G	302	LPP	C29-C30-C31-C32
3	H	302	LPP	C11-C12-C13-C14
3	H	301	LPP	C13-C14-C15-C16
3	G	301	LPP	C38-C39-C40-C41
3	H	302	LPP	C21-C22-C23-C24
3	G	301	LPP	C13-C14-C15-C16
3	H	302	LPP	C34-C35-C36-C37
3	H	301	LPP	C20-C21-C22-C23
3	G	302	LPP	C30-C31-C32-C33
3	H	301	LPP	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	H	301	LPP	C32-C33-C34-C35
3	H	302	LPP	C38-C39-C40-C41
3	G	301	LPP	C18-C19-C20-C21
3	H	302	LPP	C14-C15-C16-C17
3	H	302	LPP	C19-C20-C21-C22
3	H	302	LPP	C37-C38-C39-C40
3	G	302	LPP	C32-C33-C34-C35
3	G	301	LPP	C36-C37-C38-C39
3	G	301	LPP	C19-C20-C21-C22
3	G	302	LPP	C33-C34-C35-C36
3	G	301	LPP	C32-C33-C34-C35
3	G	301	LPP	C40-C41-C42-C43
3	H	301	LPP	C6-C7-C8-O27
3	H	302	LPP	C31-C32-C33-C34
3	G	301	LPP	C29-C30-C31-C32
3	H	301	LPP	C35-C36-C37-C38
3	G	302	LPP	C34-C35-C36-C37
3	H	302	LPP	C12-C11-O9-C7
3	H	302	LPP	O10-C11-O9-C7
3	G	301	LPP	C22-C23-C24-C25
3	G	301	LPP	C21-C22-C23-C24
3	H	302	LPP	C35-C36-C37-C38
3	G	301	LPP	C6-C7-C8-O27
3	G	301	LPP	C17-C18-C19-C20
3	H	302	LPP	C16-C17-C18-C19
3	H	301	LPP	C33-C34-C35-C36
3	H	302	LPP	C32-C33-C34-C35
3	H	301	LPP	C15-C16-C17-C18
3	G	301	LPP	C30-C29-O27-C8
3	H	301	LPP	C18-C19-C20-C21
3	H	302	LPP	O5-C6-C7-C8
3	H	302	LPP	C40-C41-C42-C43
3	G	302	LPP	C35-C36-C37-C38
3	G	301	LPP	C20-C21-C22-C23
3	G	301	LPP	C30-C31-C32-C33
3	G	301	LPP	O28-C29-O27-C8
3	G	302	LPP	C23-C24-C25-C26
3	G	301	LPP	C41-C42-C43-C44
3	H	301	LPP	C41-C42-C43-C44
3	H	301	LPP	O5-C6-C7-C8
3	G	301	LPP	C14-C15-C16-C17
3	H	302	LPP	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
3	G	302	LPP	C15-C16-C17-C18
3	H	302	LPP	C6-C7-C8-O27
3	G	301	LPP	O5-C6-C7-O9
3	H	302	LPP	O5-C6-C7-O9
3	G	302	LPP	C19-C20-C21-C22
3	G	302	LPP	O9-C7-C8-O27
3	H	301	LPP	O9-C7-C8-O27
3	G	301	LPP	C39-C40-C41-C42
3	G	301	LPP	O5-C6-C7-C8
3	G	301	LPP	C31-C32-C33-C34
3	H	302	LPP	C6-O5-P1-O3
3	G	301	LPP	C37-C38-C39-C40
3	G	301	LPP	C7-C6-O5-P1
3	H	301	LPP	C38-C39-C40-C41
3	H	301	LPP	O27-C29-C30-C31
3	G	302	LPP	C14-C15-C16-C17
3	H	302	LPP	C18-C19-C20-C21
3	G	302	LPP	C36-C37-C38-C39
3	G	302	LPP	C6-C7-C8-O27
3	H	302	LPP	C36-C37-C38-C39
3	H	301	LPP	C34-C35-C36-C37
3	H	302	LPP	C30-C31-C32-C33
3	G	302	LPP	C38-C39-C40-C41
3	G	302	LPP	C21-C22-C23-C24

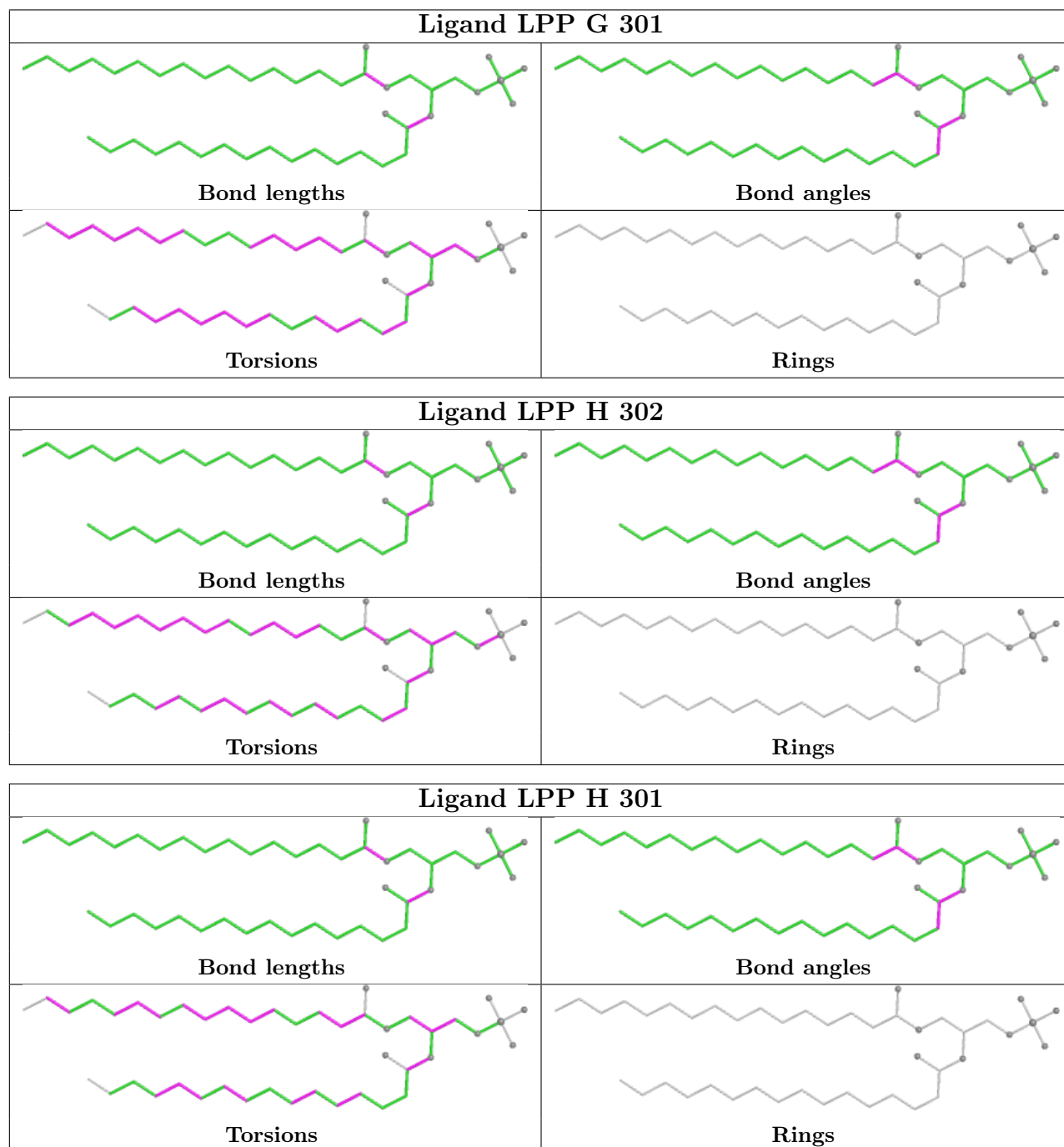
There are no ring outliers.

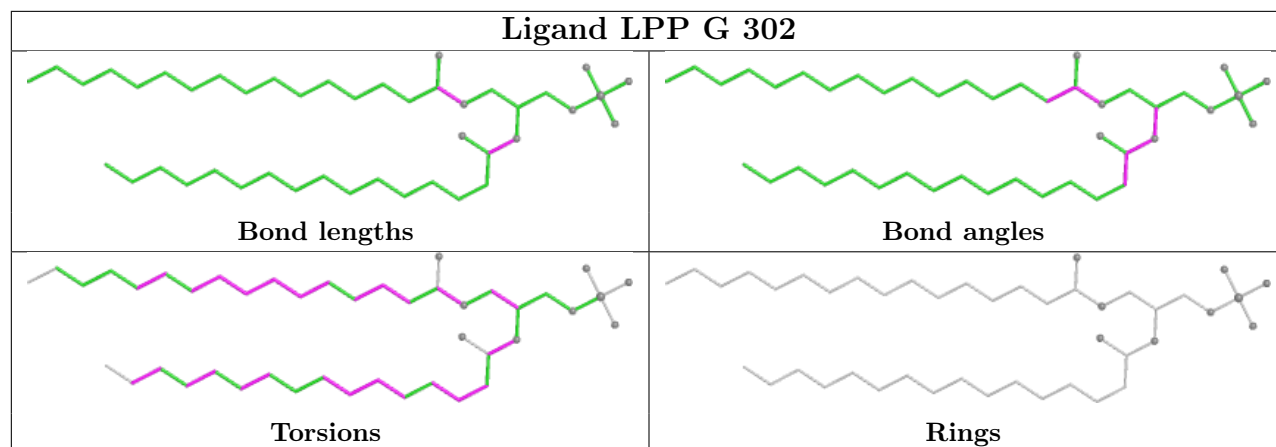
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	301	LPP	5	0
3	H	302	LPP	5	0
3	H	301	LPP	1	0
3	G	302	LPP	5	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, 95th 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 ²)	Q<0.9
1	A	117/123 (95%)	0.38	3 (2%) 57 59	39, 59, 91, 103	0
1	B	115/123 (93%)	0.07	1 (0%) 81 83	33, 48, 79, 106	0
1	C	111/123 (90%)	0.39	2 (1%) 67 69	38, 51, 72, 93	0
1	D	113/123 (91%)	0.49	3 (2%) 56 58	44, 65, 83, 92	0
1	E	114/123 (92%)	0.54	4 (3%) 47 48	44, 65, 87, 100	0
1	F	113/123 (91%)	0.44	5 (4%) 39 40	36, 60, 81, 94	0
2	G	188/197 (95%)	0.50	10 (5%) 32 32	50, 67, 97, 132	0
2	H	190/197 (96%)	0.55	10 (5%) 32 32	38, 70, 105, 119	0
2	I	185/197 (93%)	0.82	15 (8%) 18 18	42, 84, 116, 125	0
All	All	1246/1329 (93%)	0.49	53 (4%) 40 41	33, 64, 102, 132	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	167	GLY	3.9
2	G	128	ASP	3.8
2	G	126	PRO	3.7
2	H	168	ILE	3.6
2	G	127	SER	3.1
2	H	203	ALA	3.1
2	I	148	SER	3.1
2	H	57	ALA	3.0
2	I	23	ALA	3.0
1	D	136	LEU	3.0
1	A	43	TYR	3.0
1	E	126	GLY	2.8
2	G	209	ALA	2.8
1	F	66	GLY	2.7
2	I	143	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	112	TYR	2.6
2	G	141	LYS	2.6
2	I	33	THR	2.6
2	G	117	ILE	2.5
1	A	65	ILE	2.5
2	I	31	GLN	2.4
1	B	151	ASN	2.4
1	C	148	ASN	2.4
2	H	144	VAL	2.4
2	G	210	GLU	2.4
2	I	27	GLN	2.4
1	F	54	VAL	2.4
2	H	23	ALA	2.4
1	D	71	VAL	2.4
1	E	150	VAL	2.4
2	I	63	LEU	2.4
1	F	109	GLU	2.4
2	I	164	ILE	2.3
1	F	145	PHE	2.3
2	G	142	GLY	2.3
1	E	106	LEU	2.3
2	I	62	ILE	2.3
2	I	109	LEU	2.3
1	C	54	VAL	2.3
2	I	138	ARG	2.3
2	I	144	VAL	2.2
2	I	47	ALA	2.2
1	D	150	VAL	2.2
2	G	125	LYS	2.2
2	H	145	TYR	2.2
1	F	150	VAL	2.1
2	H	113	ASP	2.1
2	I	37	LEU	2.1
2	G	119	VAL	2.1
2	H	66	VAL	2.0
1	A	123	LEU	2.0
2	H	142	GLY	2.0
1	E	43	TYR	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](#)

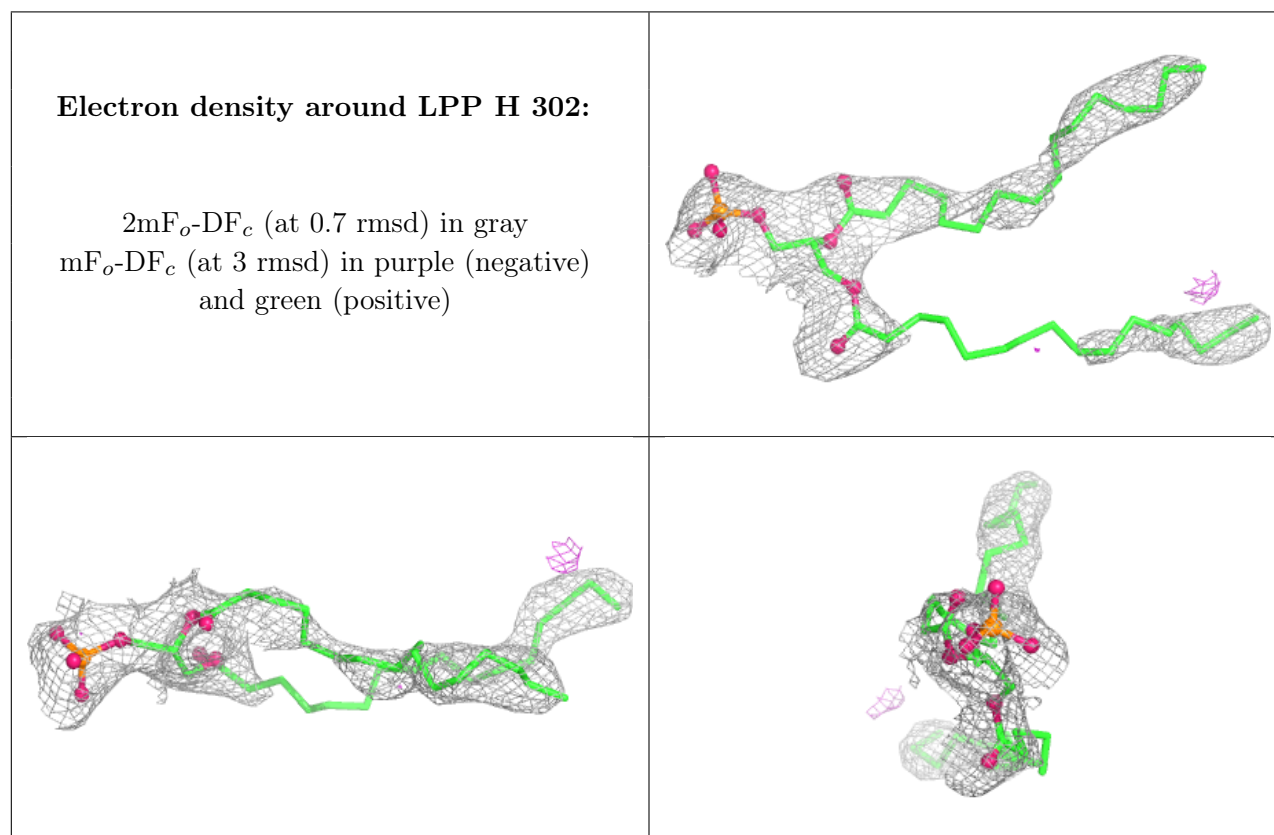
There are no oligosaccharides in this entry.

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, 95th 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.

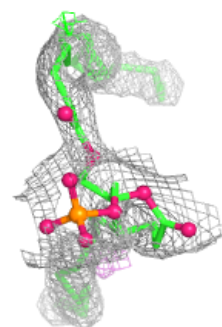
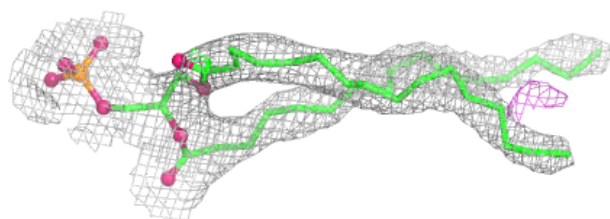
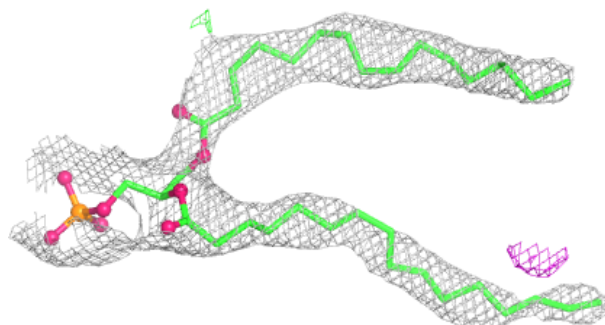
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LPP	H	302	44/44	0.82	0.17	61,94,125,139	0
3	LPP	G	301	44/44	0.88	0.14	56,73,119,135	0
3	LPP	H	301	44/44	0.89	0.14	46,79,120,129	0
3	LPP	G	302	44/44	0.89	0.14	46,70,117,129	0

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.

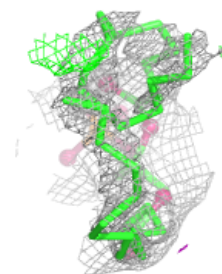
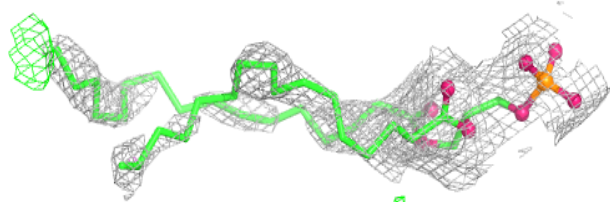
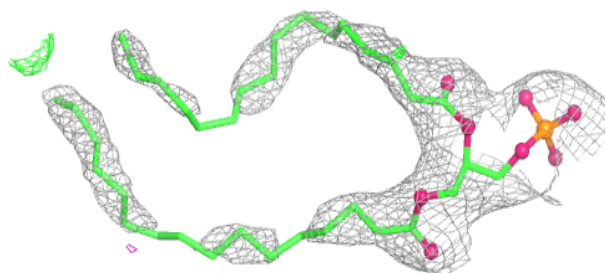


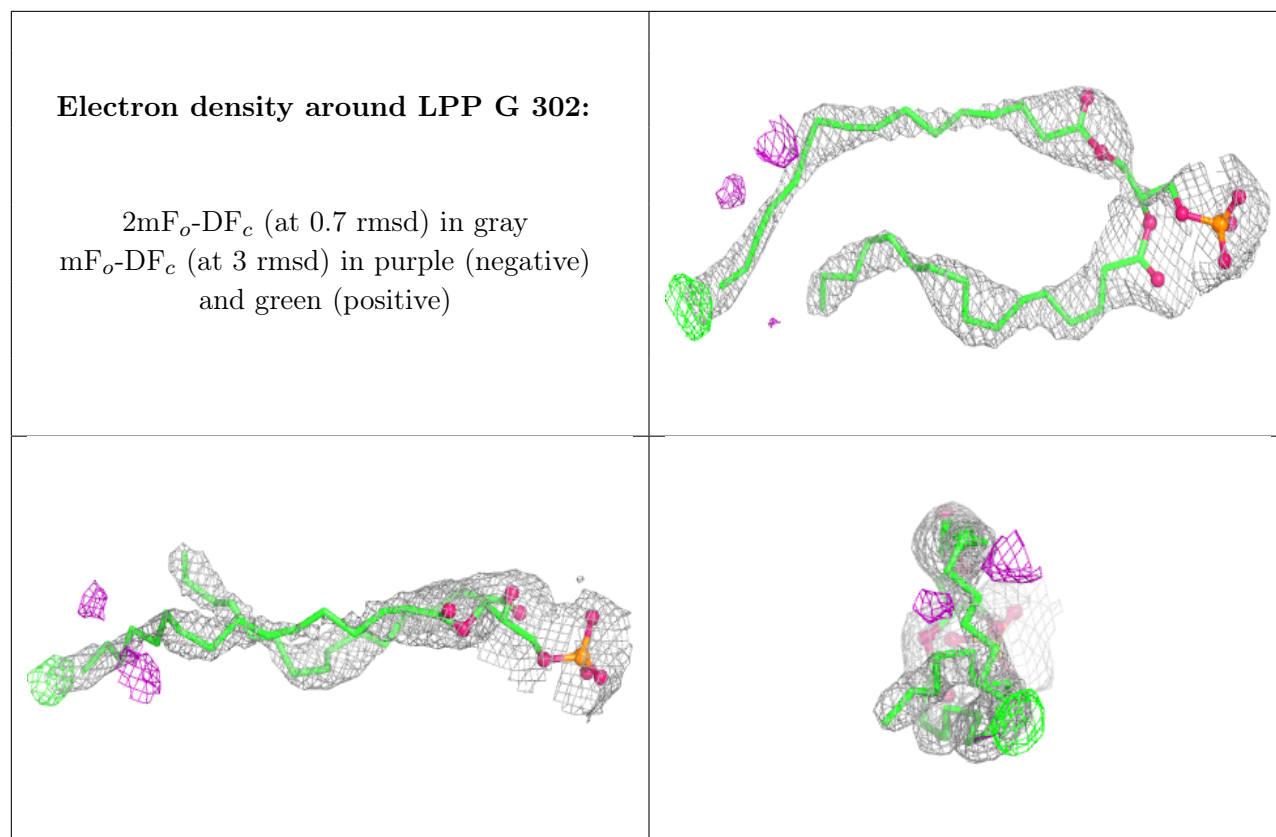
Electron density around LPP G 301:

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

**Electron density around LPP H 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.