



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2024 – 12:08 PM EDT

PDB ID : 4G4S  
Title : Structure of Proteasome-Pba1-Pba2 Complex  
Authors : Kish-Trier, E.; Robinson, H.; Stadtmueller, B.M.; Hill, C.P.  
Deposited on : 2012-07-16  
Resolution : 2.49 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>.

---

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

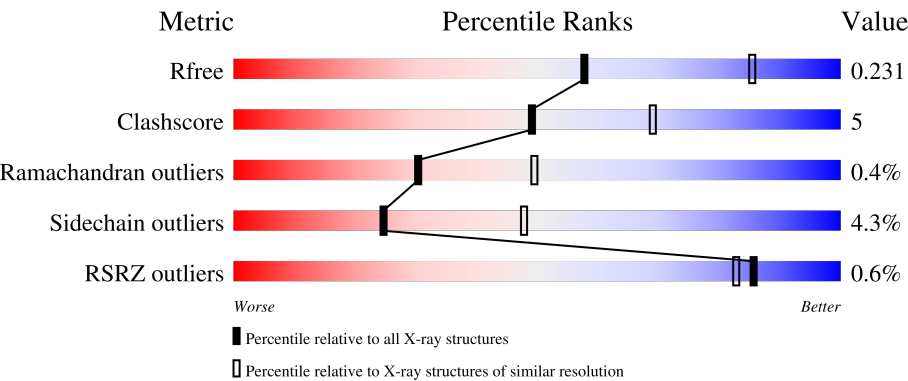
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

# 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 2.49 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 <sub>free</sub>	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	252	<div><div></div><div>82%12%••</div></div>
2	B	250	<div><div></div><div>82%15%••</div></div>
3	C	258	<div><div>%</div><div>76%14%•8%</div></div>
4	D	254	<div><div></div><div>71%13%•13%</div></div>
5	E	261	<div><div></div><div>82%12%••</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
6	F	235	 82% 17% .
7	G	288	 % 75% 9% • 15%
8	H	196	 93% 7%
9	I	232	 81% 13% 5%
10	J	205	 85% 13% .
11	K	198	 85% 13% ..
12	L	212	 92% 7%
13	M	222	 87% 12% .
14	N	233	 85% 14% .
15	O	276	 2% 58% 12% • 28%
16	P	269	 3% 49% 19% • 29%

## 2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 28531 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 Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1912	1216	320	368	8			

- Molecule 2 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	246	Total	C	N	O	S	0	0	0
			1881	1200	308	370	3			

- Molecule 3 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1855	1175	308	369	3			

- Molecule 4 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	220	Total	C	N	O	S	0	0	0
			1722	1081	298	339	4			

- Molecule 5 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	250	Total	C	N	O	S	0	0	0
			1927	1206	324	389	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ACE	-	acetylation	UNP P32379

- Molecule 6 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	235	Total	C	N	O	S	0	0	0
			1806	1136	313	352	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ACE	-	acetylation	UNP P40302

- Molecule 7 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	246	Total	C	N	O	S	0	0	0
			1909	1213	331	360	5			

- Molecule 8 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 9 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	220	Total	C	N	O	S	0	0	0
			1670	1054	291	319	6			

- Molecule 10 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	203	Total	C	N	O	S	0	0	0
			1575	1007	257	303	8			

- Molecule 11 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 12 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 13 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 14 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 15 is a protein called Proteasome chaperone 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	200	Total	C	N	O	S	0	0	0
			1544	1004	238	290	12			

- Molecule 16 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	190	Total	C	N	O	S	0	0	0
			1544	1004	242	290	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-1	GLY	-	expression tag	UNP P36040
P	0	PRO	-	expression tag	UNP P36040

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

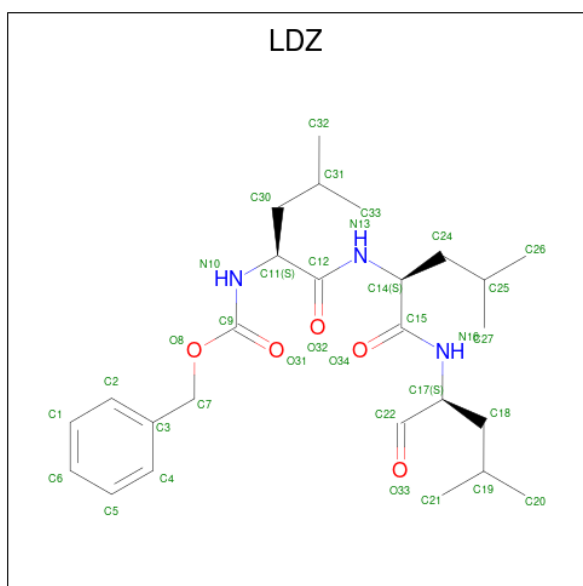
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		
17	H	1	Total	Mg	0	0
			1	1		
17	I	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	2	Total	Mg	0	0
			2	2		
17	L	1	Total	Mg	0	0
			1	1		
17	M	2	Total	Mg	0	0
			2	2		

- Molecule 18 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucinamide (three-letter code: LDZ) (formula: C<sub>26</sub>H<sub>41</sub>N<sub>3</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	L	1	Total	C	N	O	0	0
			34	26	3	5		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	81	Total	O	0	0
			81	81		
19	B	30	Total	O	0	0
			30	30		
19	C	31	Total	O	0	0
			31	31		
19	D	29	Total	O	0	0
			29	29		
19	E	49	Total	O	0	0
			49	49		

Continued on next page...

*Continued from previous page...*

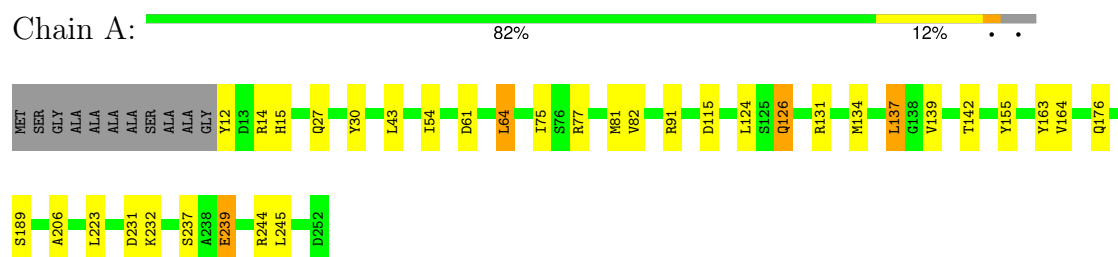
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	F	43	Total 43	O 43	0	0
19	G	53	Total 53	O 53	0	0
19	H	82	Total 82	O 82	0	0
19	I	65	Total 65	O 65	0	0
19	J	69	Total 69	O 69	0	0
19	K	61	Total 61	O 61	0	0
19	L	55	Total 55	O 55	0	0
19	M	81	Total 81	O 81	0	0
19	N	100	Total 100	O 100	0	0
19	O	6	Total 6	O 6	0	0
19	P	11	Total 11	O 11	0	0



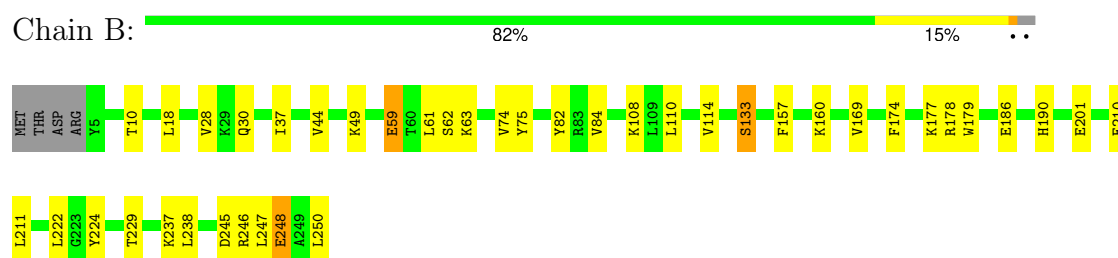
### 3 Residue-property plots [i](#)

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.

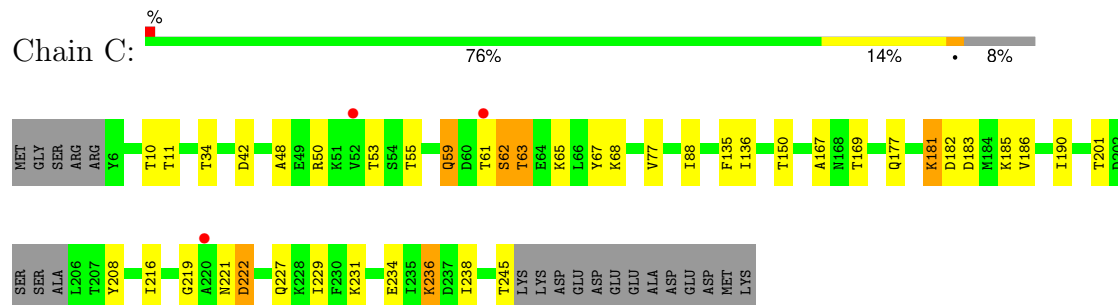
- Molecule 1: Proteasome component C7-alpha



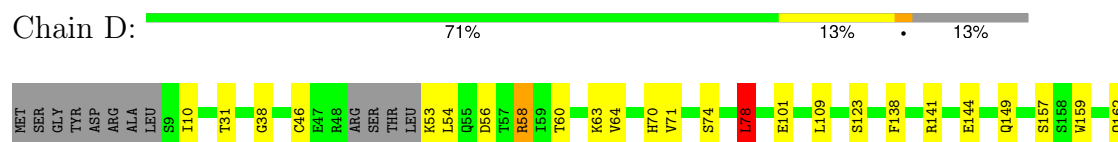
- Molecule 2: Proteasome component Y7

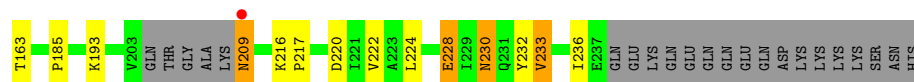


- Molecule 3: Proteasome component Y13



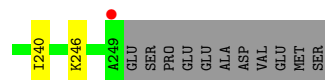
- Molecule 4: Proteasome component PRE6





• Molecule 5: Proteasome component PUP2

Chain E: 82% 12% . .



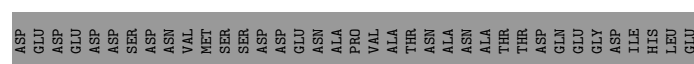
• Molecule 6: Proteasome component PRE5

Chain F: 82% 17% .



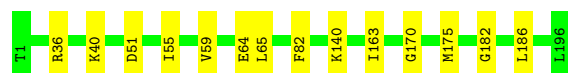
• Molecule 7: Proteasome component C1

Chain G: % 75% 9% 15%



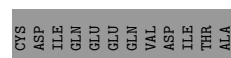
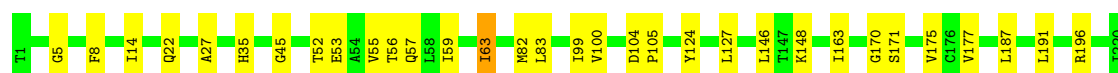
• Molecule 8: Proteasome component PRE3

Chain H: 93% 7%

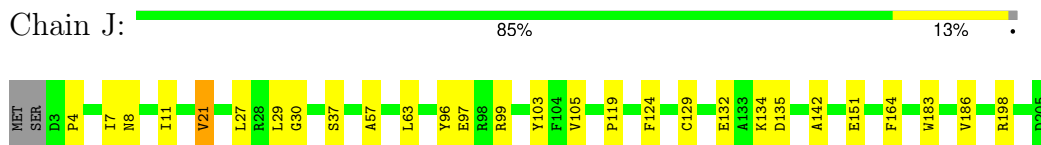


• Molecule 9: Proteasome component PUP1

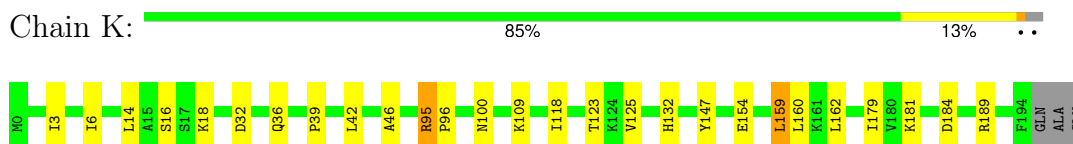
Chain I: 81% 13% 5%



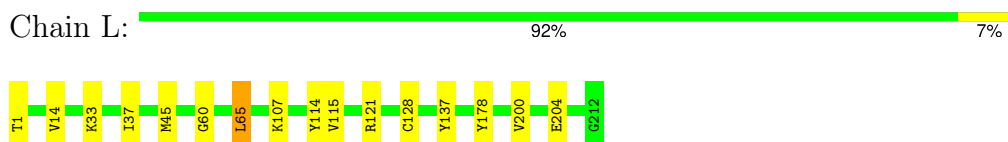
- Molecule 10: Proteasome component PUP3



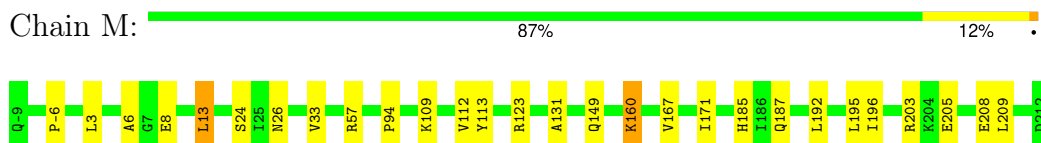
- Molecule 11: Proteasome component C11



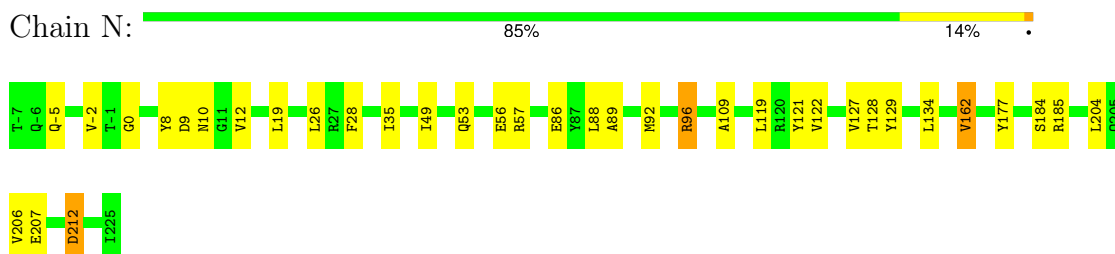
- Molecule 12: Proteasome component PRE2



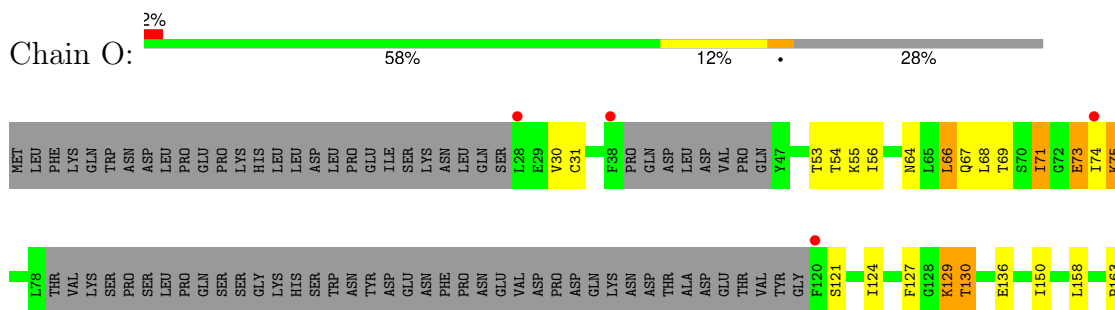
- Molecule 13: Proteasome component C5

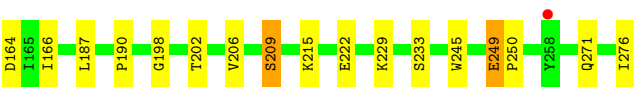


- Molecule 14: Proteasome component PRE4

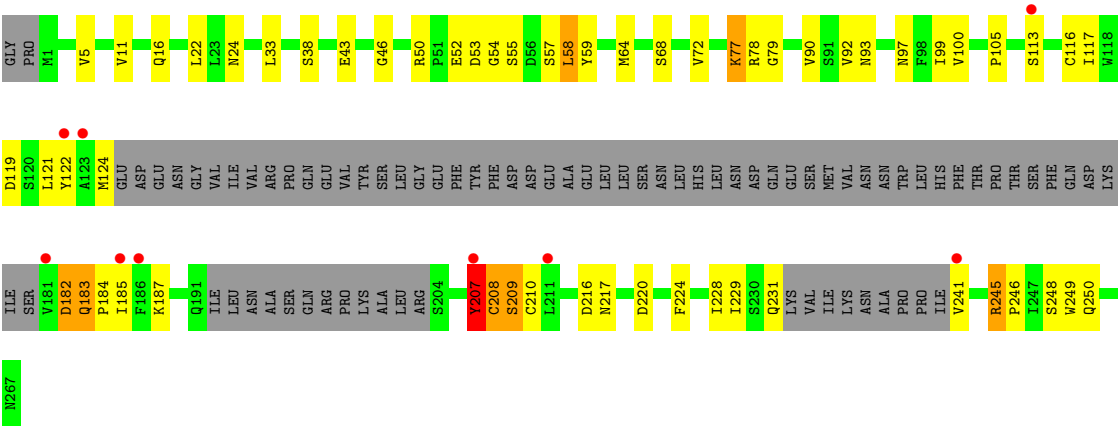


- Molecule 15: Proteasome chaperone 1





● Molecule 16: Proteasome assembly chaperone 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.41Å 182.51Å 388.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 2.49 29.78 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.78-2.49) 93.4 (29.78-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-0.46 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.183 , 0.232 0.184 , 0.231	Depositor DCC
$R_{free}$ test set	2267 reflections (1.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28531	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: ACE, MG, LDZ

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	0.43	0/1950	0.61	0/2640
2	B	0.38	0/1918	0.55	0/2597
3	C	0.34	0/1884	0.54	0/2551
4	D	0.38	0/1748	0.55	0/2367
5	E	0.39	0/1952	0.61	1/2630 (0.0%)
6	F	0.40	0/1832	0.59	1/2475 (0.0%)
7	G	0.40	0/1949	0.56	0/2631
8	H	0.42	0/1541	0.59	0/2087
9	I	0.42	0/1701	0.57	0/2307
10	J	0.41	0/1605	0.57	0/2166
11	K	0.42	0/1589	0.59	0/2142
12	L	0.44	0/1681	0.60	0/2274
13	M	0.43	0/1795	0.57	0/2420
14	N	0.44	0/1855	0.64	0/2514
15	O	0.35	0/1577	0.57	0/2132
16	P	0.37	0/1579	0.56	0/2139
All	All	0.40	0/28156	0.58	2/38072 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	0	ACE	C-N-CA	9.99	146.67	121.70
5	E	0	ACE	O-C-N	-6.91	111.65	122.70

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	1912	0	1902	19	0
2	B	1881	0	1893	24	0
3	C	1855	0	1851	22	0
4	D	1722	0	1732	23	0
5	E	1927	0	1903	26	0
6	F	1806	0	1809	26	0
7	G	1909	0	1904	18	0
8	H	1512	0	1481	6	0
9	I	1670	0	1679	17	0
10	J	1575	0	1566	16	0
11	K	1561	0	1569	17	0
12	L	1644	0	1595	15	0
13	M	1757	0	1711	16	0
14	N	1824	0	1832	22	0
15	O	1544	0	1568	25	0
16	P	1544	0	1517	34	0
17	A	1	0	0	0	0
17	H	1	0	0	0	0
17	I	1	0	0	0	0
17	J	2	0	0	0	0
17	L	1	0	0	0	0
17	M	2	0	0	0	0
18	L	34	0	41	4	0
19	A	81	0	0	2	0
19	B	30	0	0	0	0
19	C	31	0	0	0	0
19	D	29	0	0	1	0
19	E	49	0	0	1	0
19	F	43	0	0	0	0
19	G	53	0	0	0	0
19	H	82	0	0	0	0
19	I	65	0	0	0	0
19	J	69	0	0	1	0
19	K	61	0	0	1	0
19	L	55	0	0	0	0
19	M	81	0	0	2	0
19	N	100	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	O	6	0	0	0	0
19	P	11	0	0	0	0
All	All	28531	0	27553	292	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 (292) 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)
10:J:97:GLU:OE1	19:J:463:HOH:O	1.95	0.83
16:P:57:SER:O	16:P:59:TYR:N	2.13	0.80
4:D:216:LYS:HB2	4:D:220:ASP:HB3	1.65	0.79
3:C:190:ILE:HG21	3:C:238:ILE:HD11	1.68	0.76
16:P:53:ASP:O	16:P:55:SER:N	2.19	0.75
19:D:312:HOH:O	5:E:29:GLU:HG3	1.88	0.73
1:A:61:ASP:HB3	1:A:64:LEU:HD22	1.74	0.69
13:M:131:ALA:O	19:M:436:HOH:O	2.11	0.68
15:O:129:LYS:HD2	15:O:130:THR:HG22	1.74	0.68
9:I:148:LYS:HD2	9:I:177:VAL:HG11	1.75	0.68
11:K:154:GLU:OE2	19:K:260:HOH:O	2.11	0.68
3:C:216:ILE:HG12	3:C:227:GLN:HG2	1.74	0.67
16:P:217:ASN:ND2	16:P:220:ASP:OD2	2.27	0.67
2:B:62:SER:OG	2:B:237:LYS:NZ	2.29	0.66
13:M:13:LEU:HD13	13:M:33:VAL:HG13	1.78	0.66
5:E:131:GLU:O	19:E:329:HOH:O	2.13	0.66
15:O:75:LYS:HE2	15:O:150:ILE:HD11	1.78	0.65
19:A:477:HOH:O	7:G:121:GLN:HG2	1.97	0.65
16:P:224:PHE:O	16:P:228:ILE:HG13	1.98	0.63
16:P:182:ASP:OD1	16:P:182:ASP:N	2.27	0.63
3:C:77:VAL:HG22	3:C:135:PHE:HE1	1.63	0.63
7:G:1:MET:H3	7:G:20:ARG:HH22	1.47	0.63
5:E:72:ARG:NH2	5:E:225:GLN:O	2.32	0.63
15:O:73:GLU:HG3	15:O:124:ILE:HD11	1.80	0.62
2:B:211:LEU:HD22	2:B:238:LEU:HD22	1.82	0.62
1:A:75:ILE:HD11	1:A:81:MET:HE2	1.81	0.62
7:G:16:SER:OG	7:G:18:ASP:OD1	2.17	0.61
4:D:101:GLU:OE2	12:L:121:ARG:NH2	2.34	0.61
1:A:126:GLN:HG2	2:B:84:VAL:HG21	1.82	0.61
2:B:186:GLU:OE1	2:B:246:ARG:NH1	2.33	0.60
1:A:43:LEU:HD11	1:A:206:ALA:HB1	1.82	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:68:LEU:HD23	15:O:127:PHE:HB3	1.84	0.60
16:P:33:LEU:HB3	16:P:72:VAL:HG23	1.82	0.60
3:C:62:SER:OG	3:C:63:THR:N	2.33	0.60
5:E:0:ACE:H2	5:E:2:PHE:H	1.67	0.59
13:M:33:VAL:HG12	13:M:195:LEU:HD22	1.83	0.59
12:L:1:THR:OG1	12:L:33:LYS:NZ	2.19	0.59
9:I:53:GLU:OE2	9:I:57:GLN:NE2	2.36	0.59
9:I:196:ARG:HH21	10:J:151:GLU:HG3	1.68	0.58
14:N:8:TYR:CZ	14:N:162:VAL:HG13	2.38	0.58
6:F:88:LEU:HD11	6:F:108:ALA:HB1	1.84	0.58
1:A:137:LEU:HB3	1:A:139:VAL:HG22	1.84	0.58
12:L:33:LYS:HA	12:L:45:MET:HE2	1.85	0.58
16:P:119:ASP:HB3	16:P:209:SER:HA	1.86	0.57
7:G:1:MET:N	7:G:20:ARG:HH22	2.01	0.57
16:P:57:SER:C	16:P:59:TYR:H	2.05	0.57
16:P:77:LYS:O	16:P:79:GLY:N	2.38	0.57
15:O:71:ILE:O	15:O:124:ILE:N	2.35	0.56
11:K:95:ARG:HB3	11:K:95:ARG:HH21	1.71	0.56
5:E:224:LYS:HG2	5:E:225:GLN:HG2	1.87	0.56
9:I:63:ILE:HG12	9:I:82:MET:HE1	1.88	0.56
14:N:177:TYR:CZ	14:N:185:ARG:HB2	2.41	0.56
4:D:157:SER:HB2	5:E:59:LEU:HD21	1.88	0.56
15:O:31:CYS:SG	16:P:93:ASN:HB3	2.46	0.55
3:C:177:GLN:HG3	4:D:54:LEU:HD22	1.89	0.55
11:K:147:TYR:HA	11:K:159:LEU:HD21	1.89	0.55
1:A:82:VAL:HG12	1:A:142:THR:HB	1.89	0.55
5:E:97:VAL:HG21	12:L:65:LEU:HD13	1.87	0.55
15:O:158:LEU:HD22	15:O:163:PRO:HG3	1.87	0.55
5:E:85:ALA:O	5:E:89:ILE:HG12	2.07	0.55
15:O:55:LYS:HG2	15:O:136:GLU:HA	1.88	0.55
6:F:0:ACE:H2	6:F:4:ASN:H	1.71	0.55
9:I:175:VAL:HG22	9:I:187:LEU:HD12	1.88	0.54
4:D:38:GLY:HA2	4:D:185:PRO:HG2	1.88	0.54
4:D:56:ASP:OD1	4:D:58:ARG:HG3	2.07	0.54
15:O:209:SER:O	15:O:209:SER:OG	2.25	0.54
15:O:30:VAL:HG13	16:P:97:ASN:ND2	2.23	0.54
5:E:133:LEU:HB3	5:E:134:MET:HE3	1.89	0.54
6:F:201:LEU:HD11	6:F:206:LEU:HG	1.89	0.54
4:D:159:TRP:CE2	5:E:59:LEU:HD23	2.42	0.54
15:O:190:PRO:HB3	16:P:248:SER:HB2	1.90	0.53
14:N:12:VAL:HG21	14:N:109:ALA:HB1	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:51:ASP:O	8:H:55:ILE:HG12	2.08	0.53
10:J:124:PHE:HA	10:J:129:CYS:O	2.08	0.53
10:J:135:ASP:OD1	10:J:135:ASP:N	2.42	0.52
3:C:77:VAL:HG22	3:C:135:PHE:CE1	2.44	0.52
16:P:5:VAL:HG12	16:P:116:CYS:HB3	1.91	0.52
14:N:8:TYR:CE2	14:N:162:VAL:HG13	2.45	0.52
5:E:20:ARG:NH1	15:O:222:GLU:OE1	2.38	0.52
6:F:63:ILE:HG21	6:F:214:ALA:HB2	1.91	0.52
13:M:149:GLN:HB3	13:M:160:LYS:HE2	1.92	0.52
2:B:59:GLU:H	2:B:59:GLU:CD	2.12	0.52
3:C:42:ASP:N	3:C:42:ASP:OD1	2.44	0.51
3:C:48:ALA:HB1	3:C:65:LYS:HE3	1.92	0.51
5:E:0:ACE:H3	6:F:1:MET:HB2	1.92	0.51
6:F:201:LEU:HD22	6:F:204:GLU:HG3	1.92	0.51
3:C:135:PHE:O	3:C:150:THR:HA	2.10	0.51
7:G:95:GLU:OE2	7:G:115:ARG:HD2	2.10	0.51
14:N:185:ARG:HG3	14:N:206:VAL:HB	1.92	0.51
8:H:59:VAL:HG11	8:H:82:PHE:CE2	2.45	0.51
12:L:200:VAL:O	12:L:204:GLU:HB2	2.10	0.51
2:B:49:LYS:HE3	2:B:210:GLU:OE1	2.10	0.51
16:P:24:ASN:ND2	16:P:246:PRO:HG3	2.26	0.51
16:P:59:TYR:CD1	16:P:64:MET:HE1	2.45	0.51
15:O:198:GLY:O	15:O:202:THR:HG23	2.11	0.50
3:C:186:VAL:O	3:C:190:ILE:HG13	2.12	0.50
16:P:207:TYR:OH	16:P:228:ILE:HG12	2.11	0.50
10:J:63:LEU:HD11	10:J:105:VAL:HG21	1.92	0.50
4:D:46:CYS:HB3	4:D:63:LYS:HZ3	1.77	0.50
10:J:11:ILE:HG21	10:J:142:ALA:HB3	1.94	0.50
16:P:100:VAL:O	16:P:105:PRO:HD3	2.12	0.50
6:F:59:TYR:CE1	6:F:209:ASP:HB3	2.46	0.50
6:F:227:GLY:O	6:F:230:VAL:HG22	2.11	0.50
7:G:1:MET:H2	7:G:2:THR:C	2.14	0.49
7:G:114:ASP:O	7:G:118:GLN:HG2	2.12	0.49
1:A:91:ARG:HD2	19:A:417:HOH:O	2.11	0.49
1:A:126:GLN:CG	2:B:84:VAL:HG21	2.42	0.49
6:F:176:LEU:HA	6:F:179:PHE:CE2	2.47	0.49
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.95	0.49
6:F:40:SER:HB2	6:F:183:ASP:OD1	2.13	0.49
16:P:53:ASP:C	16:P:55:SER:H	2.13	0.49
15:O:215:LYS:HD3	15:O:245:TRP:CE3	2.48	0.48
13:M:203:ARG:NH2	13:M:205:GLU:OE2	2.45	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:27:LEU:HD21	10:J:186:VAL:HG13	1.96	0.48
11:K:100:ASN:HB3	11:K:132:HIS:CE1	2.49	0.48
14:N:88:LEU:O	14:N:92:MET:HG2	2.13	0.48
16:P:184:PRO:HG2	16:P:208:CYS:SG	2.53	0.48
7:G:101:LYS:O	14:N:57:ARG:NH2	2.46	0.48
3:C:221:ASN:N	3:C:222:ASP:HA	2.29	0.48
2:B:247:LEU:O	2:B:250:LEU:HB2	2.13	0.48
11:K:18:LYS:HD3	11:K:179:ILE:HG13	1.95	0.47
15:O:249:GLU:HG2	15:O:250:PRO:HD2	1.94	0.47
2:B:222:LEU:HG	2:B:224:TYR:CE1	2.49	0.47
3:C:231:LYS:HB2	3:C:234:GLU:HG3	1.97	0.47
12:L:37:ILE:HG23	12:L:60:GLY:HA2	1.97	0.47
6:F:132:LEU:HB2	6:F:147:PHE:HB3	1.96	0.47
10:J:63:LEU:HD21	10:J:103:TYR:CD2	2.49	0.47
10:J:164:PHE:CE1	10:J:198:ARG:HD2	2.50	0.47
9:I:59:ILE:HG12	9:I:83:LEU:HG	1.97	0.47
10:J:21:VAL:HG13	10:J:119:PRO:HB3	1.97	0.47
10:J:96:TYR:CE1	10:J:99:ARG:HD3	2.50	0.47
11:K:6:ILE:HD12	11:K:160:LEU:HG	1.97	0.47
16:P:11:VAL:HG11	16:P:122:TYR:HB2	1.95	0.47
16:P:38:SER:OG	16:P:43:GLU:OE2	2.31	0.47
11:K:118:ILE:HA	11:K:123:THR:O	2.14	0.47
1:A:15:HIS:NE2	7:G:7:GLY:O	2.46	0.46
6:F:156:LEU:HD13	6:F:159:THR:HB	1.96	0.46
1:A:163:TYR:O	2:B:61:LEU:HD11	2.15	0.46
9:I:22:GLN:HG3	9:I:27:ALA:HB2	1.98	0.46
10:J:132:GLU:O	10:J:134:LYS:NZ	2.39	0.46
2:B:110:LEU:O	2:B:114:VAL:HG23	2.16	0.46
4:D:64:VAL:HG22	4:D:74:SER:HB3	1.98	0.46
7:G:176:LEU:O	7:G:180:VAL:HG23	2.16	0.46
18:L:301:LDZ:H1	13:M:94:PRO:HG3	1.98	0.46
14:N:119:LEU:HG	14:N:134:LEU:HD12	1.97	0.46
6:F:0:ACE:H2	6:F:3:ARG:HB3	1.98	0.46
13:M:113:TYR:CE2	13:M:123:ARG:HB2	2.51	0.46
14:N:35:ILE:CD1	14:N:56:GLU:HG2	2.46	0.46
15:O:75:LYS:HE2	15:O:75:LYS:HB3	1.76	0.46
16:P:11:VAL:HG21	16:P:122:TYR:HB2	1.98	0.46
2:B:63:LYS:HB3	2:B:63:LYS:HE2	1.78	0.45
11:K:159:LEU:HD12	11:K:159:LEU:HA	1.82	0.45
2:B:74:VAL:HG22	2:B:75:TYR:H	1.80	0.45
3:C:236:LYS:HA	3:C:236:LYS:HZ2	1.82	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASP:HB3	1:A:155:TYR:CZ	2.51	0.45
16:P:121:LEU:HD12	16:P:122:TYR:H	1.81	0.45
9:I:8:PHE:HB2	9:I:146:LEU:O	2.17	0.45
5:E:45:GLY:HA2	5:E:153:TYR:CE1	2.52	0.45
16:P:117:ILE:O	16:P:207:TYR:HB3	2.16	0.45
5:E:222:ILE:HD13	5:E:228:PHE:HB2	1.98	0.45
13:M:196:ILE:HB	13:M:203:ARG:HG3	1.99	0.45
15:O:53:THR:OG1	15:O:54:THR:N	2.50	0.45
16:P:77:LYS:HB3	16:P:77:LYS:HE2	1.86	0.45
4:D:138:PHE:CE2	4:D:217:PRO:HG3	2.52	0.45
10:J:4:PRO:HA	10:J:7:ILE:HD12	1.98	0.45
14:N:35:ILE:HD13	14:N:56:GLU:HG2	1.98	0.45
4:D:159:TRP:CZ2	5:E:59:LEU:HD23	2.52	0.44
12:L:1:THR:HB	18:L:301:LDZ:C22	2.47	0.44
5:E:236:THR:O	5:E:240:ILE:HG13	2.17	0.44
13:M:167:VAL:O	13:M:171:ILE:HG12	2.18	0.44
4:D:230:ASN:HA	4:D:233:VAL:CG1	2.48	0.44
5:E:246:LYS:HB3	5:E:246:LYS:HE2	1.72	0.44
7:G:2:THR:O	7:G:2:THR:OG1	2.31	0.44
16:P:52:GLU:OE1	16:P:245:ARG:HB2	2.18	0.44
3:C:68:LYS:HG3	3:C:229:ILE:HD11	1.98	0.44
2:B:28:VAL:HG11	2:B:133:SER:HB2	2.00	0.44
2:B:174:PHE:CE2	2:B:178:ARG:HG3	2.52	0.44
4:D:162:GLN:OE1	4:D:163:THR:N	2.39	0.44
5:E:17:PRO:HA	6:F:24:TYR:CG	2.53	0.44
16:P:52:GLU:OE2	16:P:250:GLN:NE2	2.40	0.44
2:B:160:LYS:HD3	2:B:179:TRP:CH2	2.52	0.44
7:G:221:LEU:HD23	7:G:221:LEU:HA	1.87	0.44
11:K:36:GLN:NE2	11:K:39:PRO:HA	2.33	0.43
16:P:229:ILE:O	16:P:231:GLN:HA	2.17	0.43
10:J:8:ASN:HA	10:J:30:GLY:O	2.18	0.43
11:K:14:LEU:HD12	11:K:42:LEU:HD23	2.00	0.43
6:F:100:ASN:HB2	14:N:86:GLU:HG2	2.01	0.43
7:G:241:ASP:O	7:G:245:LYS:HD3	2.18	0.43
9:I:104:ASP:HB2	9:I:105:PRO:HD2	2.00	0.43
13:M:8:GLU:O	13:M:109:LYS:HA	2.18	0.43
6:F:0:ACE:H2	6:F:4:ASN:N	2.32	0.43
9:I:99:ILE:HG13	9:I:127:LEU:HD12	2.01	0.43
1:A:164:VAL:HG23	2:B:61:LEU:HG	2.00	0.43
6:F:33:SER:OG	6:F:49:LEU:O	2.35	0.43
6:F:171:TYR:HB2	6:F:199:GLN:HG3	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:112:LEU:HD13	6:F:147:PHE:CD1	2.54	0.43
13:M:-6:PRO:O	14:N:96:ARG:HD2	2.19	0.43
3:C:136:ILE:HG12	3:C:150:THR:HG22	2.01	0.43
4:D:101:GLU:CD	12:L:121:ARG:HH22	2.22	0.43
4:D:193:LYS:CG	4:D:236:ILE:HD11	2.48	0.43
13:M:185:HIS:CE1	13:M:187:GLN:HB2	2.54	0.43
14:N:89:ALA:HA	14:N:122:VAL:HG21	2.01	0.43
16:P:245:ARG:HG2	16:P:249:TRP:CE3	2.54	0.43
12:L:1:THR:HG1	12:L:33:LYS:HZ3	1.55	0.43
14:N:122:VAL:HA	14:N:127:VAL:O	2.19	0.43
2:B:245:ASP:O	2:B:248:GLU:HG3	2.19	0.43
3:C:208:TYR:CG	3:C:236:LYS:HG2	2.54	0.43
4:D:141:ARG:NH2	12:L:107:LYS:HD2	2.33	0.43
14:N:-2:VAL:HG12	14:N:49:ILE:HG13	1.99	0.43
16:P:99:ILE:HD12	16:P:187:LYS:HD3	2.01	0.43
5:E:2:PHE:CE1	16:P:16:GLN:HB3	2.54	0.42
10:J:37:SER:HB2	11:K:125:VAL:HG21	2.00	0.42
12:L:14:VAL:HB	12:L:178:TYR:HB2	2.01	0.42
18:L:301:LDZ:H9	18:L:301:LDZ:H39	1.68	0.42
14:N:9:ASP:OD1	14:N:10:ASN:N	2.51	0.42
15:O:166:ILE:HG12	15:O:215:LYS:HG3	2.01	0.42
15:O:187:LEU:HD13	16:P:46:GLY:HA2	2.00	0.42
3:C:10:THR:HG23	3:C:11:THR:HG23	2.02	0.42
4:D:70:HIS:HD2	4:D:138:PHE:O	2.02	0.42
6:F:62:LYS:HD3	15:O:276:ILE:HG22	2.01	0.42
7:G:237:GLN:NE2	7:G:241:ASP:OD1	2.53	0.42
9:I:5:GLY:O	9:I:124:TYR:HA	2.19	0.42
9:I:163:ILE:HG23	9:I:170:GLY:HA2	2.01	0.42
3:C:50:ARG:NE	3:C:59:GLN:OE1	2.52	0.42
5:E:198:LEU:HD23	5:E:198:LEU:HA	1.87	0.42
6:F:78:ALA:HB3	6:F:79:PRO:HD3	2.02	0.42
11:K:109:LYS:HB3	11:K:109:LYS:HE2	1.70	0.42
14:N:0:GLY:HA2	19:N:375:HOH:O	2.19	0.42
16:P:183:GLN:OE1	16:P:183:GLN:N	2.52	0.42
4:D:71:VAL:HG11	4:D:109:LEU:HD23	2.00	0.42
4:D:228:GLU:H	4:D:228:GLU:HG2	1.59	0.42
1:A:237:SER:OG	1:A:239:GLU:HG3	2.19	0.42
5:E:75:GLY:N	5:E:222:ILE:HD11	2.34	0.42
16:P:207:TYR:HE2	16:P:228:ILE:HG23	1.84	0.42
8:H:40:LYS:HE2	8:H:182:GLY:HA2	2.01	0.42
9:I:35:HIS:HB3	9:I:56:THR:HG21	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:19:LEU:HD21	14:N:26:LEU:HD22	2.01	0.42
15:O:64:ASN:O	15:O:67:GLN:N	2.50	0.42
1:A:126:GLN:HG2	2:B:84:VAL:CG2	2.48	0.42
7:G:60:VAL:HA	7:G:61:PRO:HD3	1.88	0.42
14:N:19:LEU:HD12	14:N:28:PHE:O	2.20	0.42
4:D:209:ASN:N	4:D:209:ASN:HD22	2.18	0.42
9:I:45:GLY:HA3	9:I:52:THR:HG21	2.01	0.42
12:L:128:CYS:HB2	12:L:137:TYR:CE2	2.55	0.42
15:O:66:LEU:HD22	15:O:127:PHE:CD1	2.54	0.42
3:C:67:TYR:CG	3:C:88:ILE:HD13	2.55	0.41
10:J:57:ALA:HB3	11:K:123:THR:HG23	2.02	0.41
3:C:219:GLY:C	3:C:221:ASN:H	2.24	0.41
9:I:63:ILE:HG12	9:I:82:MET:CE	2.50	0.41
11:K:3:ILE:HG13	11:K:46:ALA:HB2	2.02	0.41
14:N:53:GLN:HA	14:N:56:GLU:HG3	2.03	0.41
1:A:14:ARG:O	1:A:27:GLN:NE2	2.53	0.41
1:A:30:TYR:CD1	7:G:17:PRO:HA	2.55	0.41
2:B:37:ILE:HB	2:B:44:VAL:HG12	2.02	0.41
5:E:12:VAL:HA	5:E:23:GLN:HB2	2.01	0.41
6:F:0:ACE:CH3	6:F:3:ARG:HB3	2.50	0.41
8:H:175:MET:HB2	8:H:186:LEU:HB2	2.01	0.41
4:D:10:ILE:HD13	5:E:136:ARG:HB3	2.01	0.41
11:K:32:ASP:OD2	11:K:181:LYS:NZ	2.43	0.41
15:O:74:ILE:HA	15:O:121:SER:HB2	2.02	0.41
6:F:128:TYR:O	6:F:149:PRO:HB3	2.21	0.41
13:M:26:ASN:HB3	14:N:129:TYR:CE1	2.55	0.41
1:A:115:ASP:HB3	1:A:155:TYR:CE1	2.55	0.41
5:E:25:GLU:OE1	15:O:229:LYS:NZ	2.46	0.41
15:O:54:THR:OG1	15:O:56:ILE:HG22	2.21	0.41
2:B:75:TYR:HB3	2:B:82:TYR:CD1	2.56	0.41
2:B:177:LYS:N	2:B:177:LYS:HD3	2.35	0.41
5:E:184:LEU:HD13	5:E:184:LEU:HA	1.91	0.41
6:F:121:GLN:HG3	7:G:130:ARG:HG3	2.03	0.41
12:L:115:VAL:HG22	12:L:121:ARG:HG3	2.02	0.41
1:A:77:ARG:O	1:A:232:LYS:HA	2.21	0.41
7:G:214:LEU:HD21	7:G:216:ILE:HD11	2.03	0.41
12:L:1:THR:HB	18:L:301:LDZ:O33	2.20	0.41
12:L:114:TYR:O	12:L:121:ARG:HA	2.21	0.41
4:D:232:TYR:O	4:D:236:ILE:HG12	2.21	0.41
11:K:184:ASP:OD2	11:K:189:ARG:NH1	2.52	0.41
13:M:57:ARG:HD2	19:M:476:HOH:O	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:LEU:HD12	8:H:65:LEU:HA	1.89	0.40
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.88	0.40
2:B:10:THR:HG22	2:B:18:LEU:HD22	2.03	0.40
2:B:190:HIS:NE2	2:B:250:LEU:O	2.50	0.40
6:F:159:THR:OG1	6:F:160:ALA:N	2.54	0.40
11:K:95:ARG:HA	11:K:96:PRO:HD3	1.89	0.40
1:A:131:ARG:HD2	1:A:134:MET:HE1	2.03	0.40
3:C:181:LYS:H	3:C:181:LYS:HG2	1.70	0.40
5:E:184:LEU:HD13	6:F:56:LEU:HG	2.03	0.40
3:C:34:THR:OG1	3:C:167:ALA:O	2.36	0.40
4:D:78:LEU:HA	4:D:78:LEU:HD12	1.88	0.40
9:I:14:ILE:HD13	9:I:14:ILE:HG21	1.85	0.40
13:M:6:ALA:HB2	13:M:112:VAL:HG23	2.03	0.40
14:N:121:TYR:O	14:N:128:THR:HA	2.21	0.40
13:M:192:LEU:HB2	13:M:209:LEU:HD11	2.04	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	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
2	B	244/250 (98%)	237 (97%)	7 (3%)	0	100	100
3	C	233/258 (90%)	222 (95%)	9 (4%)	2 (1%)	14	28
4	D	214/254 (84%)	210 (98%)	3 (1%)	1 (0%)	25	44
5	E	248/261 (95%)	242 (98%)	6 (2%)	0	100	100
6	F	233/235 (99%)	224 (96%)	9 (4%)	0	100	100
7	G	244/288 (85%)	239 (98%)	4 (2%)	1 (0%)	30	49
8	H	194/196 (99%)	188 (97%)	6 (3%)	0	100	100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	218/232 (94%)	215 (99%)	2 (1%)	1 (0%)	25	44
10	J	201/205 (98%)	197 (98%)	4 (2%)	0	100	100
11	K	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
12	L	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
13	M	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
14	N	231/233 (99%)	223 (96%)	7 (3%)	1 (0%)	30	49
15	O	194/276 (70%)	178 (92%)	16 (8%)	0	100	100
16	P	182/269 (68%)	155 (85%)	20 (11%)	7 (4%)	2	3
All	All	3498/3841 (91%)	3372 (96%)	113 (3%)	13 (0%)	30	49

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	54	GLY
16	P	58	LEU
3	C	63	THR
7	G	2	THR
16	P	78	ARG
16	P	208	CYS
16	P	216	ASP
3	C	62	SER
4	D	78	LEU
16	P	77	LYS
14	N	212	ASP
9	I	171	SER
16	P	207	TYR

### 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	207/210 (99%)	194 (94%)	13 (6%)	15	30

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	205/209 (98%)	196 (96%)	9 (4%)	24	47
3	C	198/216 (92%)	185 (93%)	13 (7%)	14	28
4	D	196/226 (87%)	182 (93%)	14 (7%)	12	25
5	E	205/215 (95%)	197 (96%)	8 (4%)	27	52
6	F	193/193 (100%)	187 (97%)	6 (3%)	35	62
7	G	203/239 (85%)	192 (95%)	11 (5%)	18	37
8	H	162/162 (100%)	159 (98%)	3 (2%)	52	77
9	I	179/190 (94%)	176 (98%)	3 (2%)	56	79
10	J	171/173 (99%)	168 (98%)	3 (2%)	54	78
11	K	173/175 (99%)	169 (98%)	4 (2%)	45	72
12	L	169/169 (100%)	168 (99%)	1 (1%)	84	94
13	M	185/185 (100%)	180 (97%)	5 (3%)	40	67
14	N	199/199 (100%)	192 (96%)	7 (4%)	31	57
15	O	178/251 (71%)	165 (93%)	13 (7%)	11	24
16	P	173/245 (71%)	157 (91%)	16 (9%)	7	15
All	All	2996/3257 (92%)	2867 (96%)	129 (4%)	25	48

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TYR
1	A	54	ILE
1	A	64	LEU
1	A	124	LEU
1	A	126	GLN
1	A	137	LEU
1	A	176	GLN
1	A	189	SER
1	A	223	LEU
1	A	231	ASP
1	A	239	GLU
1	A	244	ARG
1	A	245	LEU
2	B	30	GLN
2	B	59	GLU
2	B	108	LYS
2	B	133	SER

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	157	PHE
2	B	169	VAL
2	B	201	GLU
2	B	229	THR
2	B	248	GLU
3	C	53	THR
3	C	55	THR
3	C	59	GLN
3	C	61	THR
3	C	169	THR
3	C	181	LYS
3	C	182	ASP
3	C	183	ASP
3	C	185	LYS
3	C	201	THR
3	C	222	ASP
3	C	236	LYS
3	C	245	THR
4	D	31	THR
4	D	53	LYS
4	D	58	ARG
4	D	60	THR
4	D	78	LEU
4	D	123	SER
4	D	144	GLU
4	D	149	GLN
4	D	209	ASN
4	D	222	VAL
4	D	224	LEU
4	D	228	GLU
4	D	230	ASN
4	D	233	VAL
5	E	6	SER
5	E	7	GLU
5	E	8	TYR
5	E	21	LEU
5	E	48	LEU
5	E	184	LEU
5	E	201	LEU
5	E	224	LYS
6	F	11	VAL
6	F	55	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	F	88	LEU
6	F	112	LEU
6	F	145	LEU
6	F	202	ARG
7	G	1	MET
7	G	3	SER
7	G	10	LEU
7	G	18	ASP
7	G	60	VAL
7	G	72	ARG
7	G	121	GLN
7	G	169	ARG
7	G	179	LEU
7	G	208	LYS
7	G	218	TRP
8	H	36	ARG
8	H	64	GLU
8	H	140	LYS
9	I	55	VAL
9	I	63	ILE
9	I	100	VAL
10	J	21	VAL
10	J	29	LEU
10	J	183	TRP
11	K	16	SER
11	K	95	ARG
11	K	159	LEU
11	K	162	LEU
12	L	65	LEU
13	M	3	LEU
13	M	13	LEU
13	M	24	SER
13	M	160	LYS
13	M	208	GLU
14	N	-5	GLN
14	N	96	ARG
14	N	162	VAL
14	N	184	SER
14	N	204	LEU
14	N	207	GLU
14	N	212	ASP
15	O	66	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	O	69	THR
15	O	71	ILE
15	O	73	GLU
15	O	75	LYS
15	O	129	LYS
15	O	130	THR
15	O	164	ASP
15	O	206	VAL
15	O	209	SER
15	O	233	SER
15	O	249	GLU
15	O	271	GLN
16	P	22	LEU
16	P	50	ARG
16	P	58	LEU
16	P	68	SER
16	P	90	VAL
16	P	92	VAL
16	P	113	SER
16	P	124	MET
16	P	182	ASP
16	P	183	GLN
16	P	185	ILE
16	P	207	TYR
16	P	209	SER
16	P	210	CYS
16	P	241	VAL
16	P	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	LDZ	L	301	-	33,34,34	1.54	6 (18%)	42,44,44	2.07	10 (23%)

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
18	LDZ	L	301	-	-	7/38/39/39	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	301	LDZ	O8-C9	4.02	1.43	1.35
18	L	301	LDZ	C17-N16	-3.81	1.41	1.46
18	L	301	LDZ	C11-N10	3.05	1.52	1.45
18	L	301	LDZ	C4-C3	2.47	1.43	1.38
18	L	301	LDZ	C7-C3	2.36	1.56	1.50
18	L	301	LDZ	C11-C12	2.30	1.58	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	301	LDZ	C22-C17-N16	-7.40	95.21	109.50
18	L	301	LDZ	O8-C9-N10	5.34	121.88	110.45
18	L	301	LDZ	O31-C9-N10	-4.52	117.46	124.86

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	301	LDZ	O8-C7-C3	3.85	118.74	109.40
18	L	301	LDZ	O34-C15-N16	-3.01	117.57	122.96
18	L	301	LDZ	C14-C15-N16	2.35	121.64	116.63
18	L	301	LDZ	O33-C22-C17	-2.34	118.76	124.77
18	L	301	LDZ	C24-C14-C15	-2.29	105.17	110.59
18	L	301	LDZ	O32-C12-N13	-2.18	119.06	122.96
18	L	301	LDZ	O8-C9-O31	-2.05	120.33	124.26

There are no chirality outliers.

All (7) torsion outliers are listed below:

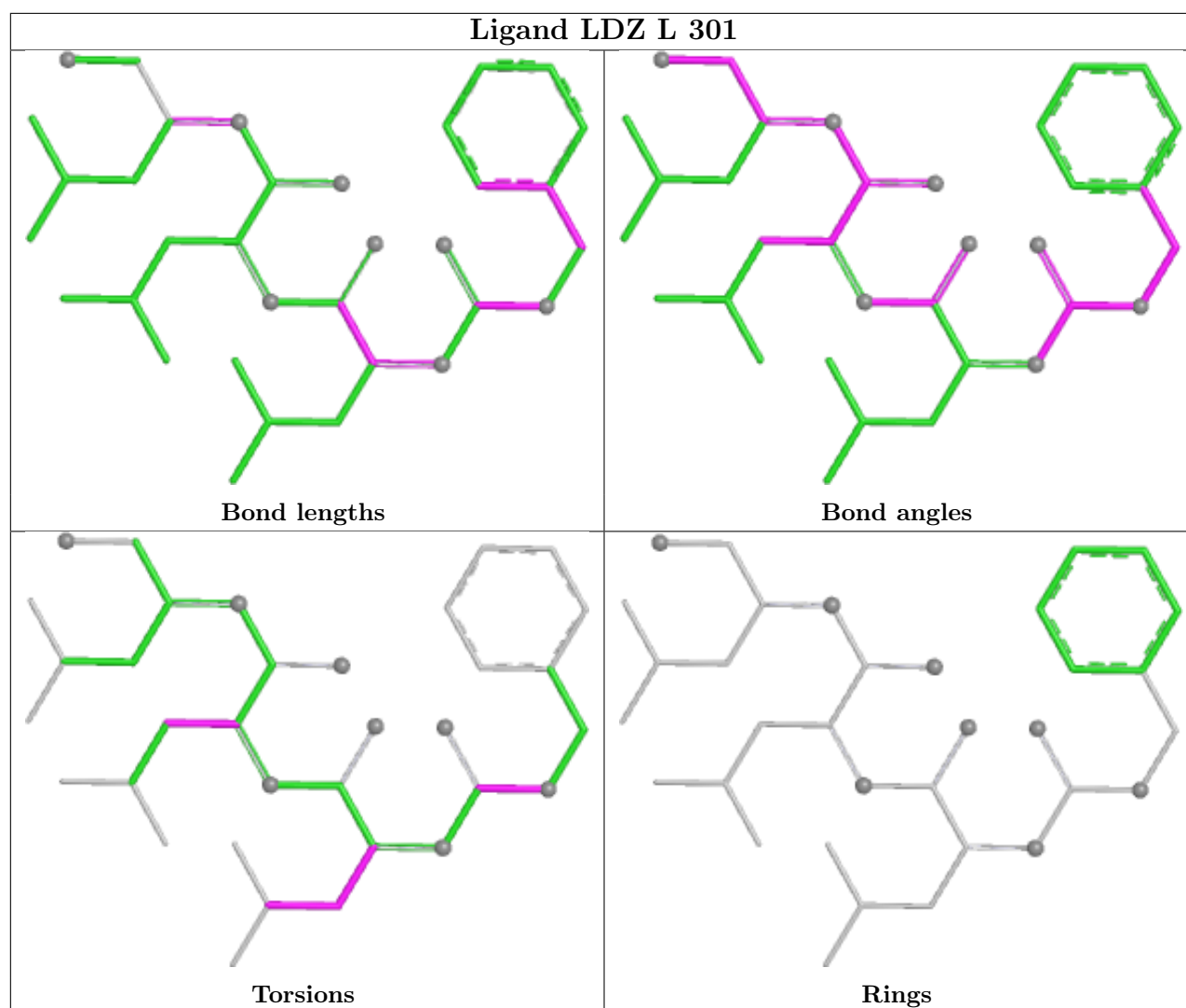
Mol	Chain	Res	Type	Atoms
18	L	301	LDZ	O31-C9-O8-C7
18	L	301	LDZ	N10-C9-O8-C7
18	L	301	LDZ	N10-C11-C30-C31
18	L	301	LDZ	C12-C11-C30-C31
18	L	301	LDZ	C11-C30-C31-C32
18	L	301	LDZ	N13-C14-C24-C25
18	L	301	LDZ	C15-C14-C24-C25

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	L	301	LDZ	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	241/252 (95%)	-0.86	0 <span>100</span> <span>100</span>	11, 20, 37, 52	0
2	B	246/250 (98%)	-0.61	0 <span>100</span> <span>100</span>	15, 26, 54, 71	0
3	C	237/258 (91%)	-0.23	3 (1%) <span>74</span> <span>71</span>	15, 36, 76, 114	0
4	D	220/254 (86%)	-0.43	1 (0%) <span>87</span> <span>85</span>	14, 32, 61, 77	0
5	E	249/261 (95%)	-0.76	1 (0%) <span>89</span> <span>86</span>	14, 23, 50, 64	0
6	F	234/235 (99%)	-0.86	0 <span>100</span> <span>100</span>	10, 21, 36, 66	0
7	G	246/288 (85%)	-0.80	2 (0%) <span>82</span> <span>79</span>	12, 21, 45, 68	0
8	H	196/196 (100%)	-1.06	0 <span>100</span> <span>100</span>	9, 14, 25, 50	0
9	I	220/232 (94%)	-0.92	0 <span>100</span> <span>100</span>	11, 19, 32, 55	0
10	J	203/205 (99%)	-0.97	0 <span>100</span> <span>100</span>	11, 17, 31, 47	0
11	K	195/198 (98%)	-0.96	0 <span>100</span> <span>100</span>	11, 18, 32, 58	0
12	L	212/212 (100%)	-1.01	0 <span>100</span> <span>100</span>	11, 16, 29, 40	0
13	M	222/222 (100%)	-0.94	0 <span>100</span> <span>100</span>	12, 18, 30, 53	0
14	N	233/233 (100%)	-1.03	0 <span>100</span> <span>100</span>	9, 15, 27, 36	0
15	O	200/276 (72%)	-0.01	5 (2%) <span>58</span> <span>55</span>	20, 42, 66, 73	0
16	P	190/269 (70%)	0.29	9 (4%) <span>37</span> <span>34</span>	27, 47, 67, 69	0
All	All	3544/3841 (92%)	-0.70	21 (0%) <span>85</span> <span>83</span>	9, 22, 57, 114	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	1	MET	4.1
16	P	181	VAL	4.1
3	C	220	ALA	3.1
3	C	61	THR	3.1
5	E	249	ALA	3.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
16	P	241	VAL	2.7
15	O	28	LEU	2.7
7	G	2	THR	2.6
3	C	52	VAL	2.5
16	P	186	PHE	2.4
15	O	74	ILE	2.3
16	P	123	ALA	2.3
4	D	209	ASN	2.3
16	P	211	LEU	2.2
15	O	38	PHE	2.2
16	P	207	TYR	2.1
15	O	120	PHE	2.1
15	O	258	TYR	2.1
16	P	122	TYR	2.1
16	P	113	SER	2.1
16	P	185	ILE	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

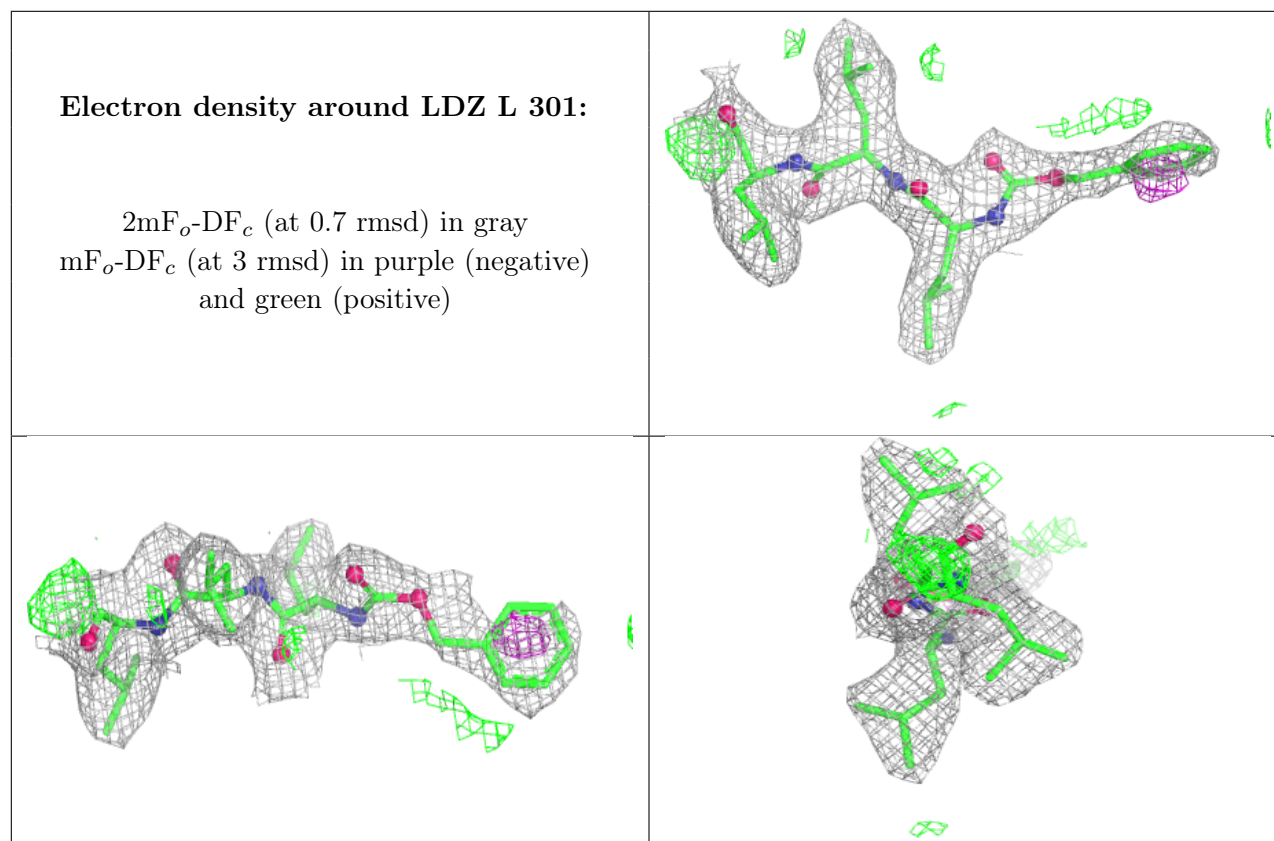
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
17	MG	J	302	1/1	0.88	0.07	34,34,34,34	0
17	MG	M	301	1/1	0.89	0.08	24,24,24,24	0
17	MG	L	302	1/1	0.91	0.04	22,22,22,22	0
17	MG	J	301	1/1	0.93	0.06	26,26,26,26	0
18	LDZ	L	301	34/34	0.93	0.09	7,18,42,50	0
17	MG	M	302	1/1	0.95	0.08	17,17,17,17	0
17	MG	I	301	1/1	0.96	0.06	18,18,18,18	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	MG	A	301	1/1	0.98	0.08	21,21,21,21	0
17	MG	H	201	1/1	0.99	0.03	20,20,20,20	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.