



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:30 PM UTC

PDB ID : 3D29 / pdb\_00003d29  
Title : Proteasome Inhibition by Fellutamide B  
Authors : Groll, M.; Hines, J.; Fahnestock, M.; Crews, M.C.  
Deposited on : 2008-05-07  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

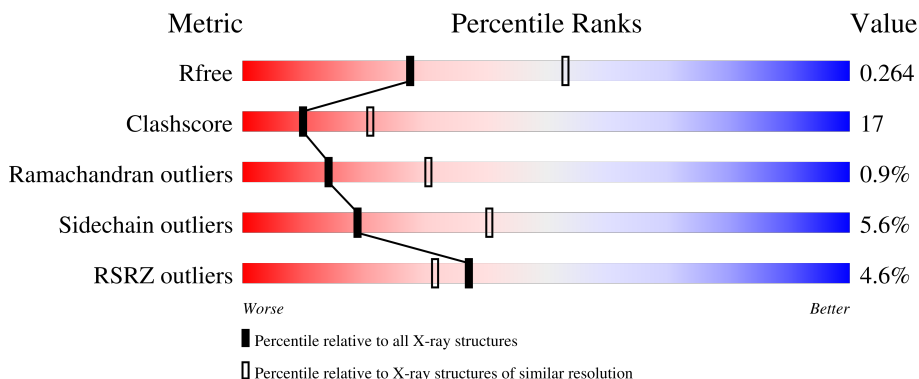
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

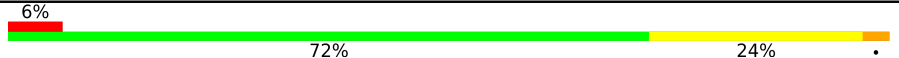
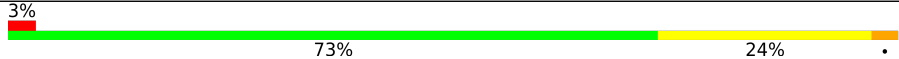



The reported resolution of this entry is 2.60 Å.

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



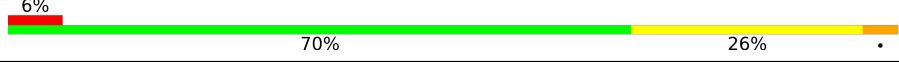
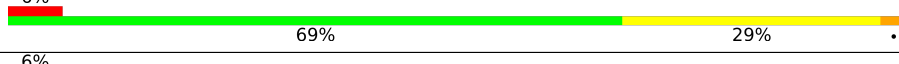

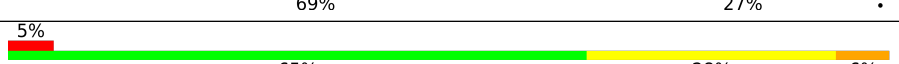
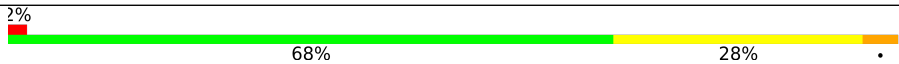










Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	250	
1	O	250	
2	B	244	
2	P	244	
3	C	241	

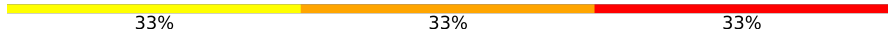


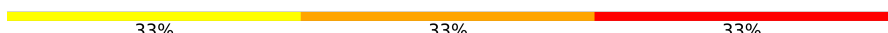
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Mol	Chain	Length	Quality of chain
3	Q	241	 12% 59% 39%
4	D	242	 6% 70% 26%
4	R	242	 6% 69% 29%
5	E	233	 6% 64% 30% 6%
5	S	233	 6% 63% 33%
6	F	244	 4% 68% 28%
6	T	244	 2% 69% 27%
7	G	243	 5% 65% 28% 6%
7	U	243	 5% 64% 30% 5%
8	H	222	 2% 68% 28%
8	V	222	 2% 70% 27%
9	I	204	 0% 72% 27%
9	W	204	 0% 68% 30%
10	J	198	 3% 65% 31%
10	X	198	 4% 61% 36%
11	K	212	 5% 67% 31%
11	Y	212	 7% 68% 28%
12	L	222	 6% 66% 27% 6%
12	Z	222	 5% 67% 25% 8%
13	1	233	 0% 71% 26%
13	M	233	 0% 72% 24%
14	2	196	 3% 68% 30%
14	N	196	 0% 71% 27%
15	a	3	 0% 67% 33%
15	b	3	 0% 67% 33%

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Mol	Chain	Length	Quality of chain
15	c	3	 33% 33% 33%
15	d	3	 67% 33%
15	e	3	 67% 33%
15	f	3	 33% 33% 33%

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 51114 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 PRE8 isoform 1.

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

- Molecule 2 is a protein called PRE9 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	244	1905	1201	321	380	3	0	0	0
2	P	244	1905	1201	321	380	3	0	0	0

- Molecule 3 is a protein called PRE6 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	241	1891	1181	331	375	4	0	0	0
3	Q	241	1891	1181	331	375	4	0	0	0

- Molecule 4 is a protein called PUP2 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	242	1862	1162	314	379	7	0	0	0
4	R	242	1862	1162	314	379	7	0	0	0

- Molecule 5 is a protein called PRE5 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called PRE10 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 7 is a protein called SCL1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called PUP3 isoform 1.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called proteasome endopeptidase complex.

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 PRE7 isoform 1.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	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	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called Fellutamide B.

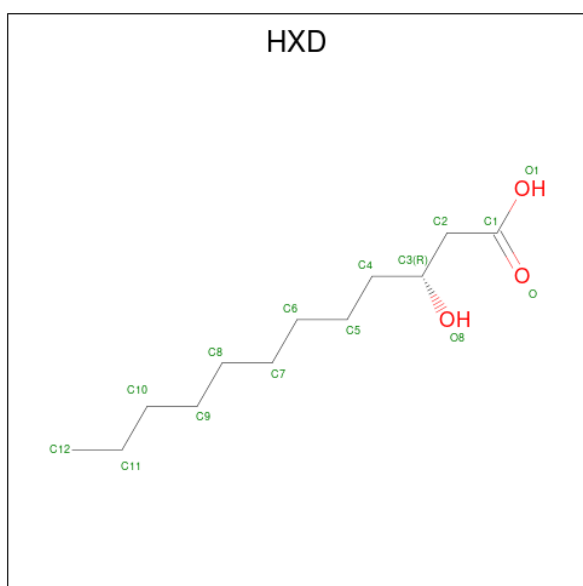
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	a	3	Total	C	N	O	0	0	0
			25	15	5	5			
15	b	3	Total	C	N	O	0	0	0
			25	15	5	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	c	3	Total 25	C 15	N 5	O 5	0	0	0
15	d	3	Total 25	C 15	N 5	O 5	0	0	0
15	e	3	Total 25	C 15	N 5	O 5	0	0	0
15	f	3	Total 25	C 15	N 5	O 5	0	0	0

- Molecule 16 is (3R)-3-HYDROXYDODECANOIC ACID (CCD ID: HXD) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
16	a	1	Total 14	C 12	O 2	0	0
16	b	1	Total 14	C 12	O 2	0	0
16	c	1	Total 14	C 12	O 2	0	0
16	d	1	Total 14	C 12	O 2	0	0
16	e	1	Total 14	C 12	O 2	0	0
16	f	1	Total 14	C 12	O 2	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	55	Total O 55 55	0	0
17	B	36	Total O 36 36	0	0
17	C	46	Total O 46 46	0	0
17	D	42	Total O 42 42	0	0
17	E	23	Total O 23 23	0	0
17	F	46	Total O 46 46	0	0
17	G	62	Total O 62 62	0	0
17	H	51	Total O 51 51	0	0
17	I	66	Total O 66 66	0	0
17	J	53	Total O 53 53	0	0
17	K	42	Total O 42 42	0	0
17	L	56	Total O 56 56	0	0
17	M	68	Total O 68 68	0	0
17	N	59	Total O 59 59	0	0
17	O	35	Total O 35 35	0	0
17	P	29	Total O 29 29	0	0
17	Q	26	Total O 26 26	0	0
17	R	31	Total O 31 31	0	0
17	S	20	Total O 20 20	0	0
17	T	39	Total O 39 39	0	0
17	U	61	Total O 61 61	0	0
17	V	48	Total O 48 48	0	0

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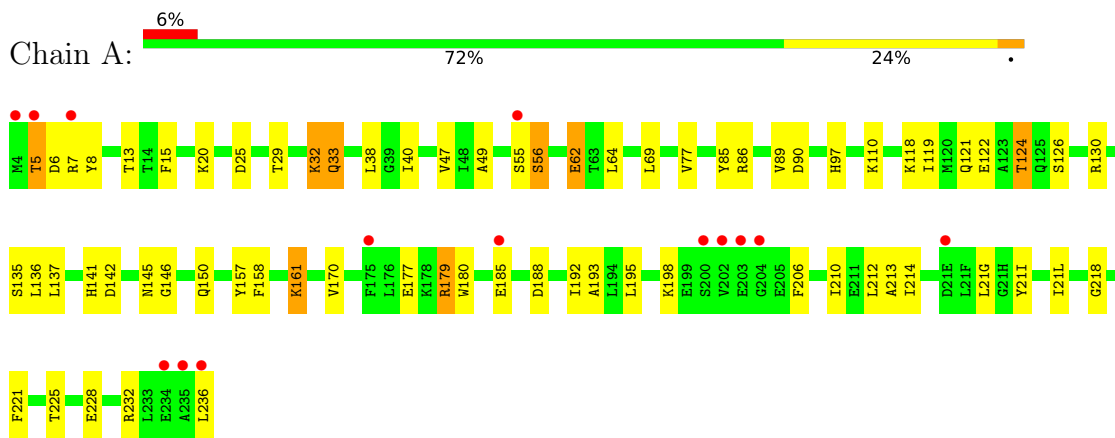
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
17	W	59	Total O 59 59	0	0
17	X	46	Total O 46 46	0	0
17	Y	48	Total O 48 48	0	0
17	Z	52	Total O 52 52	0	0
17	1	74	Total O 74 74	0	0
17	2	59	Total O 59 59	0	0

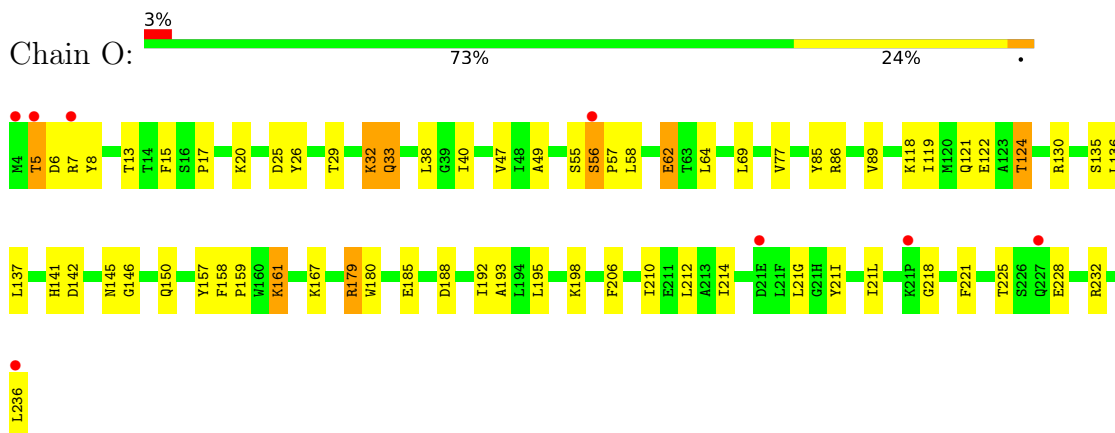
### 3 Residue-property plots [i](#)

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.

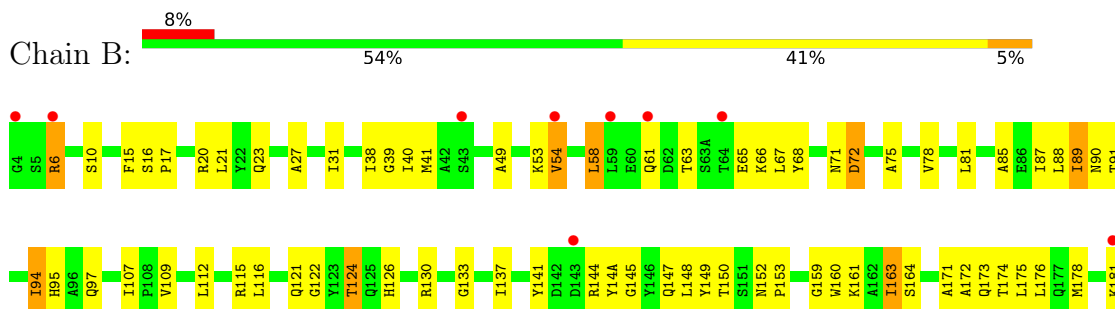
- Molecule 1: PRE8 isoform 1

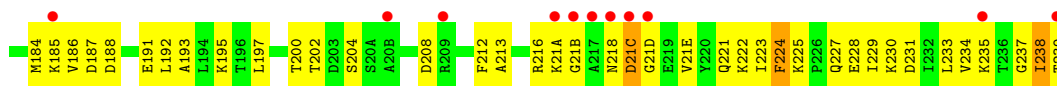


- Molecule 1: PRE8 isoform 1

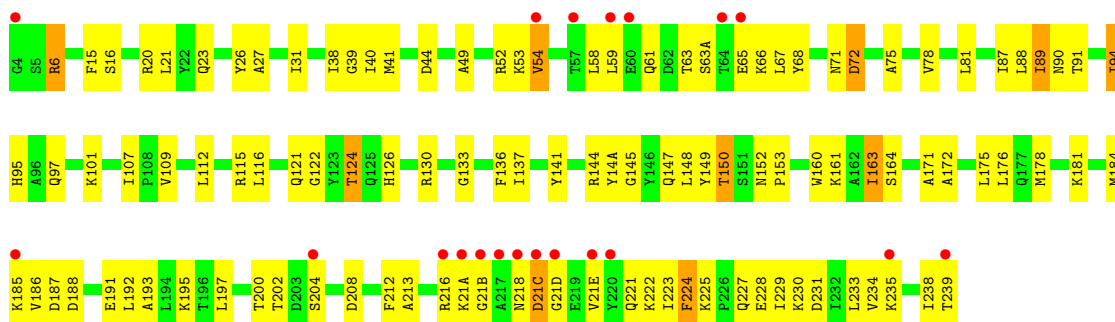


- Molecule 2: PRE9 isoform 1

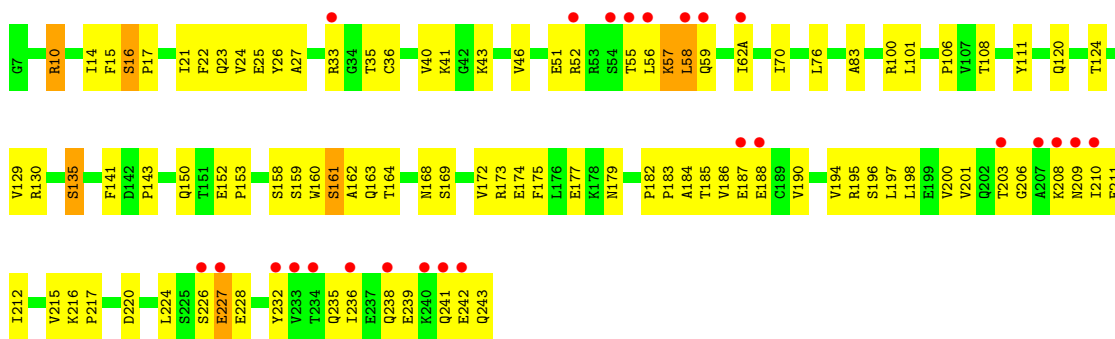




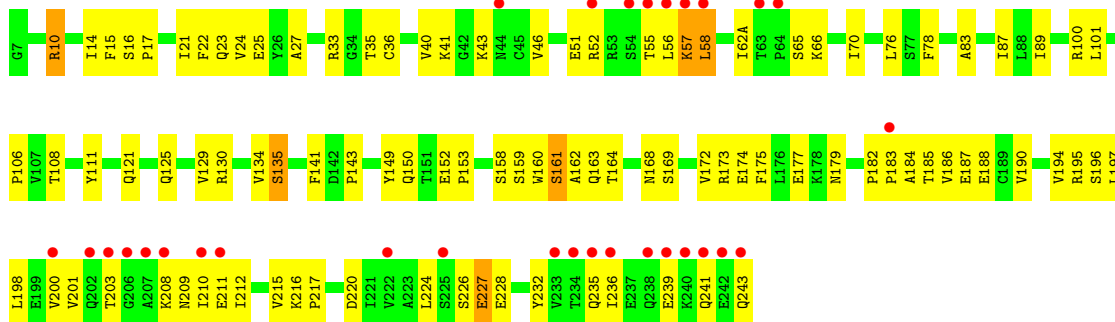
- Molecule 2: PRE9 isoform 1



- Molecule 3: PRE6 isoform 1

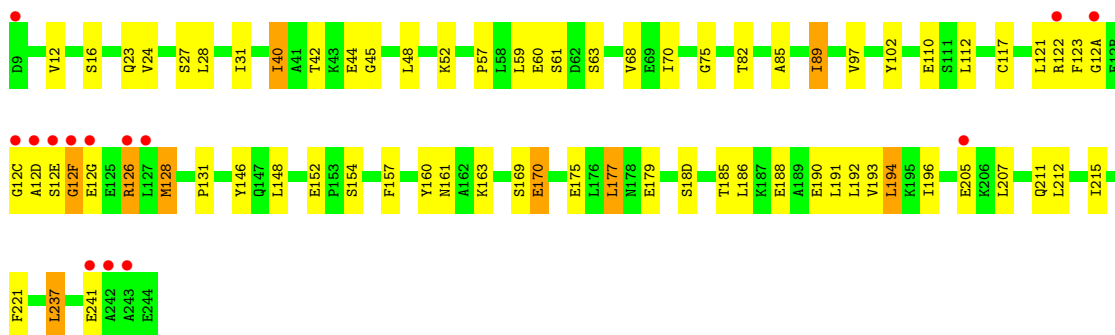


- Molecule 3: PRE6 isoform 1

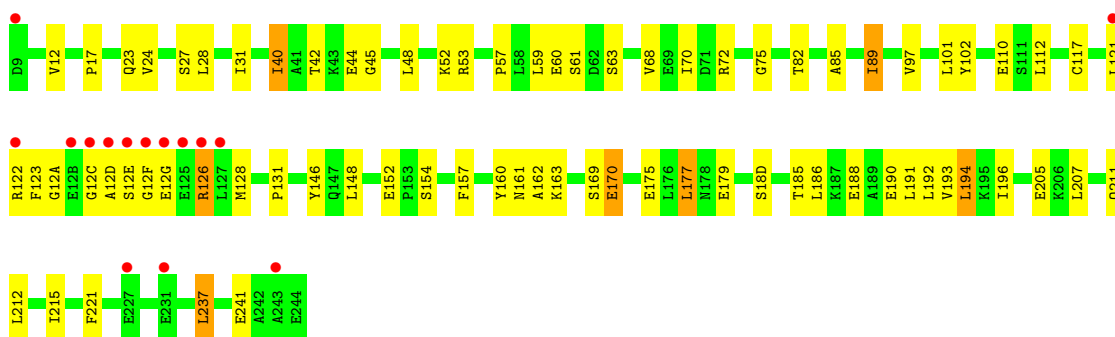


- Molecule 4: PUP2 isoform 1

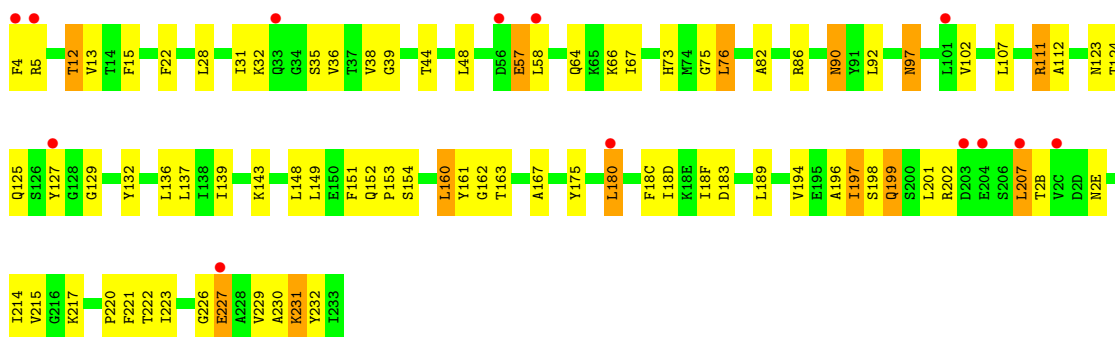




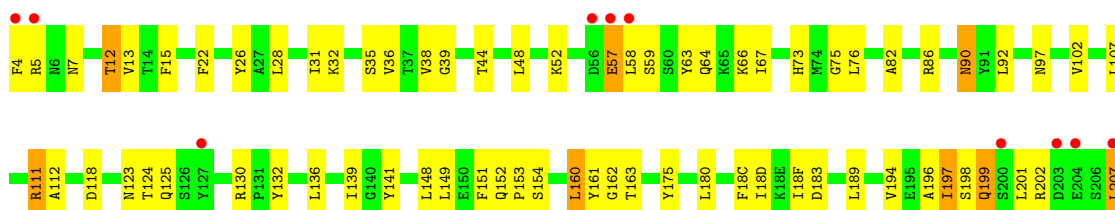
- Molecule 4: PUP2 isoform 1

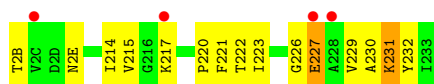


- Molecule 5: PRE5 isoform 1

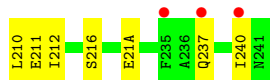


- Molecule 5: PRE5 isoform 1

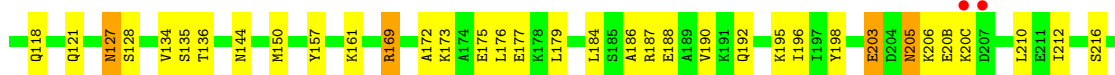




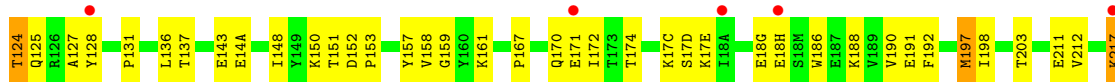
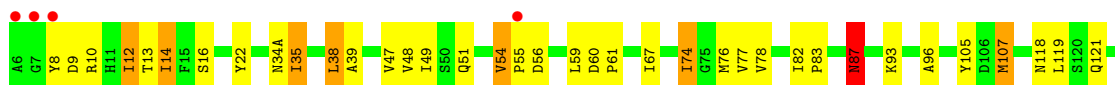
- Molecule 6: PRE10 isoform 1



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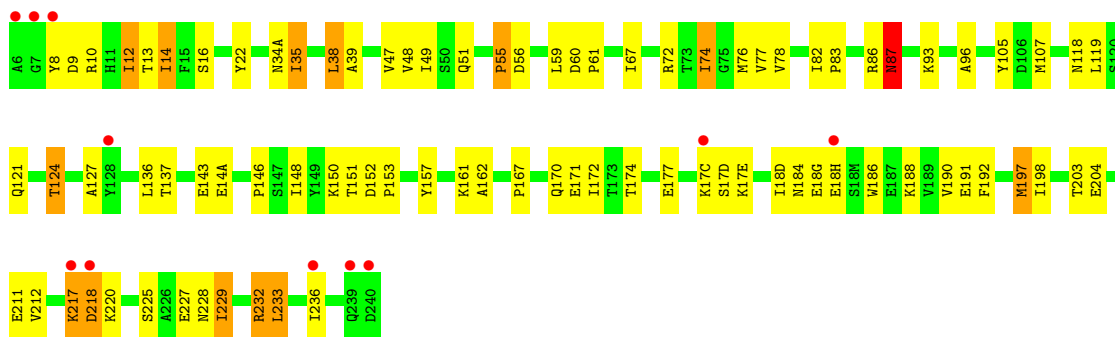


- Molecule 7: SCL1 isoform 1

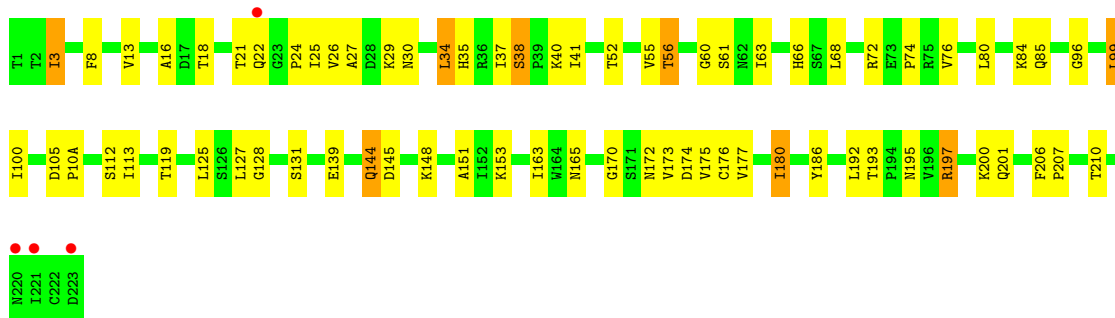


- Molecule 7: SCL1 isoform 1

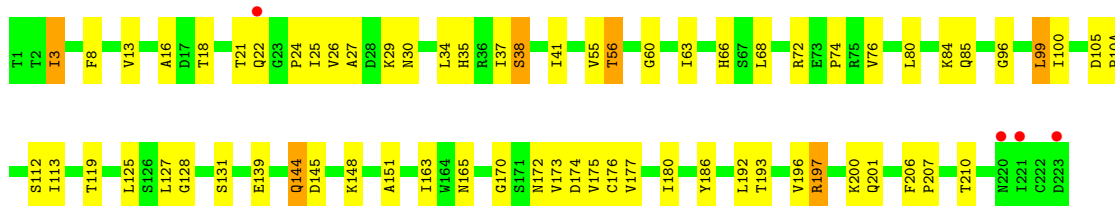




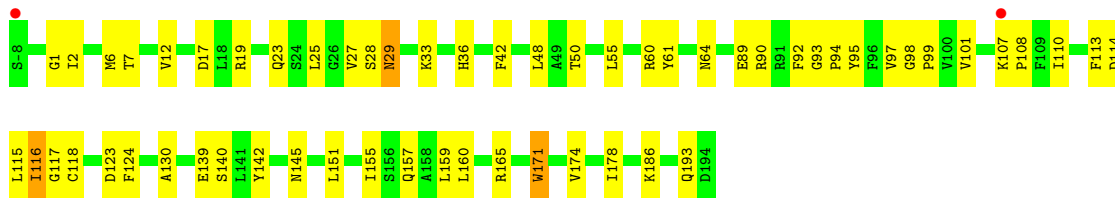
• Molecule 8: proteasome endopeptidase complex



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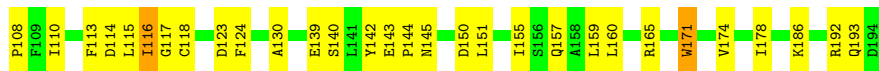


• Molecule 9: PUP3 isoform 1



• Molecule 9: PUP3 isoform 1

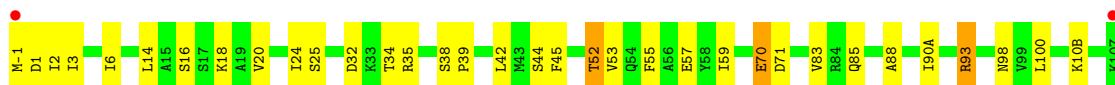




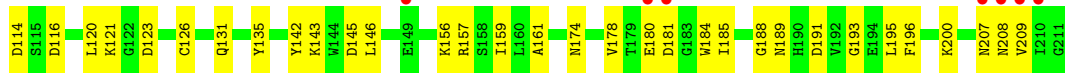
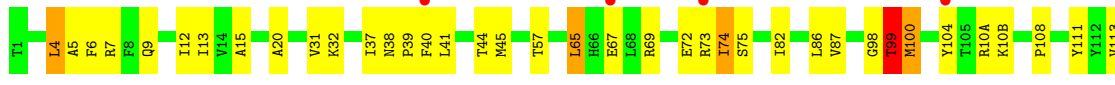
● Molecule 10: Proteasome subunit beta



● Molecule 10: Proteasome subunit beta



● Molecule 11: proteasome endopeptidase complex

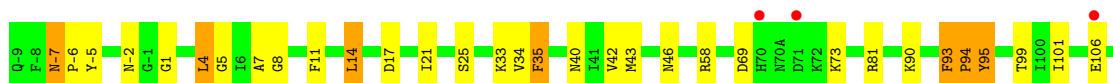


● Molecule 11: proteasome endopeptidase complex

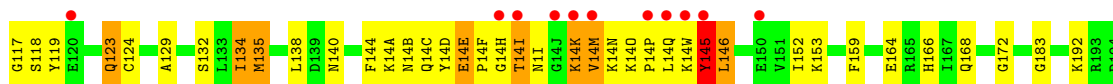
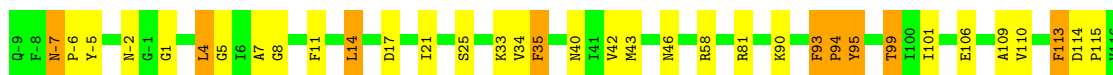




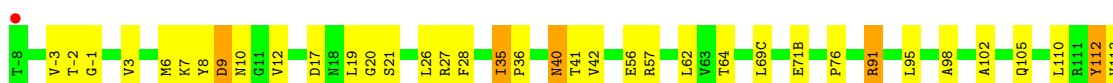
- Molecule 12: PRE7 isoform 1



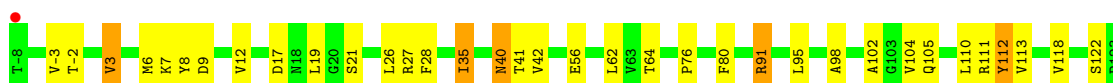
- Molecule 12: PRE7 isoform 1



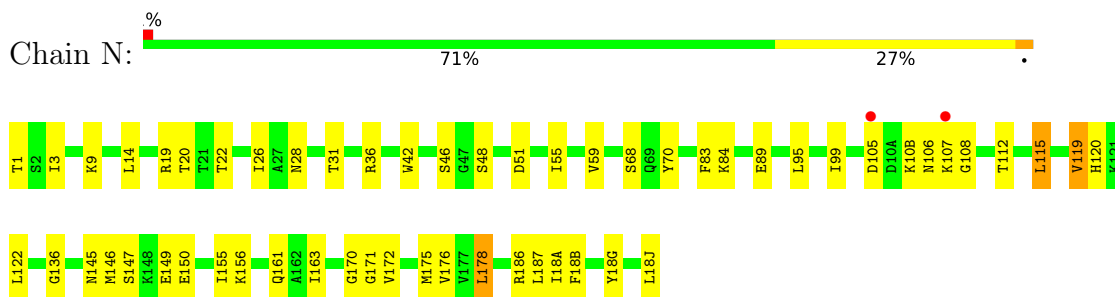
- Molecule 13: Proteasome subunit beta



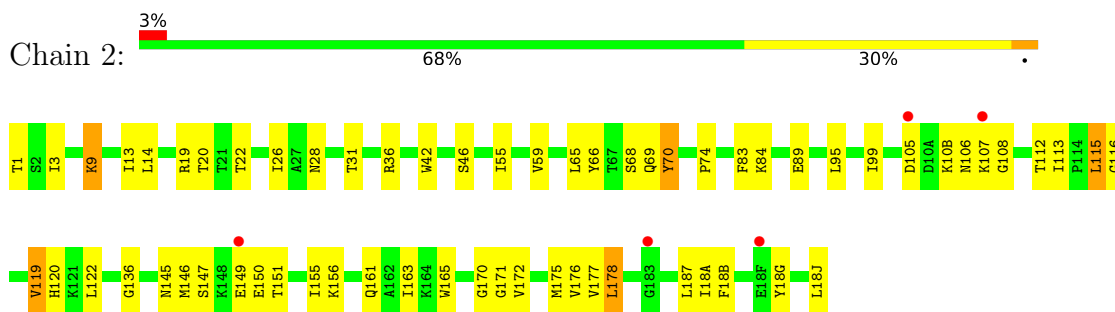
- Molecule 13: Proteasome subunit beta



- Molecule 14: Proteasome subunit beta type-1



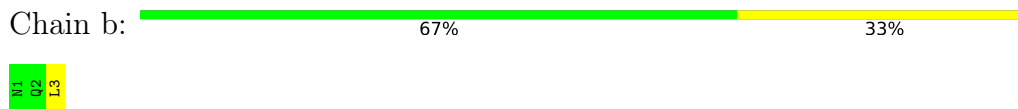
- Molecule 14: Proteasome subunit beta type-1



- Molecule 15: Fellutamide B



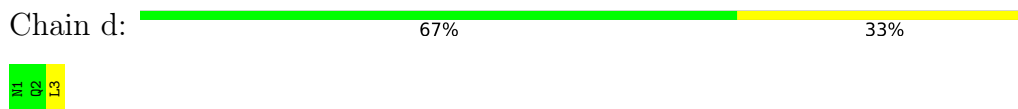
- Molecule 15: Fellutamide B



- Molecule 15: Fellutamide B



- Molecule 15: Fellutamide B



- Molecule 15: Fellutamide B



- Molecule 15: Fellutamide B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.27Å 301.58Å 143.45Å 90.00° 112.70° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.60) 97.7 (15.00-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.56Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.240 , 0.266 0.239 , 0.264	Depositor DCC
$R_{free}$ test set	15699 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtrriage
Anisotropy	0.795	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	51114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.44	0/1952	0.91	2/2642 (0.1%)
1	O	0.41	0/1952	0.92	2/2642 (0.1%)
2	B	0.42	0/1935	0.92	9/2618 (0.3%)
2	P	0.43	0/1935	0.91	8/2618 (0.3%)
3	C	0.41	0/1920	0.90	7/2598 (0.3%)
3	Q	0.40	0/1920	0.90	6/2598 (0.2%)
4	D	0.41	0/1887	0.88	8/2541 (0.3%)
4	R	0.41	0/1887	0.88	7/2541 (0.3%)
5	E	0.42	0/1823	0.93	6/2463 (0.2%)
5	S	0.42	0/1823	0.93	6/2463 (0.2%)
6	F	0.44	0/1937	0.94	7/2614 (0.3%)
6	T	0.45	0/1937	0.95	7/2614 (0.3%)
7	G	0.49	1/1959 (0.1%)	0.97	11/2652 (0.4%)
7	U	0.47	0/1959	0.96	9/2652 (0.3%)
8	H	0.47	0/1716	0.94	4/2326 (0.2%)
8	V	0.45	0/1716	0.94	4/2326 (0.2%)
9	I	0.45	0/1611	1.05	15/2174 (0.7%)
9	W	0.46	0/1611	1.05	14/2174 (0.6%)
10	J	0.47	0/1613	0.99	9/2173 (0.4%)
10	X	0.46	0/1613	1.00	10/2173 (0.5%)
11	K	0.47	0/1681	0.97	7/2274 (0.3%)
11	Y	0.47	0/1681	0.98	6/2274 (0.3%)
12	L	0.47	0/1795	1.05	14/2420 (0.6%)
12	Z	0.46	1/1795 (0.1%)	1.04	13/2420 (0.5%)
13	1	0.47	0/1855	0.96	8/2514 (0.3%)
13	M	0.47	0/1855	0.95	7/2514 (0.3%)
14	2	0.48	0/1541	0.96	5/2087 (0.2%)
14	N	0.49	0/1541	0.98	4/2087 (0.2%)
15	a	2.24	1/24 (4.2%)	1.75	0/30
15	b	2.41	1/24 (4.2%)	1.56	0/30
15	c	2.70	2/24 (8.3%)	2.01	0/30
15	d	2.16	1/24 (4.2%)	1.74	0/30

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
15	e	2.33	1/24 (4.2%)	1.53	0/30
15	f	2.75	2/24 (8.3%)	2.05	0/30
All	All	0.47	10/50594 (0.0%)	0.96	215/68372 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
12	Z	0	1
All	All	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	3	LEU	C-OXT	9.92	1.43	1.23
15	f	3	LEU	C-OXT	9.67	1.42	1.23
15	e	3	LEU	C-OXT	9.39	1.42	1.23
15	c	3	LEU	C-OXT	9.24	1.42	1.23
15	a	3	LEU	C-OXT	8.90	1.41	1.23

The worst 5 of 215 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	27	ARG	N-CA-C	11.70	123.58	111.07
13	M	27	ARG	N-CA-C	11.41	123.28	111.07
11	Y	188	GLY	N-CA-C	9.44	124.58	112.68
12	L	93	PHE	CA-C-N	9.18	129.25	119.89
12	L	93	PHE	C-N-CA	9.18	129.25	119.89

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
12	Z	145	TYR	Sidechain

## 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	1926	62	0
1	O	1915	0	1926	62	0
2	B	1905	0	1901	104	0
2	P	1905	0	1901	97	0
3	C	1891	0	1900	109	0
3	Q	1891	0	1900	107	0
4	D	1862	0	1836	53	0
4	R	1862	0	1836	58	0
5	E	1795	0	1797	75	0
5	S	1795	0	1797	72	0
6	F	1897	0	1886	62	0
6	T	1897	0	1886	56	0
7	G	1921	0	1910	83	0
7	U	1921	0	1910	88	0
8	H	1685	0	1687	63	0
8	V	1685	0	1687	55	0
9	I	1581	0	1574	49	0
9	W	1581	0	1574	51	0
10	J	1585	0	1590	66	0
10	X	1585	0	1590	68	0
11	K	1644	0	1594	71	0
11	Y	1644	0	1594	74	0
12	L	1757	0	1711	52	0
12	Z	1757	0	1711	50	0
13	1	1824	0	1832	53	0
13	M	1824	0	1832	54	0
14	2	1512	0	1480	58	0
14	N	1512	0	1480	51	0
15	a	25	0	24	0	0
15	b	25	0	24	0	0
15	c	25	0	25	7	0
15	d	25	0	24	0	0
15	e	25	0	25	0	0
15	f	25	0	25	6	0
16	a	14	0	23	3	0
16	b	14	0	23	0	0
16	c	14	0	23	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	d	14	0	23	3	0
16	e	14	0	23	0	0
16	f	14	0	23	1	0
17	1	74	0	0	4	0
17	2	59	0	0	1	0
17	A	55	0	0	4	0
17	B	36	0	0	2	0
17	C	46	0	0	1	0
17	D	42	0	0	2	0
17	E	23	0	0	1	0
17	F	46	0	0	2	0
17	G	62	0	0	3	0
17	H	51	0	0	3	0
17	I	66	0	0	2	0
17	J	53	0	0	4	0
17	K	42	0	0	6	0
17	L	56	0	0	5	0
17	M	68	0	0	6	0
17	N	59	0	0	2	0
17	O	35	0	0	0	0
17	P	29	0	0	2	0
17	Q	26	0	0	2	0
17	R	31	0	0	3	0
17	S	20	0	0	1	0
17	T	39	0	0	2	0
17	U	61	0	0	6	0
17	V	48	0	0	3	0
17	W	59	0	0	1	0
17	X	46	0	0	6	0
17	Y	48	0	0	13	0
17	Z	52	0	0	3	0
All	All	51114	0	49533	1729	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 17.

The worst 5 of 1729 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)
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.10	1.16
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.33	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.33	1.10
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.10	1.09
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.11	1.09

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%)	231 (93%)	15 (6%)	2 (1%)	16	34
1	O	248/250 (99%)	232 (94%)	13 (5%)	3 (1%)	10	23
2	B	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	7	15
2	P	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	7	15
3	C	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	9	21
3	Q	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	9	21
4	D	240/242 (99%)	221 (92%)	12 (5%)	7 (3%)	3	6
4	R	240/242 (99%)	221 (92%)	13 (5%)	6 (2%)	4	8
5	E	231/233 (99%)	214 (93%)	13 (6%)	4 (2%)	7	15
5	S	231/233 (99%)	213 (92%)	16 (7%)	2 (1%)	14	30
6	F	242/244 (99%)	230 (95%)	9 (4%)	3 (1%)	10	23
6	T	242/244 (99%)	230 (95%)	9 (4%)	3 (1%)	10	23
7	G	241/243 (99%)	229 (95%)	12 (5%)	0	100	100
7	U	241/243 (99%)	229 (95%)	11 (5%)	1 (0%)	30	51
8	H	220/222 (99%)	210 (96%)	8 (4%)	2 (1%)	14	30
8	V	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	24	46
9	I	202/204 (99%)	194 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	W	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
10	J	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	24	46
10	X	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	24	46
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	24	46
11	Y	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	24	46
12	L	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	24	46
12	Z	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	24	46
13	1	231/233 (99%)	217 (94%)	14 (6%)	0	100	100
13	M	231/233 (99%)	217 (94%)	14 (6%)	0	100	100
14	2	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
15	a	1/3 (33%)	1 (100%)	0	0	100	100
15	b	1/3 (33%)	1 (100%)	0	0	100	100
15	c	1/3 (33%)	1 (100%)	0	0	100	100
15	d	1/3 (33%)	1 (100%)	0	0	100	100
15	e	1/3 (33%)	1 (100%)	0	0	100	100
15	f	1/3 (33%)	1 (100%)	0	0	100	100
All	All	6318/6386 (99%)	5954 (94%)	310 (5%)	54 (1%)	14	30

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	56	SER
3	C	58	LEU
4	D	12(G)	GLU
10	J	192	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	199 (95%)	10 (5%)	23	47
1	O	209/209 (100%)	199 (95%)	10 (5%)	23	47
2	B	203/203 (100%)	196 (97%)	7 (3%)	32	60
2	P	203/203 (100%)	196 (97%)	7 (3%)	32	60
3	C	213/213 (100%)	206 (97%)	7 (3%)	33	61
3	Q	213/213 (100%)	206 (97%)	7 (3%)	33	61
4	D	198/198 (100%)	185 (93%)	13 (7%)	15	34
4	R	198/198 (100%)	185 (93%)	13 (7%)	15	34
5	E	192/192 (100%)	175 (91%)	17 (9%)	9	20
5	S	192/192 (100%)	175 (91%)	17 (9%)	9	20
6	F	201/201 (100%)	189 (94%)	12 (6%)	17	37
6	T	201/201 (100%)	188 (94%)	13 (6%)	15	35
7	G	207/207 (100%)	194 (94%)	13 (6%)	16	36
7	U	207/207 (100%)	194 (94%)	13 (6%)	16	36
8	H	181/181 (100%)	172 (95%)	9 (5%)	22	46
8	V	181/181 (100%)	173 (96%)	8 (4%)	25	50
9	I	172/172 (100%)	168 (98%)	4 (2%)	44	71
9	W	172/172 (100%)	167 (97%)	5 (3%)	37	65
10	J	175/175 (100%)	168 (96%)	7 (4%)	28	55
10	X	175/175 (100%)	169 (97%)	6 (3%)	32	60
11	K	169/169 (100%)	160 (95%)	9 (5%)	20	43
11	Y	169/169 (100%)	159 (94%)	10 (6%)	18	38
12	L	185/185 (100%)	160 (86%)	25 (14%)	4	7
12	Z	185/185 (100%)	160 (86%)	25 (14%)	4	7
13	1	199/199 (100%)	190 (96%)	9 (4%)	24	50
13	M	199/199 (100%)	190 (96%)	9 (4%)	24	50
14	2	162/162 (100%)	155 (96%)	7 (4%)	26	51
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	51
15	a	3/3 (100%)	3 (100%)	0	100	100
15	b	3/3 (100%)	3 (100%)	0	100	100
15	c	3/3 (100%)	2 (67%)	1 (33%)	0	0
15	d	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	e	3/3 (100%)	3 (100%)	0	100	100
15	f	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	5350/5350 (100%)	5049 (94%)	301 (6%)	19	40

5 of 301 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	V	55	VAL
13	1	112	TYR
9	W	29	ASN
12	Z	14	LEU
15	f	1	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 223 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	95	HIS
15	c	1	ASN
5	S	123	ASN
14	2	145	ASN
12	Z	27	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	HXD	a	4	15	12,13,14	0.62	0	13,13,15	0.85	1 (7%)
16	HXD	d	4	15	12,13,14	0.59	0	13,13,15	0.84	1 (7%)
16	HXD	e	4	15	12,13,14	0.74	0	13,13,15	0.67	0
16	HXD	c	4	15	12,13,14	1.14	1 (8%)	13,13,15	1.05	1 (7%)
16	HXD	f	4	15	12,13,14	1.13	2 (16%)	13,13,15	1.00	1 (7%)
16	HXD	b	4	15	12,13,14	0.77	0	13,13,15	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	HXD	a	4	15	-	2/12/12/13	-
16	HXD	d	4	15	-	2/12/12/13	-
16	HXD	e	4	15	-	5/12/12/13	-
16	HXD	c	4	15	-	3/12/12/13	-
16	HXD	f	4	15	-	3/12/12/13	-
16	HXD	b	4	15	-	5/12/12/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	f	4	HXD	C5-C6	-2.21	1.40	1.51
16	f	4	HXD	C5-C4	2.10	1.61	1.52
16	c	4	HXD	C5-C4	2.06	1.60	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	d	4	HXD	C3-C2-C1	2.37	116.74	112.70
16	a	4	HXD	C3-C2-C1	2.37	116.73	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	f	4	HXD	O-C1-C2	-2.13	119.19	125.38
16	c	4	HXD	O-C1-C2	-2.03	119.48	125.38

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	c	4	HXD	C1-C2-C3-C4
16	c	4	HXD	C1-C2-C3-O8
16	f	4	HXD	C1-C2-C3-C4
16	f	4	HXD	C1-C2-C3-O8
16	b	4	HXD	O8-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	a	4	HXD	3	0
16	d	4	HXD	3	0
16	c	4	HXD	1	0
16	f	4	HXD	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	0.20	14 (5%) 30 24	34, 52, 85, 106	0
1	O	250/250 (100%)	0.20	8 (3%) 50 44	35, 54, 85, 105	0
2	B	244/244 (100%)	0.46	20 (8%) 17 14	37, 56, 89, 116	0
2	P	244/244 (100%)	0.46	20 (8%) 17 14	40, 56, 89, 116	0
3	C	241/241 (100%)	0.68	25 (10%) 11 9	39, 61, 110, 124	0
3	Q	241/241 (100%)	0.76	30 (12%) 8 6	41, 62, 110, 124	0
4	D	242/242 (100%)	0.49	14 (5%) 29 23	43, 58, 94, 121	0
4	R	242/242 (100%)	0.50	15 (6%) 26 21	44, 59, 95, 122	0
5	E	233/233 (100%)	0.37	13 (5%) 30 24	42, 55, 82, 109	0
5	S	233/233 (100%)	0.37	14 (6%) 27 22	41, 54, 82, 109	0
6	F	244/244 (100%)	0.19	10 (4%) 41 36	36, 50, 89, 106	0
6	T	244/244 (100%)	0.12	6 (2%) 58 52	34, 50, 89, 106	0
7	G	243/243 (100%)	0.02	13 (5%) 32 26	33, 47, 75, 112	0
7	U	243/243 (100%)	0.10	11 (4%) 38 32	33, 47, 75, 111	0
8	H	222/222 (100%)	-0.18	4 (1%) 67 63	30, 44, 62, 100	0
8	V	222/222 (100%)	-0.16	4 (1%) 67 63	29, 45, 63, 100	0
9	I	204/204 (100%)	-0.17	2 (0%) 79 76	35, 45, 63, 80	0
9	W	204/204 (100%)	-0.15	1 (0%) 87 85	36, 46, 64, 80	0
10	J	198/198 (100%)	0.02	6 (3%) 52 47	38, 49, 69, 122	0
10	X	198/198 (100%)	0.06	8 (4%) 42 37	38, 49, 69, 122	0
11	K	212/212 (100%)	0.11	11 (5%) 33 27	34, 47, 72, 86	0
11	Y	212/212 (100%)	0.19	14 (6%) 24 19	35, 47, 74, 86	0
12	L	222/222 (100%)	0.10	13 (5%) 28 23	33, 48, 74, 89	0
12	Z	222/222 (100%)	0.07	11 (4%) 34 28	34, 47, 74, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1	233/233 (100%)	-0.32	1 (0%) 88 86	31, 43, 57, 61	0
13	M	233/233 (100%)	-0.20	1 (0%) 88 86	32, 43, 57, 63	0
14	2	196/196 (100%)	-0.27	5 (2%) 57 51	31, 41, 61, 81	0
14	N	196/196 (100%)	-0.27	2 (1%) 79 76	31, 40, 60, 81	0
15	a	3/3 (100%)	-0.23	0 100 100	41, 41, 44, 46	0
15	b	3/3 (100%)	0.17	0 100 100	34, 34, 42, 47	0
15	c	3/3 (100%)	0.20	0 100 100	43, 43, 48, 51	0
15	d	3/3 (100%)	-0.09	0 100 100	44, 44, 44, 47	0
15	e	3/3 (100%)	-0.12	0 100 100	37, 37, 44, 50	0
15	f	3/3 (100%)	0.15	0 100 100	43, 43, 50, 51	0
All	All	6386/6386 (100%)	0.15	296 (4%) 37 32	29, 50, 84, 124	0

The worst 5 of 296 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	145	TYR	8.2
4	R	12(E)	SER	8.0
3	Q	56	LEU	7.4
11	K	208	ASN	7.4
3	C	56	LEU	7.3

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	HXD	f	4	14/15	0.85	0.12	50,59,61,65	0
16	HXD	d	4	14/15	0.86	0.13	43,45,60,63	0
16	HXD	c	4	14/15	0.86	0.14	49,58,60,61	0
16	HXD	a	4	14/15	0.87	0.12	43,47,59,63	0
16	HXD	e	4	14/15	0.88	0.15	34,39,56,58	0
16	HXD	b	4	14/15	0.88	0.12	37,41,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.