



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2020 – 11:19 AM EDT

PDB ID : 4NO1  
Title : yCP in complex with Z-Leu-Leu-Leu-B(OH)<sub>2</sub>  
Authors : Stein, M.L.; Cui, H.; Beck, P.; Dubiella, C.; Voss, C.; Krueger, A.; Schmidt, B.; Groll, M.  
Deposited on : 2013-11-19  
Resolution : 2.50 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 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 : 2.14.6  
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) : 2.14.6

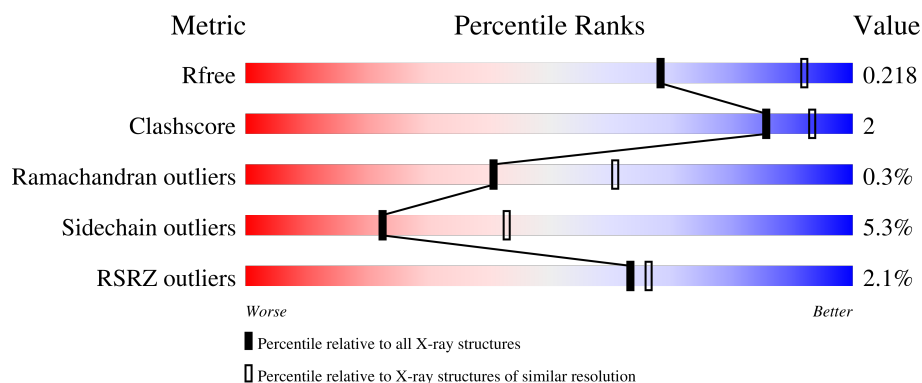
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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	250	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>.</div> </div> </div>
1	O	250	<div> <div>3%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
2	B	258	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>8% • 5%</div> </div> </div>
2	P	258	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>9% • 5%</div> </div> </div>
3	C	254	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>7% • 6%</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50397 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 subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

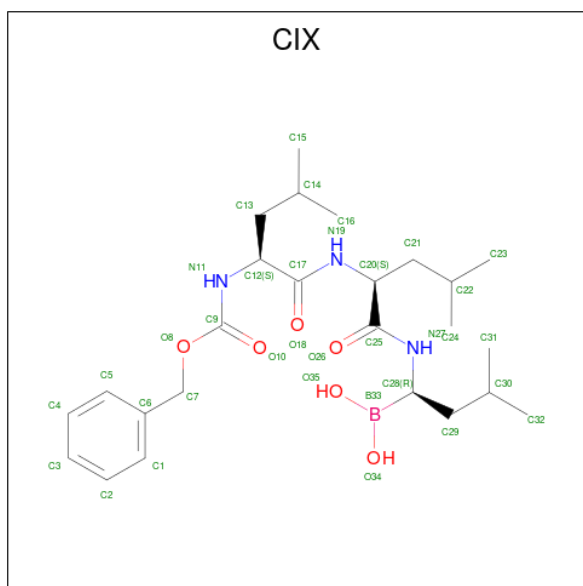
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0

- Molecule 16 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(1R)-1-(dihydroxyboranyl)-3-methylbutyl]-L-leucinamide (three-letter code: CIX) (formula:  $C_{25}H_{42}BN_3O_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	K	1	Total B C N O 35 1 25 3 6	0	0
16	Y	1	Total B C N O 35 1 25 3 6	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	39	Total O 39 39	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	41	Total O 41 41	0	0
17	C	34	Total O 34 34	0	0
17	D	19	Total O 19 19	0	0
17	E	23	Total O 23 23	0	0
17	F	35	Total O 35 35	0	0
17	G	42	Total O 42 42	0	0
17	H	41	Total O 41 41	0	0
17	I	37	Total O 37 37	0	0
17	J	36	Total O 36 36	0	0
17	K	48	Total O 48 48	0	0
17	L	47	Total O 47 47	0	0
17	M	49	Total O 49 49	0	0
17	N	42	Total O 42 42	0	0
17	O	26	Total O 26 26	0	0
17	P	21	Total O 21 21	0	0
17	Q	20	Total O 20 20	0	0
17	R	23	Total O 23 23	0	0
17	S	19	Total O 19 19	0	0
17	T	30	Total O 30 30	0	0
17	U	49	Total O 49 49	0	0
17	V	43	Total O 43 43	0	0

*Continued on next page...*



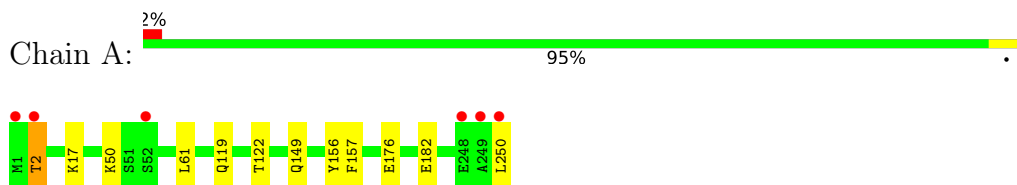
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	33	Total 33	O 33	0	0
17	X	40	Total 40	O 40	0	0
17	Y	34	Total 34	O 34	0	0
17	Z	44	Total 44	O 44	0	0
17	a	55	Total 55	O 55	0	0
17	b	53	Total 53	O 53	0	0

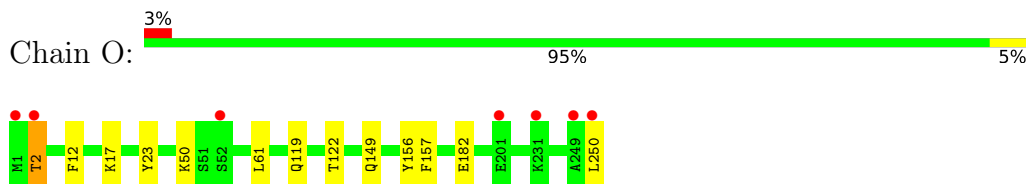
### 3 Residue-property plots

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.

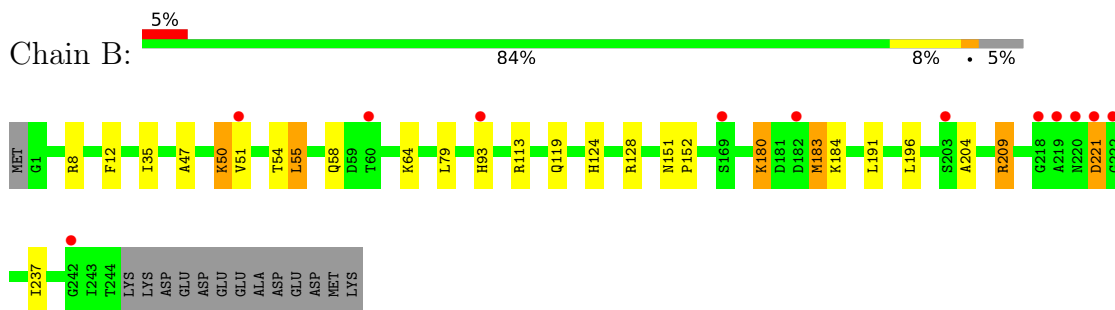
- Molecule 1: Proteasome subunit alpha type-2



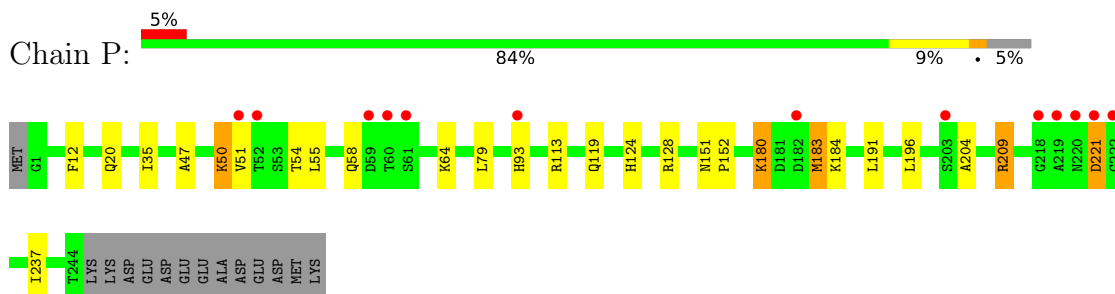
- Molecule 1: Proteasome subunit alpha type-2



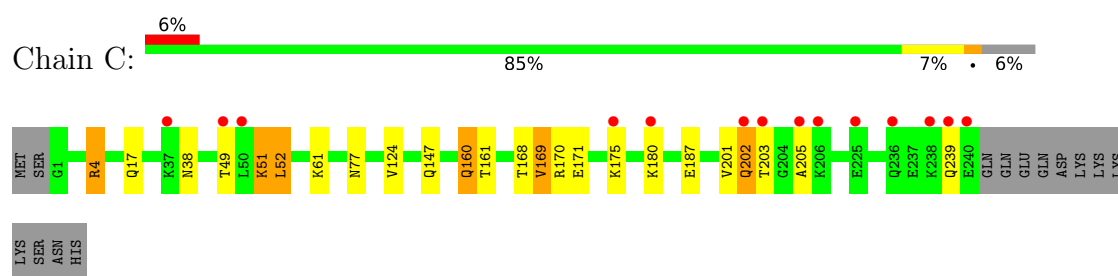
- Molecule 2: Proteasome subunit alpha type-3



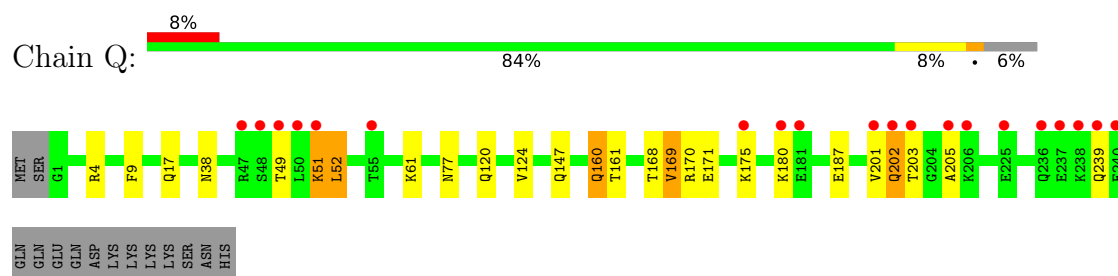
- Molecule 2: Proteasome subunit alpha type-3



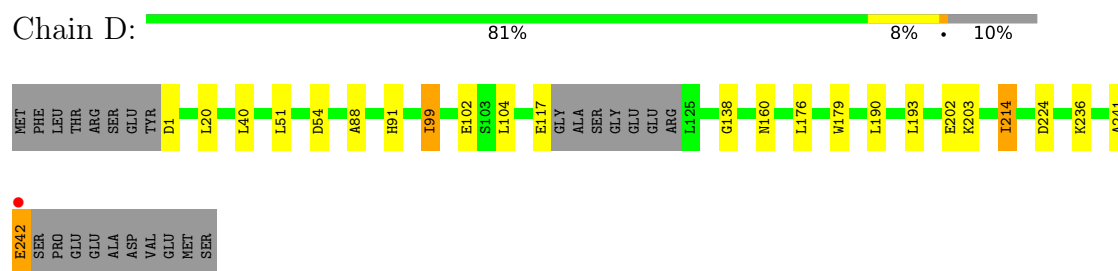
- Molecule 3: Proteasome subunit alpha type-4



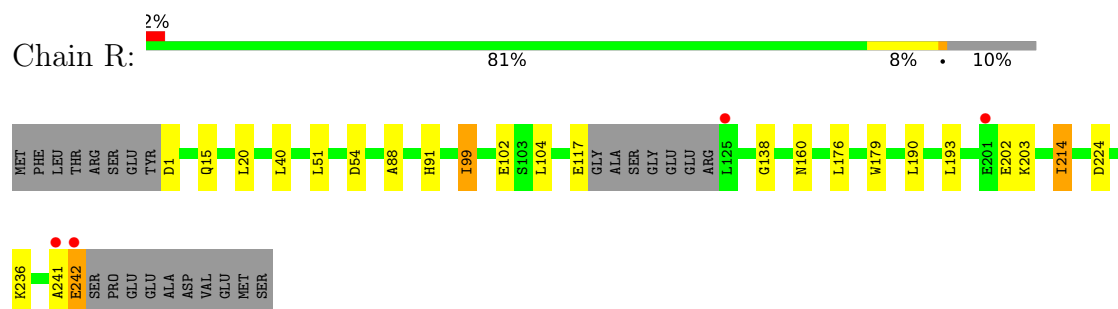
- Molecule 3: Proteasome subunit alpha type-4



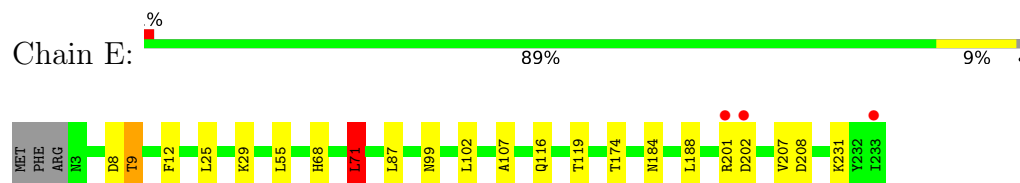
- Molecule 4: Proteasome subunit alpha type-5



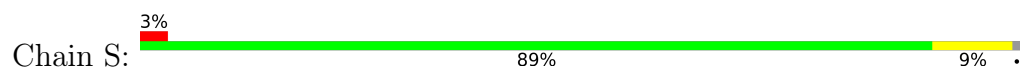
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 5: Proteasome subunit alpha type-6

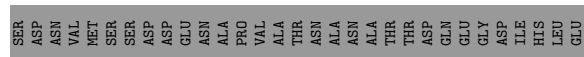
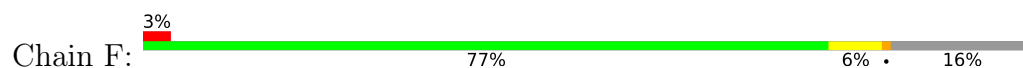


- Molecule 5: Proteasome subunit alpha type-6

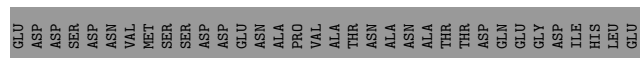
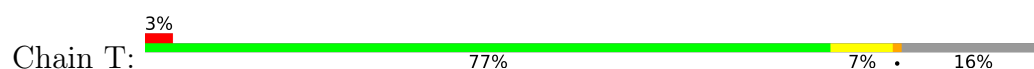




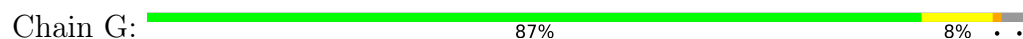
- Molecule 6: Probable proteasome subunit alpha type-7



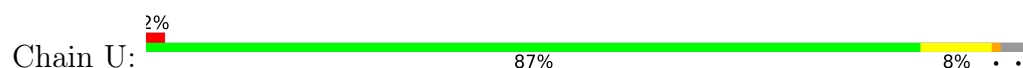
- Molecule 6: Probable proteasome subunit alpha type-7



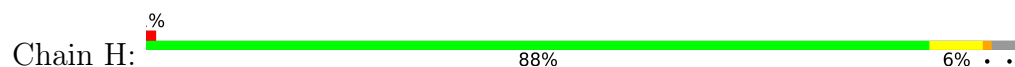
- Molecule 7: Proteasome subunit alpha type-1



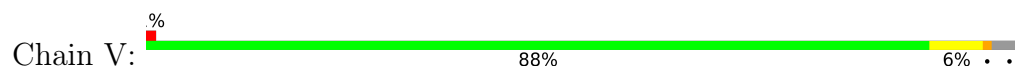
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2

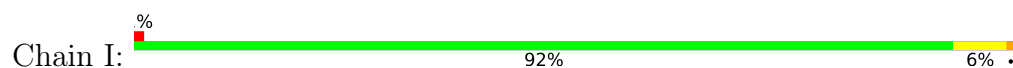


- Molecule 8: Proteasome subunit beta type-2





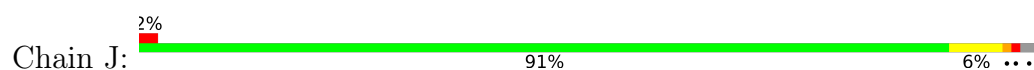
- Molecule 9: Proteasome subunit beta type-3



- Molecule 9: Proteasome subunit beta type-3



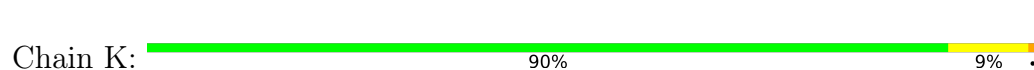
- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5




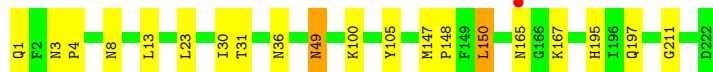
- Molecule 11: Proteasome subunit beta type-5




- Molecule 12: Proteasome subunit beta type-6



Chain L:  91% 8% .




• Molecule 12: Proteasome subunit beta type-6

Chain Z:  91% 9% .




• Molecule 13: Proteasome subunit beta type-7

Chain M:  87% 6% 5% .



• Molecule 13: Proteasome subunit beta type-7

Chain a:  90% 5% 5% .



• Molecule 14: Proteasome subunit beta type-1

Chain N:  94% 5% .



• Molecule 14: Proteasome subunit beta type-1

Chain b:  98% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.44Å 301.33Å 144.91Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-2.50) 98.9 (15.00-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.190 , 0.214 0.194 , 0.218	Depositor DCC
$R_{free}$ test set	17905 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	50397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: MG, CIX

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	0.27	0/1952	0.50	0/2642
1	O	0.28	0/1952	0.49	0/2642
2	B	0.28	0/1934	0.52	0/2618
2	P	0.28	0/1934	0.52	0/2618
3	C	0.28	0/1910	0.54	0/2586
3	Q	0.28	0/1910	0.54	0/2586
4	D	0.28	0/1837	0.51	0/2475
4	R	0.28	0/1837	0.51	0/2475
5	E	0.27	0/1800	0.51	1/2433 (0.0%)
5	S	0.27	0/1800	0.51	1/2433 (0.0%)
6	F	0.28	0/1932	0.48	0/2609
6	T	0.28	0/1932	0.48	0/2609
7	G	0.28	0/1945	0.50	0/2634
7	U	0.28	0/1945	0.50	0/2634
8	H	0.26	0/1715	0.50	0/2326
8	V	0.26	0/1715	0.50	0/2326
9	I	0.27	0/1611	0.51	0/2174
9	W	0.27	0/1611	0.50	0/2174
10	J	0.27	0/1589	0.50	0/2142
10	X	0.27	0/1589	0.50	0/2142
11	K	0.27	0/1681	0.52	1/2274 (0.0%)
11	Y	0.27	0/1681	0.52	1/2274 (0.0%)
12	L	0.27	0/1795	0.50	0/2420
12	Z	0.28	0/1795	0.50	0/2420
13	M	0.28	0/1855	0.54	0/2514
13	a	0.28	0/1855	0.54	0/2514
14	N	0.26	0/1541	0.48	0/2087
14	b	0.26	0/1541	0.48	0/2087
All	All	0.27	0/50194	0.51	4/67868 (0.0%)

There are no bond length outliers.



All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.26	127.41	115.30
11	K	4	LEU	CA-CB-CG	5.25	127.38	115.30
5	S	71	LEU	CA-CB-CG	5.09	127.01	115.30
5	E	71	LEU	CA-CB-CG	5.03	126.87	115.30

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	1915	0	1929	4	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	13	0
2	P	1904	0	1904	12	0
3	C	1881	0	1895	13	0
3	Q	1881	0	1895	14	0
4	D	1813	0	1797	7	0
4	R	1813	0	1797	9	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	8	0
6	T	1892	0	1883	8	0
7	G	1907	0	1901	7	0
7	U	1907	0	1901	8	0
8	H	1684	0	1688	6	0
8	V	1684	0	1688	7	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	6	0
10	X	1561	0	1569	5	0
11	K	1644	0	1594	12	0
11	Y	1644	0	1594	11	0
12	L	1757	0	1711	10	0
12	Z	1757	0	1711	11	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1824	0	1832	7	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	7	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	K	35	0	42	0	0
16	Y	35	0	42	1	0
17	A	39	0	0	0	0
17	B	41	0	0	0	0
17	C	34	0	0	0	0
17	D	19	0	0	0	0
17	E	23	0	0	0	0
17	F	35	0	0	1	0
17	G	42	0	0	0	0
17	H	41	0	0	0	0
17	I	37	0	0	0	0
17	J	36	0	0	0	0
17	K	48	0	0	1	0
17	L	47	0	0	0	0
17	M	49	0	0	0	0
17	N	42	0	0	1	0
17	O	26	0	0	0	0
17	P	21	0	0	0	0
17	Q	20	0	0	1	0
17	R	23	0	0	0	0
17	S	19	0	0	0	0
17	T	30	0	0	1	0
17	U	49	0	0	0	0
17	V	43	0	0	0	0
17	W	33	0	0	0	0
17	X	40	0	0	0	0
17	Y	34	0	0	0	0
17	Z	44	0	0	0	0
17	a	55	0	0	0	0
17	b	53	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	50397	0	49150	198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (198) 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)
3:C:202:GLN:HG3	3:C:203:THR:H	1.35	0.89
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.35	0.89
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.64	0.79
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.64	0.77
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.68	0.74
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.69	0.74
4:R:241:ALA:O	4:R:242:GLU:HB2	1.88	0.73
8:H:3:ILE:HG12	8:H:44:ALA:HB1	1.71	0.73
4:D:241:ALA:O	4:D:242:GLU:HB2	1.88	0.72
8:V:3:ILE:HG12	8:V:44:ALA:HB1	1.72	0.71
2:P:50:LYS:HA	2:P:50:LYS:HE3	1.72	0.71
14:N:152:VAL:HA	14:N:175:MET:HE1	1.73	0.70
2:B:50:LYS:HE3	2:B:50:LYS:HA	1.72	0.70
11:K:53:GLN:O	11:K:57:THR:HG23	1.92	0.69
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.93	0.68
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.75	0.67
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.76	0.67
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.78	0.64
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.97	0.64
3:C:51:LYS:O	3:C:52:LEU:HB2	1.98	0.63
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.79	0.63
14:N:20:THR:HG22	14:N:31:THR:OG1	2.01	0.61
7:G:23:PHE:O	7:G:26:THR:HB	2.01	0.60
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.65	0.60
10:X:1:MET:O	10:X:2:ASP:HB2	2.01	0.60
14:N:35:THR:HG21	14:N:45:ARG:HE	1.67	0.60
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.65	0.59
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.84	0.59
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.65	0.59
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.84	0.59
7:U:23:PHE:O	7:U:26:THR:HB	2.02	0.59
3:C:201:VAL:O	3:C:202:GLN:HB2	2.04	0.58
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.66	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:O	10:J:2:ASP:HB2	2.02	0.58
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.86	0.57
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.04	0.57
4:R:99:ILE:CD1	4:R:104:LEU:HB2	2.35	0.57
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.87	0.57
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.86	0.56
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.87	0.55
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.89	0.55
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.89	0.55
14:N:35:THR:HG22	17:N:302:HOH:O	2.08	0.54
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.90	0.54
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.89	0.54
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.72	0.54
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.90	0.54
13:M:161:ARG:HH11	13:M:161:ARG:HG3	1.73	0.53
2:B:12:PHE:H	3:C:17:GLN:HE22	1.55	0.53
4:D:99:ILE:CD1	4:D:104:LEU:HB2	2.35	0.53
5:E:12:PHE:H	6:F:19:GLN:HE22	1.55	0.53
9:I:98:ARG:O	9:I:126:ILE:HD11	2.09	0.53
14:N:20:THR:HG23	14:N:28:ASN:HB3	1.90	0.53
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.74	0.53
11:K:100:MET:CE	11:K:127:PHE:HB2	2.39	0.53
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.39	0.53
4:D:91:HIS:CG	4:D:99:ILE:HB	2.44	0.52
5:E:9:THR:HG21	5:E:119:THR:HA	1.91	0.52
5:S:9:THR:HG21	5:S:119:THR:HA	1.91	0.52
9:W:98:ARG:O	9:W:126:ILE:HD11	2.10	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.92	0.51
13:M:128:ARG:HH11	13:M:138:SER:HB2	1.75	0.51
5:S:12:PHE:H	6:T:19:GLN:HE22	1.57	0.51
4:R:91:HIS:CG	4:R:99:ILE:HB	2.45	0.51
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.76	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.51
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.76	0.51
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.92	0.51
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.93	0.51
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.44	0.50
11:Y:1:THR:HB	16:Y:301:CIX:O35	2.11	0.50
11:K:209:ASN:O	9:W:37:ASN:ND2	2.45	0.50
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.94	0.50
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.94	0.50
2:B:180:LYS:O	2:B:183:MET:HB2	2.12	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.49
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.93	0.49
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.95	0.49
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.95	0.49
3:C:202:GLN:HG3	3:C:203:THR:N	2.16	0.48
2:P:180:LYS:O	2:P:183:MET:HB2	2.12	0.48
12:L:8:ASN:HA	12:L:30:ILE:O	2.14	0.48
14:N:35:THR:CG2	14:N:45:ARG:HE	2.26	0.48
2:B:204:ALA:O	2:B:209:ARG:NH2	2.47	0.48
2:P:204:ALA:O	2:P:209:ARG:NH2	2.48	0.47
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.49	0.47
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.97	0.47
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.96	0.47
6:F:228:LYS:HB2	6:F:228:LYS:HE3	1.71	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.47
11:Y:104:TYR:CD1	11:Y:182:GLU:HA	2.49	0.47
11:K:104:TYR:CD1	11:K:182:GLU:HA	2.49	0.47
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.50	0.47
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.14	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.47
5:E:71:LEU:HD23	5:E:71:LEU:C	2.35	0.47
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.45	0.46
3:Q:202:GLN:HG3	3:Q:203:THR:N	2.16	0.46
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.97	0.46
5:S:71:LEU:HD23	5:S:71:LEU:C	2.36	0.46
6:F:19:GLN:NE2	17:F:323:HOH:O	2.49	0.46
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.97	0.46
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.46	0.45
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.47	0.45
6:T:19:GLN:NE2	17:T:327:HOH:O	2.47	0.45
6:F:175:LEU:HD21	6:F:191:GLN:NE2	2.32	0.45
1:O:119:GLN:O	1:O:122:THR:HB	2.17	0.45
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.98	0.45
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.64	0.45
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.99	0.45
13:M:27:LEU:HB2	13:M:192:SER:HB3	1.99	0.44
6:T:175:LEU:HD21	6:T:191:GLN:NE2	2.32	0.44
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:165:ASN:O	12:L:165:ASN:CG	2.55	0.44
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.98	0.44
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.99	0.44
3:C:168:THR:O	3:C:171:GLU:HB3	2.18	0.44
6:F:123:ASN:C	6:F:123:ASN:HD22	2.20	0.44
1:A:149:GLN:O	1:A:156:TYR:HA	2.18	0.44
12:L:195:HIS:HD2	12:L:197:GLN:H	1.65	0.44
3:Q:168:THR:O	3:Q:171:GLU:HB3	2.18	0.44
7:U:63:ILE:HD12	7:U:215:GLU:HG2	2.00	0.44
12:Z:165:ASN:O	12:Z:165:ASN:CG	2.55	0.44
7:G:26:THR:HG21	7:G:131:ILE:HD12	2.00	0.44
12:L:4:PRO:O	13:M:104:ARG:NH1	2.47	0.44
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.98	0.44
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.33	0.44
1:A:119:GLN:O	1:A:122:THR:HB	2.17	0.43
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.00	0.43
4:R:138:GLY:HA2	4:R:214:ILE:HG12	2.01	0.43
3:C:201:VAL:HG13	3:C:202:GLN:N	2.33	0.43
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.99	0.43
11:K:4:LEU:HD13	11:K:161:ILE:HD11	2.01	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.54	0.43
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.48	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.43
6:T:123:ASN:HD22	6:T:123:ASN:C	2.21	0.43
6:T:41:GLY:HA3	6:T:215:CYS:O	2.19	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.43
7:U:195:GLU:HG3	7:U:235:ARG:HG3	2.00	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.01	0.43
7:G:187:GLU:HG2	7:G:192:LYS:CB	2.48	0.43
1:O:149:GLN:O	1:O:156:TYR:HA	2.18	0.43
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.00	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.43
10:X:1:MET:HA	10:X:34:LYS:CE	2.49	0.43
7:G:63:ILE:HD12	7:G:215:GLU:HG2	2.01	0.43
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.66	0.43
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	2.01	0.43
4:D:138:GLY:HA2	4:D:214:ILE:HG12	2.01	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.42
6:F:48:LYS:HG2	6:F:62:LYS:HD2	2.02	0.42
5:E:68:HIS:HE1	5:E:102:LEU:O	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:195:GLU:HG3	7:G:235:ARG:HG3	2.00	0.42
6:F:41:GLY:HA3	6:F:215:CYS:O	2.19	0.42
5:S:68:HIS:HE1	5:S:102:LEU:O	2.01	0.42
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.34	0.42
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.68	0.42
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.02	0.41
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.68	0.41
8:H:35:HIS:HB3	8:H:56:THR:HG21	2.02	0.41
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.85	0.41
4:R:99:ILE:HD11	4:R:104:LEU:CB	2.45	0.41
10:J:1:MET:HA	10:J:34:LYS:CE	2.49	0.41
3:C:161:THR:HG21	3:C:169:VAL:HG22	2.03	0.41
8:H:43:CYS:SG	8:H:100:VAL:HG22	2.60	0.41
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.55	0.41
3:Q:120:GLN:NE2	17:Q:305:HOH:O	2.53	0.41
8:V:43:CYS:SG	8:V:100:VAL:HG22	2.60	0.41
10:X:119:ILE:HG12	10:X:125:LYS:HG3	2.02	0.41
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.02	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.03	0.41
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.55	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.41
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.68	0.41
13:M:43:ILE:HG12	13:M:43:ILE:O	2.20	0.41
3:Q:161:THR:HG21	3:Q:169:VAL:HG22	2.03	0.41
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.85	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.56	0.41
8:V:52:THR:O	8:V:56:THR:HB	2.20	0.41
8:H:52:THR:O	8:H:56:THR:HB	2.20	0.41
8:H:84:LYS:HG3	8:H:85:GLN:N	2.36	0.41
11:K:35:ILE:HG21	11:K:56:GLU:HB3	2.03	0.41
1:O:12:PHE:H	2:P:20:GLN:HE22	1.67	0.40
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.36	0.40
10:J:23:ARG:HD3	17:K:405:HOH:O	2.20	0.40
12:L:147:MET:N	12:L:148:PRO:HD2	2.36	0.40
6:T:146:MET:CE	6:T:161:THR:HB	2.51	0.40
8:V:1:THR:CG2	8:V:3:ILE:HD12	2.51	0.40
10:J:119:ILE:HG12	10:J:125:LYS:HG3	2.03	0.40
11:K:38:ASN:HB2	11:K:39:PRO:HD2	2.04	0.40
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.52	0.40
6:T:48:LYS:HG2	6:T:62:LYS:HD2	2.03	0.40
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	2.04	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.57	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	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	34	54
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	54
2	B	242/258 (94%)	233 (96%)	6 (2%)	3 (1%)	13	24
2	P	242/258 (94%)	233 (96%)	6 (2%)	3 (1%)	13	24
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	35
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	35
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	220/232 (95%)	212 (96%)	7 (3%)	1 (0%)	29	48
8	V	220/232 (95%)	212 (96%)	7 (3%)	1 (0%)	29	48
9	I	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
9	W	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	48

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	29	48
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6276/6614 (95%)	6101 (97%)	159 (2%)	16 (0%)	41	61

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
1	A	2	THR
3	C	205	ALA
1	O	2	THR
3	Q	205	ALA
8	H	9	ASN
8	V	9	ASN
2	B	221	ASP
2	P	221	ASP
2	B	183	MET
2	P	183	MET

### 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	209/209 (100%)	202 (97%)	7 (3%)	38	64
1	O	209/209 (100%)	202 (97%)	7 (3%)	38	64
2	B	203/216 (94%)	191 (94%)	12 (6%)	19	37
2	P	203/216 (94%)	191 (94%)	12 (6%)	19	37
3	C	212/226 (94%)	198 (93%)	14 (7%)	16	32
3	Q	212/226 (94%)	198 (93%)	14 (7%)	16	32
4	D	194/215 (90%)	177 (91%)	17 (9%)	10	19
4	R	194/215 (90%)	177 (91%)	17 (9%)	10	19
5	E	190/193 (98%)	174 (92%)	16 (8%)	11	21
5	S	190/193 (98%)	174 (92%)	16 (8%)	11	21
6	F	201/239 (84%)	190 (94%)	11 (6%)	21	41
6	T	201/239 (84%)	190 (94%)	11 (6%)	21	41
7	G	206/210 (98%)	193 (94%)	13 (6%)	18	34
7	U	206/210 (98%)	193 (94%)	13 (6%)	18	34
8	H	181/190 (95%)	172 (95%)	9 (5%)	24	46
8	V	181/190 (95%)	172 (95%)	9 (5%)	24	46
9	I	172/173 (99%)	166 (96%)	6 (4%)	36	62
9	W	172/173 (99%)	166 (96%)	6 (4%)	36	62
10	J	173/175 (99%)	165 (95%)	8 (5%)	27	50
10	X	173/175 (99%)	165 (95%)	8 (5%)	27	50
11	K	169/169 (100%)	164 (97%)	5 (3%)	41	68
11	Y	169/169 (100%)	164 (97%)	5 (3%)	41	68
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	65
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	65
13	M	199/208 (96%)	187 (94%)	12 (6%)	19	37
13	a	199/208 (96%)	187 (94%)	12 (6%)	19	37
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	73
14	b	162/162 (100%)	158 (98%)	4 (2%)	47	73
All	All	5312/5540 (96%)	5032 (95%)	280 (5%)	22	43

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	LYS
1	A	50	LYS
1	A	61	LEU
1	A	157	PHE
1	A	182	GLU
1	A	250	LEU
2	B	50	LYS
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	119	GLN
2	B	180	LYS
2	B	184	LYS
2	B	191	LEU
2	B	209	ARG
2	B	221	ASP
2	B	237	ILE
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	51	LYS
3	C	52	LEU
3	C	61	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	239	GLN
4	D	1	ASP
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	54	ASP
4	D	99	ILE
4	D	102	GLU
4	D	117	GLU
4	D	176	LEU
4	D	190	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	193	LEU
4	D	202	GLU
4	D	203	LYS
4	D	214	ILE
4	D	224	ASP
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	174	THR
5	E	184	ASN
5	E	188	LEU
5	E	201	ARG
5	E	202	ASP
5	E	207	VAL
5	E	208	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	148	GLU
6	F	172	LEU
6	F	181	GLU
6	F	198	LEU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	26	THR
7	G	34	LEU
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	165	LYS
7	G	166	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	G	171	THR
7	G	178	LYS
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	3	ILE
8	H	22	GLN
8	H	30	ASN
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
8	H	198	GLU
9	I	37	ASN
9	I	126	ILE
9	I	170	LEU
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	2	ASP
10	J	23	ARG
10	J	35	THR
10	J	78	GLN
10	J	126	VAL
10	J	144	LEU
10	J	174	MET
10	J	193	ASP
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	106	ARG
11	K	107	LYS
12	L	1	GLN
12	L	3	ASN
12	L	23	LEU
12	L	49	ASN
12	L	150	LEU
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	M	104	ARG
13	M	138	SER
13	M	161	ARG
13	M	187	ARG
13	M	204	THR
13	M	212	LEU
13	M	215	GLU
13	M	226	LYS
13	M	233	ILE
14	N	20	THR
14	N	36	ARG
14	N	144	GLU
14	N	178	LEU
1	O	2	THR
1	O	17	LYS
1	O	50	LYS
1	O	61	LEU
1	O	157	PHE
1	O	182	GLU
1	O	250	LEU
2	P	50	LYS
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	119	GLN
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	209	ARG
2	P	221	ASP
2	P	237	ILE
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR
3	Q	51	LYS
3	Q	52	LEU
3	Q	61	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	Q	175	LYS
3	Q	180	LYS
3	Q	187	GLU
3	Q	239	GLN
4	R	1	ASP
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	54	ASP
4	R	99	ILE
4	R	102	GLU
4	R	117	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	203	LYS
4	R	214	ILE
4	R	224	ASP
4	R	236	LYS
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	174	THR
5	S	184	ASN
5	S	188	LEU
5	S	201	ARG
5	S	202	ASP
5	S	207	VAL
5	S	208	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	148	GLU
6	T	172	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	T	181	GLU
6	T	198	LEU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	26	THR
7	U	34	LEU
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	165	LYS
7	U	166	GLN
7	U	171	THR
7	U	178	LYS
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	3	ILE
8	V	22	GLN
8	V	30	ASN
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
8	V	198	GLU
9	W	37	ASN
9	W	126	ILE
9	W	170	LEU
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	2	ASP
10	X	23	ARG
10	X	35	THR
10	X	78	GLN
10	X	126	VAL
10	X	144	LEU
10	X	174	MET
10	X	193	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	106	ARG
11	Y	107	LYS
12	Z	1	GLN
12	Z	3	ASN
12	Z	23	LEU
12	Z	49	ASN
12	Z	150	LEU
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	138	SER
13	a	161	ARG
13	a	187	ARG
13	a	204	THR
13	a	212	LEU
13	a	215	GLU
13	a	226	LYS
13	a	233	ILE
14	b	20	THR
14	b	36	ARG
14	b	144	GLU
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
4	D	160	ASN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	147	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
8	H	66	HIS
8	H	165	ASN
10	J	55	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	158	ASN
13	M	18	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	147	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
8	V	165	ASN
10	X	55	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	158	ASN
12	Z	159	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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
16	CIX	Y	301	11	31,35,35	1.00	1 (3%)	40,46,46	1.22	5 (12%)
16	CIX	K	301	11	31,35,35	0.99	1 (3%)	40,46,46	1.22	5 (12%)

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
16	CIX	Y	301	11	-	4/35/41/41	0/1/1/1
16	CIX	K	301	11	-	4/35/41/41	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	301	CIX	C7-C6	-4.13	1.40	1.50
16	K	301	CIX	C7-C6	-4.05	1.41	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	CIX	O8-C9-N11	4.58	119.82	110.50
16	K	301	CIX	O8-C9-N11	4.57	119.80	110.50
16	Y	301	CIX	O10-C9-N11	-3.04	119.88	124.85
16	K	301	CIX	O10-C9-N11	-2.97	119.97	124.85
16	Y	301	CIX	C21-C20-C25	-2.38	104.90	110.57
16	K	301	CIX	C21-C20-C25	-2.31	105.06	110.57
16	K	301	CIX	C13-C12-C17	-2.12	105.51	110.57
16	K	301	CIX	O8-C9-O10	-2.10	120.23	124.25
16	Y	301	CIX	O8-C9-O10	-2.06	120.31	124.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	CIX	C13-C12-C17	-2.03	105.73	110.57

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	301	CIX	C20-C21-C22-C24
16	K	301	CIX	C20-C21-C22-C23
16	Y	301	CIX	C20-C21-C22-C23
16	Y	301	CIX	C20-C21-C22-C24
16	Y	301	CIX	N19-C20-C21-C22
16	K	301	CIX	N19-C20-C21-C22
16	Y	301	CIX	C25-C20-C21-C22
16	K	301	CIX	C25-C20-C21-C22

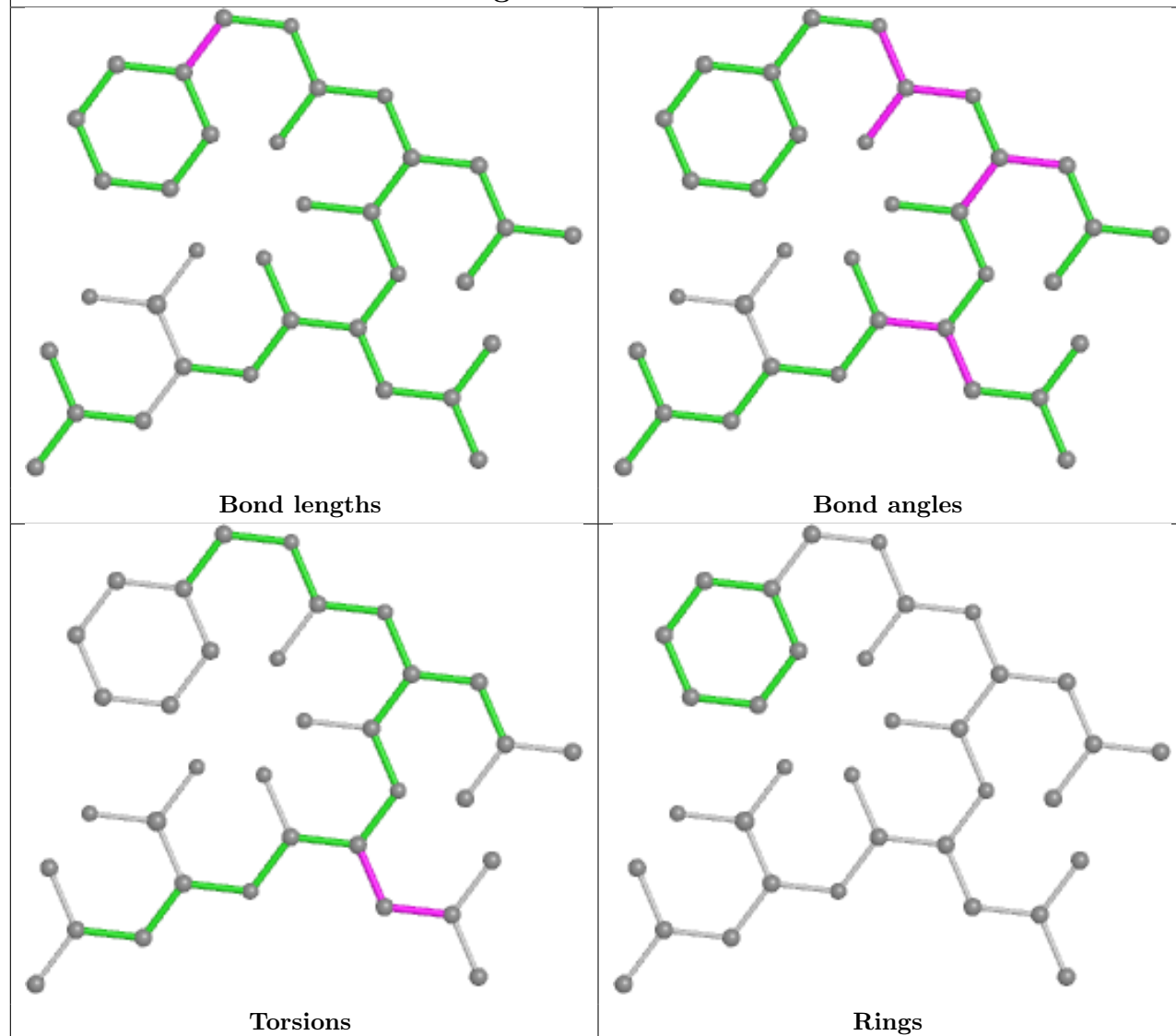
There are no ring outliers.

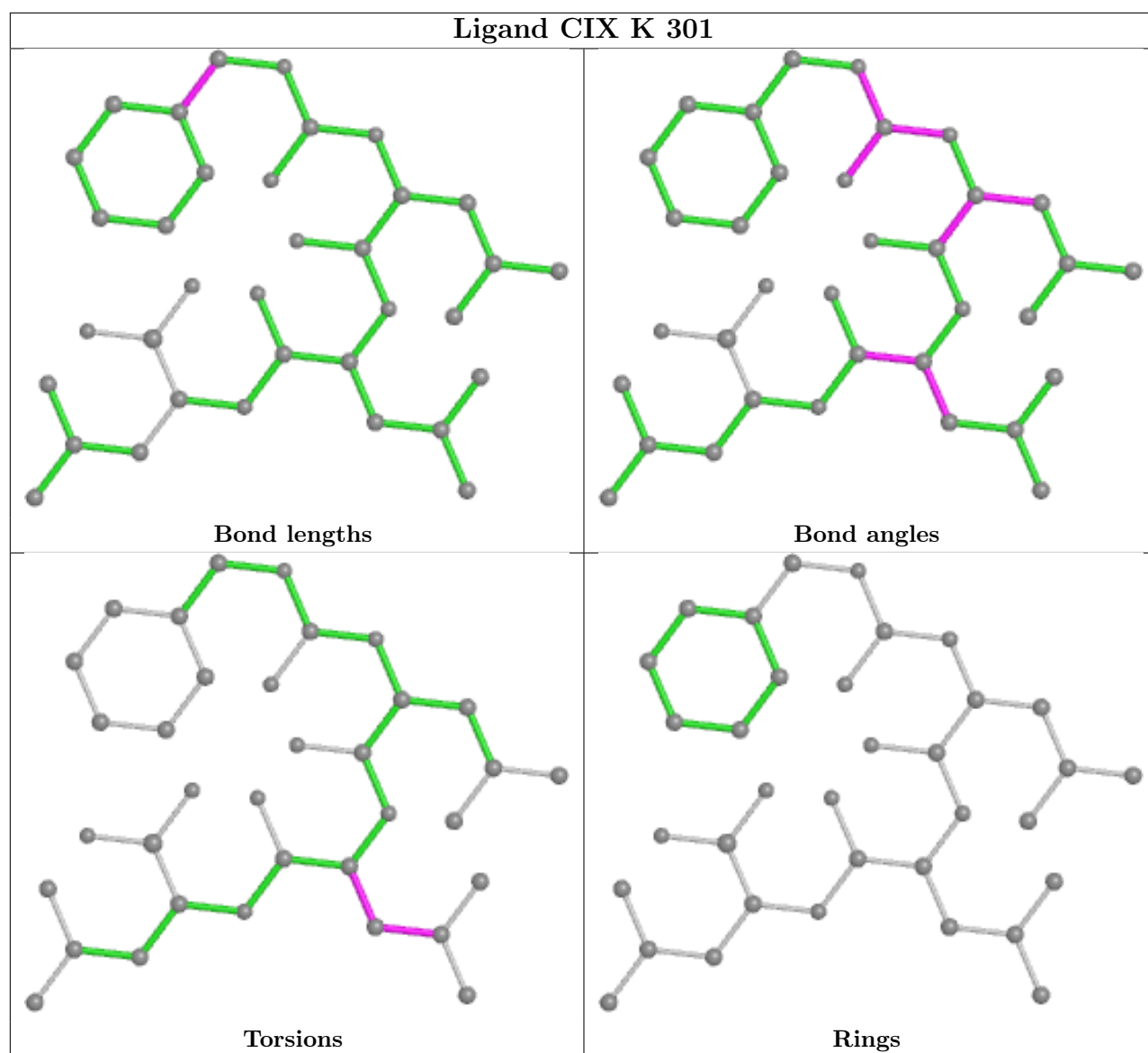
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	301	CIX	1	0

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

## Ligand CIX Y 301





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.38	6 (2%) 59 62	29, 44, 78, 117	0
1	O	250/250 (100%)	-0.33	7 (2%) 53 56	34, 48, 89, 115	0
2	B	244/258 (94%)	-0.24	12 (4%) 29 31	31, 47, 90, 141	0
2	P	244/258 (94%)	-0.22	13 (5%) 26 28	30, 50, 96, 150	0
3	C	240/254 (94%)	-0.13	14 (5%) 23 24	28, 50, 111, 135	0
3	Q	240/254 (94%)	-0.03	20 (8%) 11 11	30, 55, 119, 157	0
4	D	235/260 (90%)	-0.39	1 (0%) 92 93	32, 49, 78, 118	0
4	R	235/260 (90%)	-0.36	4 (1%) 70 72	37, 52, 79, 117	0
5	E	231/234 (98%)	-0.33	3 (1%) 77 79	29, 51, 79, 122	0
5	S	231/234 (98%)	-0.34	6 (2%) 56 59	36, 52, 81, 108	0
6	F	243/288 (84%)	-0.39	8 (3%) 46 50	30, 46, 87, 122	0
6	T	243/288 (84%)	-0.39	8 (3%) 46 50	31, 49, 87, 116	0
7	G	241/252 (95%)	-0.42	1 (0%) 92 93	28, 43, 78, 133	0
7	U	241/252 (95%)	-0.41	4 (1%) 70 72	33, 45, 74, 110	0
8	H	222/232 (95%)	-0.45	3 (1%) 75 77	29, 42, 68, 97	0
8	V	222/232 (95%)	-0.47	2 (0%) 84 86	32, 44, 66, 107	0
9	I	204/205 (99%)	-0.60	3 (1%) 73 75	28, 41, 65, 99	0
9	W	204/205 (99%)	-0.57	2 (0%) 82 84	28, 42, 69, 109	0
10	J	195/198 (98%)	-0.52	4 (2%) 63 66	30, 42, 67, 118	0
10	X	195/198 (98%)	-0.51	3 (1%) 73 75	30, 43, 66, 125	0
11	K	212/212 (100%)	-0.51	1 (0%) 91 91	30, 43, 72, 96	0
11	Y	212/212 (100%)	-0.47	2 (0%) 84 86	28, 44, 74, 96	0
12	L	222/222 (100%)	-0.59	1 (0%) 91 91	30, 43, 65, 86	0
12	Z	222/222 (100%)	-0.57	1 (0%) 91 91	28, 43, 68, 93	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.62	2 (0%) 84 86	27, 41, 58, 69	0
13	a	233/246 (94%)	-0.62	1 (0%) 92 93	27, 41, 58, 70	0
14	N	196/196 (100%)	-0.61	2 (1%) 82 84	30, 38, 61, 90	0
14	b	196/196 (100%)	-0.61	1 (0%) 91 91	28, 39, 62, 86	0
All	All	6336/6614 (95%)	-0.42	135 (2%) 63 66	27, 45, 80, 157	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	W	1	SER	7.6
3	C	206	LYS	6.9
2	P	218	GLY	6.3
2	P	51	VAL	6.0
3	Q	239	GLN	5.9
2	B	219	ALA	5.8
9	I	1	SER	5.7
2	P	219	ALA	5.7
3	C	49	THR	5.2
2	P	222	GLY	4.7
3	Q	50	LEU	4.7
2	B	220	ASN	4.6
8	V	222	ASP	4.5
3	Q	206	LYS	4.5
3	Q	240	GLU	4.4
2	B	218	GLY	4.3
2	P	221	ASP	4.2
3	C	238	LYS	4.1
6	F	202	ASP	4.1
10	X	194	ASP	4.1
5	E	202	ASP	4.0
3	Q	48	SER	4.0
3	C	202	GLN	3.9
13	a	1	THR	3.8
2	B	51	VAL	3.6
2	B	221	ASP	3.5
3	Q	49	THR	3.5
4	D	242	GLU	3.5
2	P	59	ASP	3.5
3	C	240	GLU	3.5
6	T	205	GLU	3.5
1	A	2	THR	3.5

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	R	241	ALA	3.5
3	Q	236	GLN	3.5
1	A	249	ALA	3.5
2	P	220	ASN	3.5
1	O	249	ALA	3.4
8	H	221	CYS	3.4
3	C	203	THR	3.4
1	A	1	MET	3.4
10	J	194	ASP	3.4
7	U	242	GLN	3.4
6	F	205	GLU	3.3
2	B	242	GLY	3.3
8	H	222	ASP	3.3
3	C	239	GLN	3.2
1	O	52	SER	3.2
1	O	2	THR	3.2
2	P	61	SER	3.2
3	Q	202	GLN	3.2
3	Q	238	LYS	3.2
1	A	250	LEU	3.1
3	C	225	GLU	3.1
2	P	52	THR	3.1
1	O	1	MET	3.1
5	S	202	ASP	3.0
11	Y	106	ARG	3.0
5	E	201	ARG	3.0
14	b	105	LYS	3.0
3	C	236	GLN	3.0
10	X	1	MET	3.0
7	G	242	GLN	2.9
3	Q	203	THR	2.9
3	C	205	ALA	2.9
1	O	201	GLU	2.9
3	Q	201	VAL	2.8
6	T	244	ASN	2.8
2	B	222	GLY	2.8
6	T	2	THR	2.8
7	U	2	GLY	2.8
11	Y	212	GLY	2.8
6	T	180	PRO	2.8
13	M	1	THR	2.7
1	O	250	LEU	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	203	SER	2.7
2	B	60	THR	2.7
8	H	217	ILE	2.6
6	F	2	THR	2.6
5	S	123	GLY	2.6
3	C	180	LYS	2.6
2	P	182	ASP	2.6
3	Q	55	THR	2.6
6	F	244	ASN	2.5
8	V	221	CYS	2.5
3	C	175	LYS	2.5
4	R	242	GLU	2.5
2	B	169	SER	2.4
2	P	203	SER	2.4
3	Q	181	GLU	2.4
5	S	165	GLN	2.4
6	T	243	ILE	2.4
3	Q	180	LYS	2.4
4	R	125	LEU	2.4
6	F	215	CYS	2.4
5	S	3	ASN	2.3
1	O	231	LYS	2.3
3	Q	51	LYS	2.3
6	F	180	PRO	2.3
7	U	181	LYS	2.3
14	N	105	LYS	2.3
3	Q	175	LYS	2.3
3	Q	205	ALA	2.3
5	S	201	ARG	2.3
10	J	1	MET	2.3
2	P	93	HIS	2.3
5	E	233	ILE	2.3
1	A	248	GLU	2.3
7	U	241	GLU	2.3
10	X	193	ASP	2.3
3	C	50	LEU	2.3
6	T	181	GLU	2.3
10	J	95	ARG	2.2
5	S	233	ILE	2.2
13	M	47	ASP	2.2
11	K	182	GLU	2.2
6	T	215	CYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	Q	225	GLU	2.1
6	F	181	GLU	2.1
3	C	37	LYS	2.1
2	B	93	HIS	2.1
2	B	182	ASP	2.1
6	F	201	GLU	2.1
2	P	60	THR	2.1
9	I	192	ASP	2.1
12	Z	165	ASN	2.1
14	N	195	GLN	2.1
3	Q	47	ARG	2.1
9	W	133	LYS	2.1
1	A	52	SER	2.0
3	Q	237	GLU	2.0
6	T	166	GLN	2.0
9	I	133	LYS	2.0
4	R	201	GLU	2.0
12	L	165	ASN	2.0
10	J	193	ASP	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
16	CIX	Y	301	35/35	0.85	0.20	55,70,88,90	0
16	CIX	K	301	35/35	0.87	0.19	34,69,95,98	0
15	MG	I	301	1/1	0.92	0.35	65,65,65,65	0
15	MG	H	301	1/1	0.93	0.05	60,60,60,60	0

*Continued on next page...*

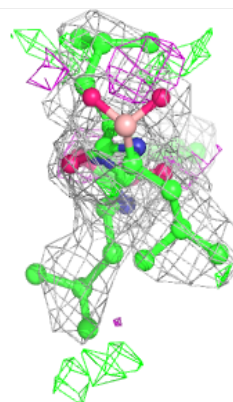
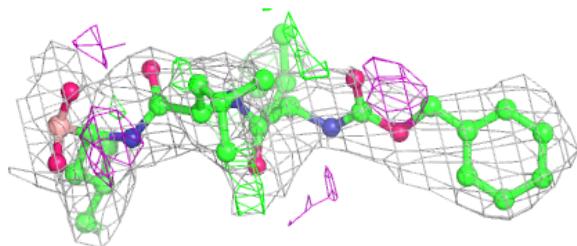
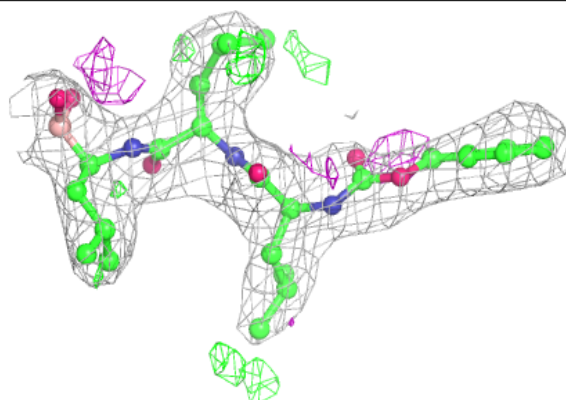
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	MG	Z	301	1/1	0.93	0.14	68,68,68,68	0
15	MG	N	201	1/1	0.96	0.06	42,42,42,42	0
15	MG	G	301	1/1	0.96	0.04	44,44,44,44	0
15	MG	V	301	1/1	0.98	0.07	48,48,48,48	0
15	MG	Y	302	1/1	0.98	0.05	42,42,42,42	0
15	MG	K	302	1/1	0.98	0.07	42,42,42,42	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.

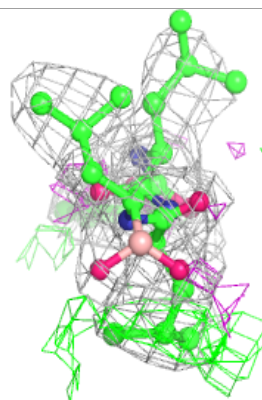
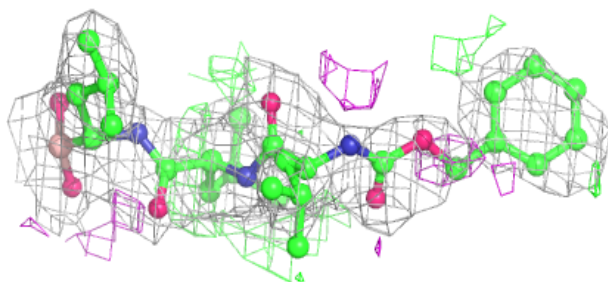
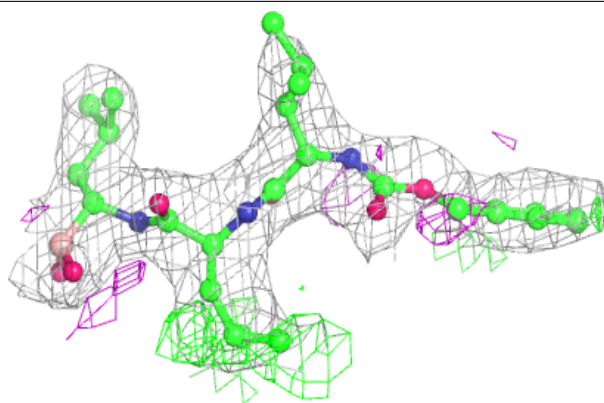
**Electron density around CIX Y 301:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CIX K 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.