



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:12 PM UTC

PDB ID : 3KRD / pdb_00003krd
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome in complex with Fellutamide B
Authors : Li, D.; Li, H.
Deposited on : 2009-11-18
Resolution : 2.50 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
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

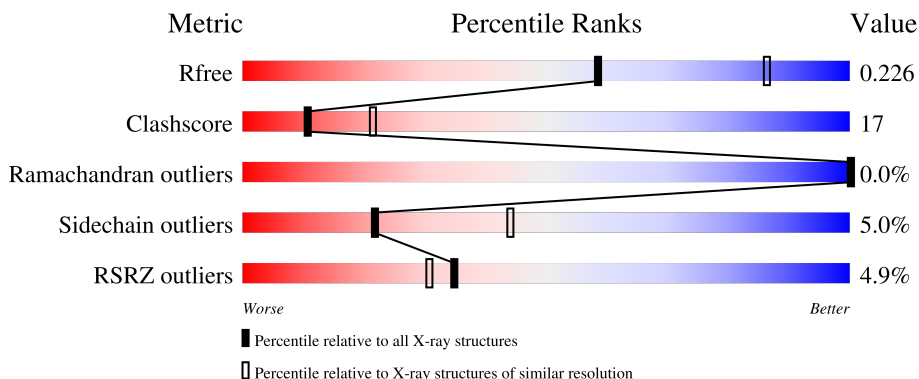
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1	248	
1	A	248	
1	B	248	
1	D	248	
1	F	248	

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Mol	Chain	Length	Quality of chain
1	I	248	6% 56% 26% 13%
1	K	248	7% 56% 28% 13%
1	M	248	9% 56% 25% 14%
1	O	248	8% 50% 30% 6% 14%
1	Q	248	7% 46% 36% 14%
1	S	248	8% 48% 36% 13%
1	U	248	8% 55% 28% 14%
1	W	248	7% 46% 36% 13%
1	Y	248	11% 48% 35% 13%
2	2	240	1% 75% 17% 8%
2	C	240	71% 21% 8%
2	E	240	75% 18% 8%
2	G	240	1% 74% 17% 8%
2	H	240	75% 17% 8%
2	J	240	1% 76% 15% 8%
2	L	240	71% 20% 8%
2	N	240	78% 14% 8%
2	P	240	1% 80% 11% 8%
2	R	240	1% 77% 16% 5% 5%
2	T	240	75% 15% 8%
2	V	240	76% 17% 5% 5%
2	X	240	74% 18% 8%
2	Z	240	1% 77% 15% 8%
3	a	3	67% 33%
3	b	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	c	3	 67% 33%
3	d	3	 67% 33%
3	e	3	 67% 33%
3	f	3	 67% 33%
3	g	3	 67% 33%
3	h	3	 67% 33%
3	i	3	 67% 33%
3	j	3	 67% 33%
3	k	3	 67% 33%
3	l	3	 67% 33%
3	m	3	 67% 33%
3	n	3	 67% 33%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 48828 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	Total 1650	C 1033	N 302	O 312	S 3	0	0	0
1	B	213	Total 1642	C 1027	N 301	O 311	S 3	0	0	0
1	D	213	Total 1646	C 1031	N 301	O 311	S 3	0	0	0
1	F	216	Total 1661	C 1040	N 304	O 314	S 3	0	0	0
1	I	215	Total 1654	C 1035	N 303	O 313	S 3	0	0	0
1	K	215	Total 1654	C 1035	N 303	O 313	S 3	0	0	0
1	M	214	Total 1650	C 1033	N 302	O 312	S 3	0	0	0
1	O	214	Total 1650	C 1033	N 302	O 312	S 3	0	0	0
1	Q	214	Total 1650	C 1033	N 302	O 312	S 3	0	0	0
1	S	215	Total 1657	C 1038	N 303	O 313	S 3	0	0	0
1	U	214	Total 1650	C 1033	N 302	O 312	S 3	0	0	0
1	W	215	Total 1654	C 1035	N 303	O 313	S 3	0	0	0
1	Y	216	Total 1661	C 1040	N 304	O 314	S 3	0	0	0
1	1	215	Total 1654	C 1035	N 303	O 313	S 3	0	0	0

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	222	1638	1027	282	324	5	0	0	0
2	E	222	1638	1027	282	324	5	0	0	0
2	G	222	1638	1027	282	324	5	0	0	0
2	H	222	1638	1027	282	324	5	0	0	0
2	J	222	1638	1027	282	324	5	0	0	0
2	L	222	1638	1027	282	324	5	0	0	0
2	N	222	1638	1027	282	324	5	0	0	0
2	P	222	1638	1027	282	324	5	0	0	0
2	R	229	1683	1054	289	335	5	0	0	0
2	T	222	1638	1027	282	324	5	0	0	0
2	V	229	1683	1054	289	335	5	0	0	0
2	X	222	1638	1027	282	324	5	0	0	0
2	Z	222	1638	1027	282	324	5	0	0	0
2	2	222	1638	1027	282	324	5	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	535	HIS	-	expression tag	UNP A5U4D6
C	536	HIS	-	expression tag	UNP A5U4D6
C	537	HIS	-	expression tag	UNP A5U4D6
C	538	HIS	-	expression tag	UNP A5U4D6
C	539	HIS	-	expression tag	UNP A5U4D6
C	540	HIS	-	expression tag	UNP A5U4D6
E	535	HIS	-	expression tag	UNP A5U4D6
E	536	HIS	-	expression tag	UNP A5U4D6
E	537	HIS	-	expression tag	UNP A5U4D6
E	538	HIS	-	expression tag	UNP A5U4D6
E	539	HIS	-	expression tag	UNP A5U4D6
E	540	HIS	-	expression tag	UNP A5U4D6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	535	HIS	-	expression tag	UNP A5U4D6
G	536	HIS	-	expression tag	UNP A5U4D6
G	537	HIS	-	expression tag	UNP A5U4D6
G	538	HIS	-	expression tag	UNP A5U4D6
G	539	HIS	-	expression tag	UNP A5U4D6
G	540	HIS	-	expression tag	UNP A5U4D6
H	535	HIS	-	expression tag	UNP A5U4D6
H	536	HIS	-	expression tag	UNP A5U4D6
H	537	HIS	-	expression tag	UNP A5U4D6
H	538	HIS	-	expression tag	UNP A5U4D6
H	539	HIS	-	expression tag	UNP A5U4D6
H	540	HIS	-	expression tag	UNP A5U4D6
J	535	HIS	-	expression tag	UNP A5U4D6
J	536	HIS	-	expression tag	UNP A5U4D6
J	537	HIS	-	expression tag	UNP A5U4D6
J	538	HIS	-	expression tag	UNP A5U4D6
J	539	HIS	-	expression tag	UNP A5U4D6
J	540	HIS	-	expression tag	UNP A5U4D6
L	535	HIS	-	expression tag	UNP A5U4D6
L	536	HIS	-	expression tag	UNP A5U4D6
L	537	HIS	-	expression tag	UNP A5U4D6
L	538	HIS	-	expression tag	UNP A5U4D6
L	539	HIS	-	expression tag	UNP A5U4D6
L	540	HIS	-	expression tag	UNP A5U4D6
N	535	HIS	-	expression tag	UNP A5U4D6
N	536	HIS	-	expression tag	UNP A5U4D6
N	537	HIS	-	expression tag	UNP A5U4D6
N	538	HIS	-	expression tag	UNP A5U4D6
N	539	HIS	-	expression tag	UNP A5U4D6
N	540	HIS	-	expression tag	UNP A5U4D6
P	535	HIS	-	expression tag	UNP A5U4D6
P	536	HIS	-	expression tag	UNP A5U4D6
P	537	HIS	-	expression tag	UNP A5U4D6
P	538	HIS	-	expression tag	UNP A5U4D6
P	539	HIS	-	expression tag	UNP A5U4D6
P	540	HIS	-	expression tag	UNP A5U4D6
R	535	HIS	-	expression tag	UNP A5U4D6
R	536	HIS	-	expression tag	UNP A5U4D6
R	537	HIS	-	expression tag	UNP A5U4D6
R	538	HIS	-	expression tag	UNP A5U4D6
R	539	HIS	-	expression tag	UNP A5U4D6
R	540	HIS	-	expression tag	UNP A5U4D6

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Chain	Residue	Modelled	Actual	Comment	Reference
T	535	HIS	-	expression tag	UNP A5U4D6
T	536	HIS	-	expression tag	UNP A5U4D6
T	537	HIS	-	expression tag	UNP A5U4D6
T	538	HIS	-	expression tag	UNP A5U4D6
T	539	HIS	-	expression tag	UNP A5U4D6
T	540	HIS	-	expression tag	UNP A5U4D6
V	535	HIS	-	expression tag	UNP A5U4D6
V	536	HIS	-	expression tag	UNP A5U4D6
V	537	HIS	-	expression tag	UNP A5U4D6
V	538	HIS	-	expression tag	UNP A5U4D6
V	539	HIS	-	expression tag	UNP A5U4D6
V	540	HIS	-	expression tag	UNP A5U4D6
X	535	HIS	-	expression tag	UNP A5U4D6
X	536	HIS	-	expression tag	UNP A5U4D6
X	537	HIS	-	expression tag	UNP A5U4D6
X	538	HIS	-	expression tag	UNP A5U4D6
X	539	HIS	-	expression tag	UNP A5U4D6
X	540	HIS	-	expression tag	UNP A5U4D6
Z	535	HIS	-	expression tag	UNP A5U4D6
Z	536	HIS	-	expression tag	UNP A5U4D6
Z	537	HIS	-	expression tag	UNP A5U4D6
Z	538	HIS	-	expression tag	UNP A5U4D6
Z	539	HIS	-	expression tag	UNP A5U4D6
Z	540	HIS	-	expression tag	UNP A5U4D6
2	535	HIS	-	expression tag	UNP A5U4D6
2	536	HIS	-	expression tag	UNP A5U4D6
2	537	HIS	-	expression tag	UNP A5U4D6
2	538	HIS	-	expression tag	UNP A5U4D6
2	539	HIS	-	expression tag	UNP A5U4D6
2	540	HIS	-	expression tag	UNP A5U4D6

- Molecule 3 is a protein called Fellutamide B.

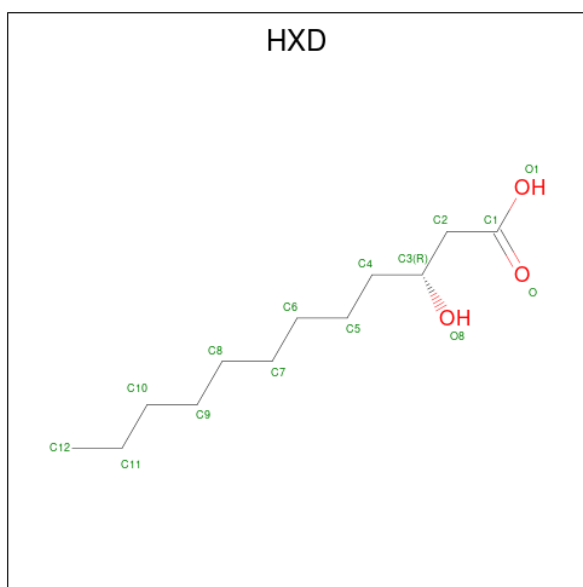
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	a	3	25	15	5	5	0	0	0
3	b	3	25	15	5	5	0	0	0
3	c	3	25	15	5	5	0	0	0
3	d	3	25	15	5	5	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	e	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	f	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	g	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	h	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	i	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	j	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	k	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	l	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	m	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	n	3	Total	C	N	O	0	0	0
			25	15	5	5			

- Molecule 4 is (3R)-3-HYDROXYDODECANOIC ACID (CCD ID: HXD) (formula: $C_{12}H_{24}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	a	1	Total	C	O	0	0
			7	5	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	b	1	Total C O 7 5 2	0	0
4	c	1	Total C O 7 5 2	0	0
4	d	1	Total C O 7 5 2	0	0
4	e	1	Total C O 7 5 2	0	0
4	f	1	Total C O 7 5 2	0	0
4	g	1	Total C O 7 5 2	0	0
4	h	1	Total C O 7 5 2	0	0
4	i	1	Total C O 7 5 2	0	0
4	j	1	Total C O 7 5 2	0	0
4	k	1	Total C O 7 5 2	0	0
4	l	1	Total C O 7 5 2	0	0
4	m	1	Total C O 7 5 2	0	0
4	n	1	Total C O 7 5 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	32	Total O 32 32	0	0
5	B	42	Total O 42 42	0	0
5	C	131	Total O 131 131	0	0
5	D	25	Total O 25 25	0	0
5	E	130	Total O 130 130	0	0
5	F	41	Total O 41 41	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	113	Total 113	O 113	0	0
5	H	126	Total 126	O 126	0	0
5	I	38	Total 38	O 38	0	0
5	J	122	Total 122	O 122	0	0
5	K	33	Total 33	O 33	0	0
5	L	132	Total 132	O 132	0	0
5	M	42	Total 42	O 42	0	0
5	N	121	Total 121	O 121	0	0
5	O	39	Total 39	O 39	0	0
5	P	111	Total 111	O 111	0	0
5	Q	34	Total 34	O 34	0	0
5	R	143	Total 143	O 143	0	0
5	S	43	Total 43	O 43	0	0
5	T	103	Total 103	O 103	0	0
5	U	33	Total 33	O 33	0	0
5	V	149	Total 149	O 149	0	0
5	W	26	Total 26	O 26	0	0
5	X	115	Total 115	O 115	0	0
5	Y	22	Total 22	O 22	0	0
5	Z	106	Total 106	O 106	0	0
5	1	55	Total 55	O 55	0	0

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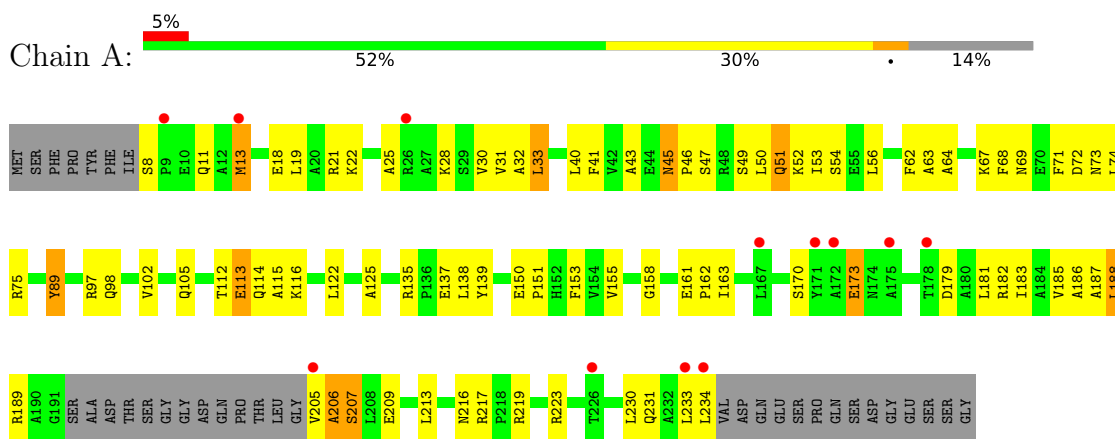
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2	118	Total 118	O 118	0	0

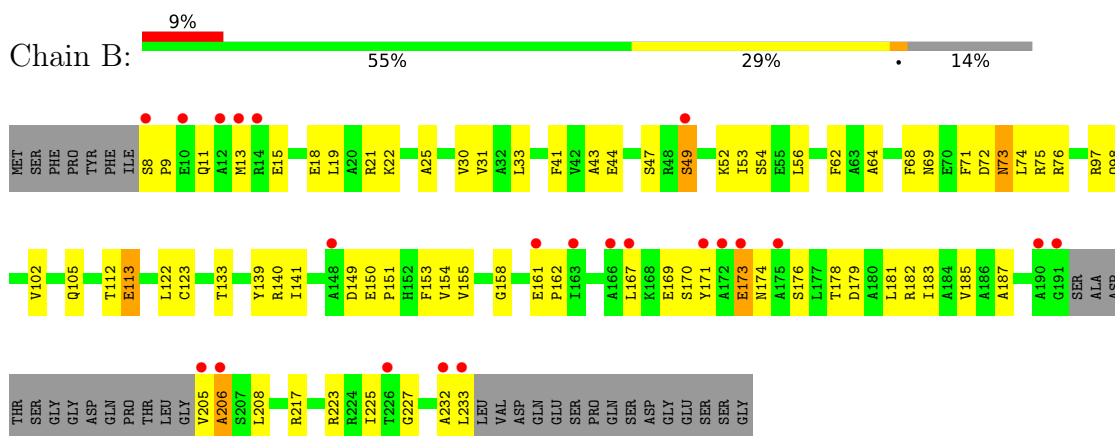
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

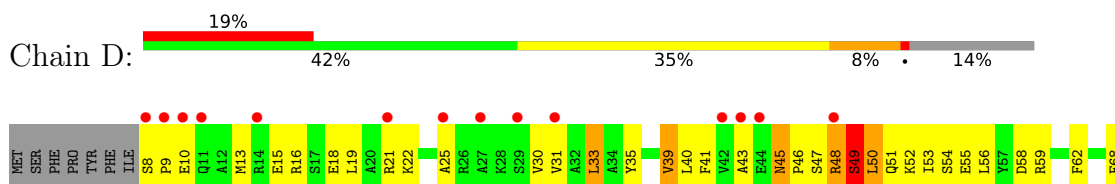
- Molecule 1: Proteasome subunit alpha

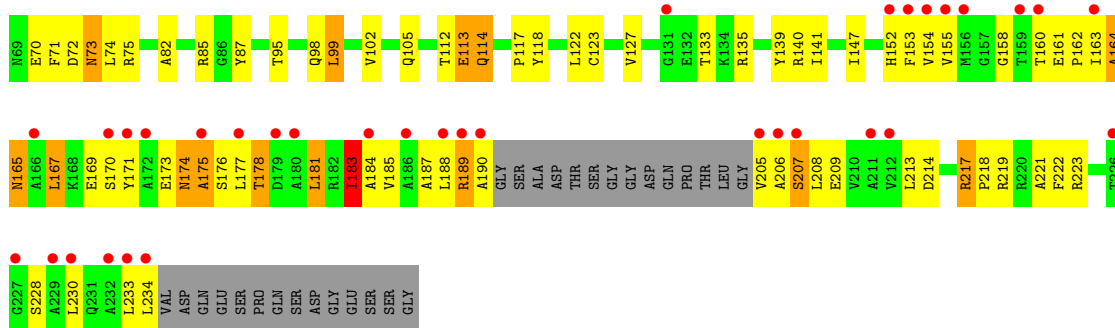


- Molecule 1: Proteasome subunit alpha

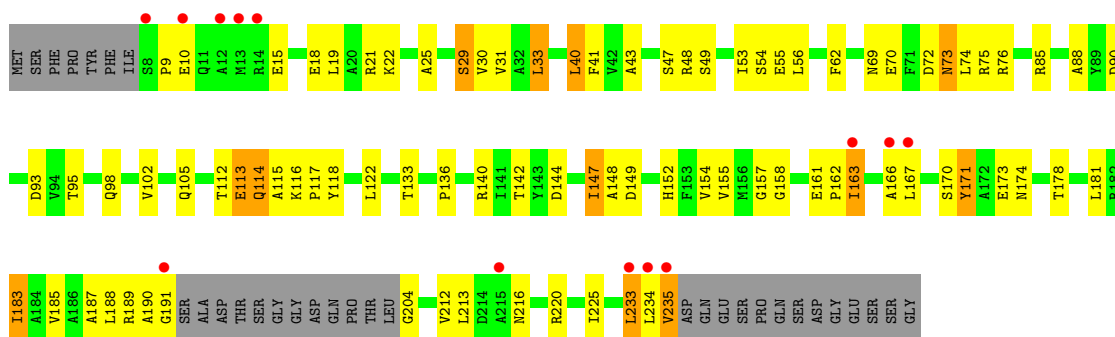


- Molecule 1: Proteasome subunit alpha

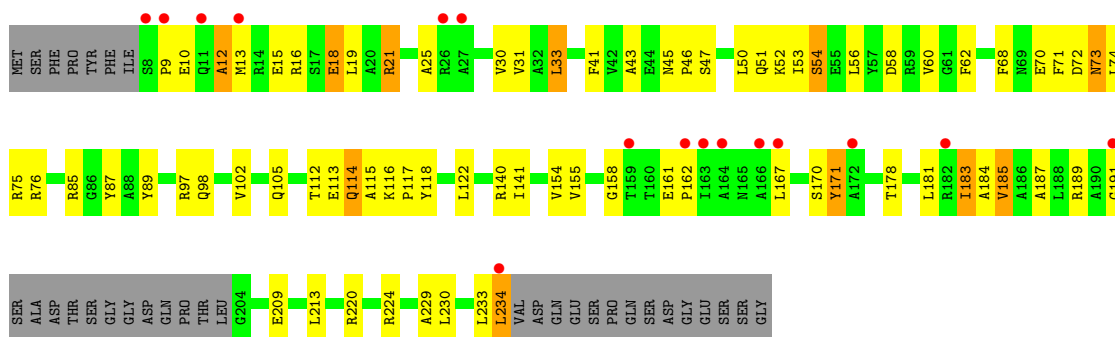




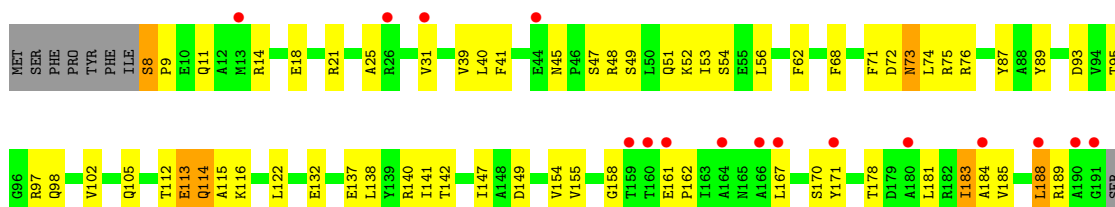
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

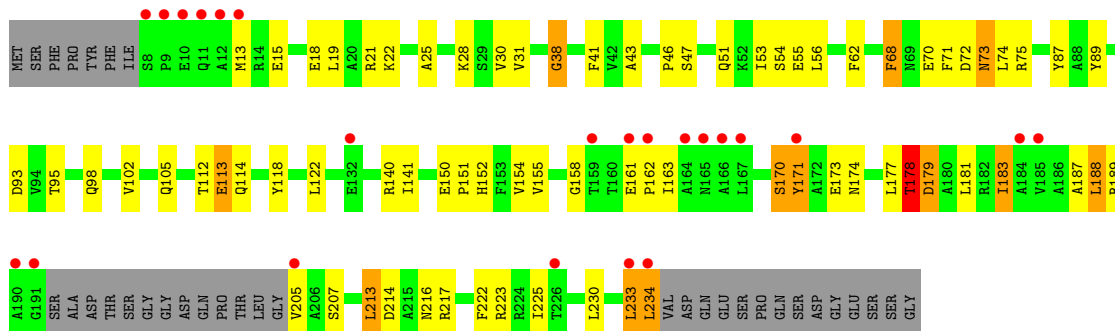


• Molecule 1: Proteasome subunit alpha

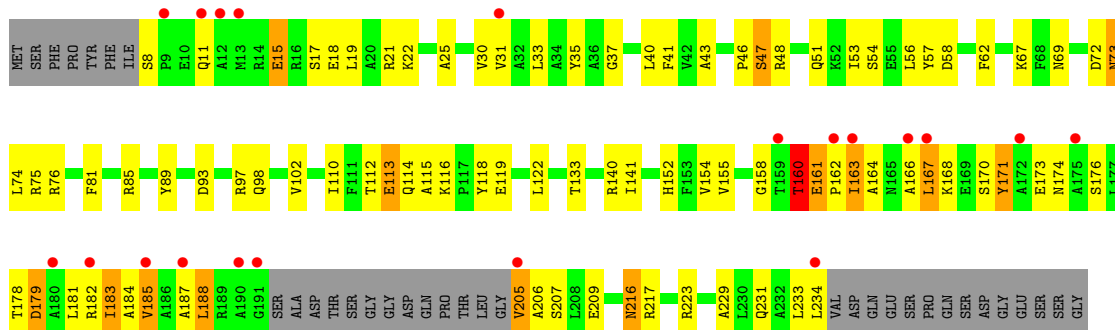




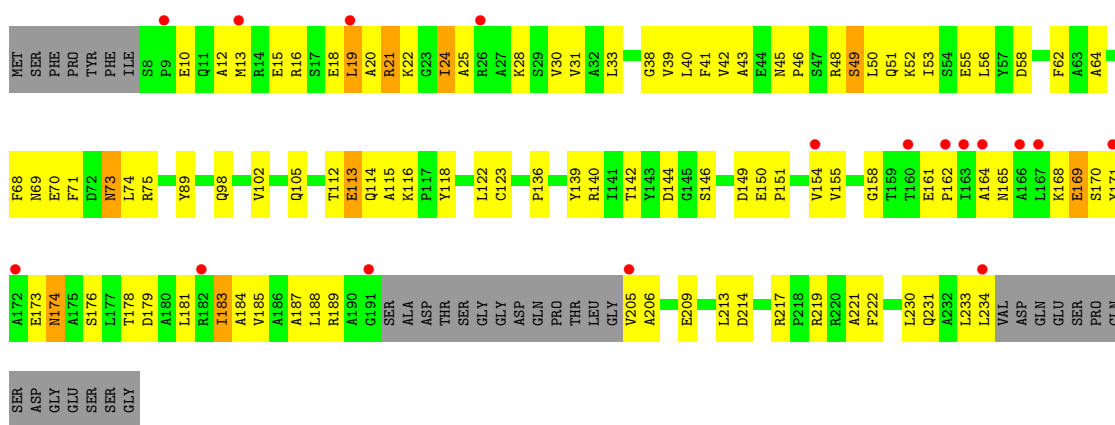
• Molecule 1: Proteasome subunit alpha



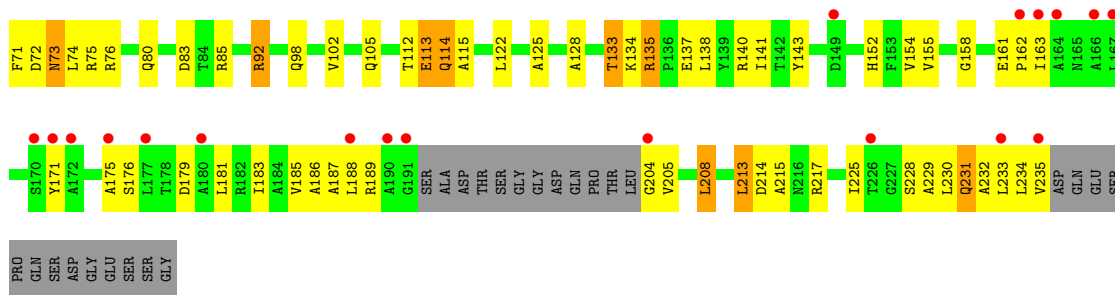
• Molecule 1: Proteasome subunit alpha



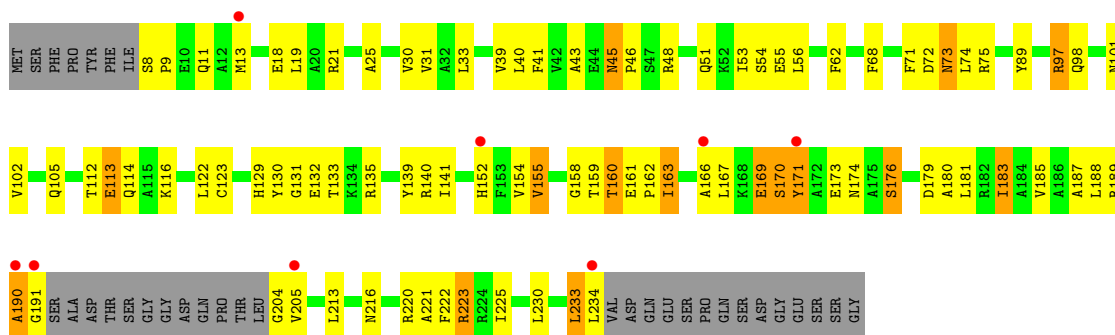
• Molecule 1: Proteasome subunit alpha



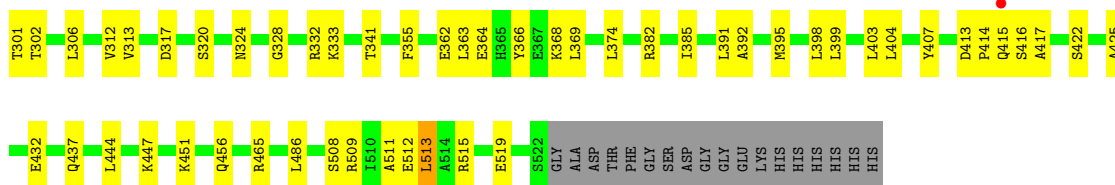
• Molecule 1: Proteasome subunit alpha



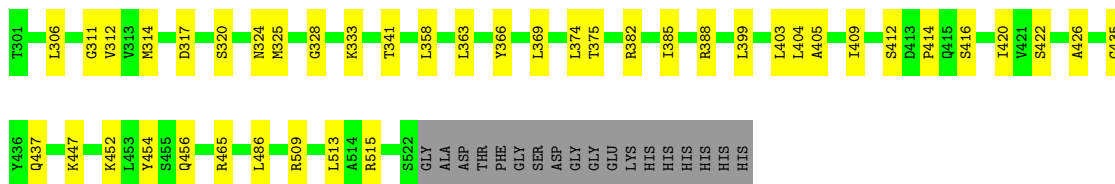
• Molecule 1: Proteasome subunit alpha



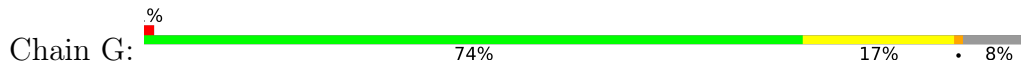
• Molecule 2: Proteasome subunit beta

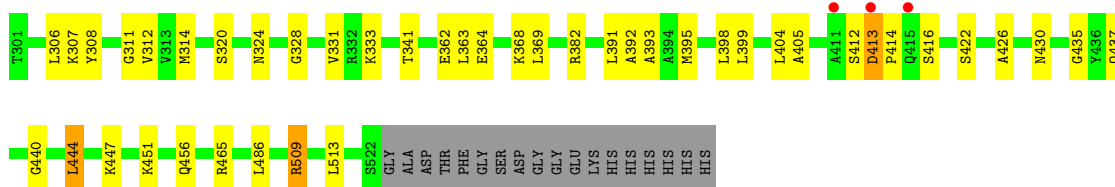


• Molecule 2: Proteasome subunit beta

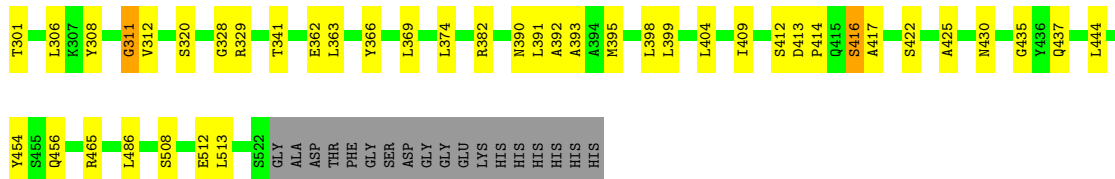


• Molecule 2: Proteasome subunit beta

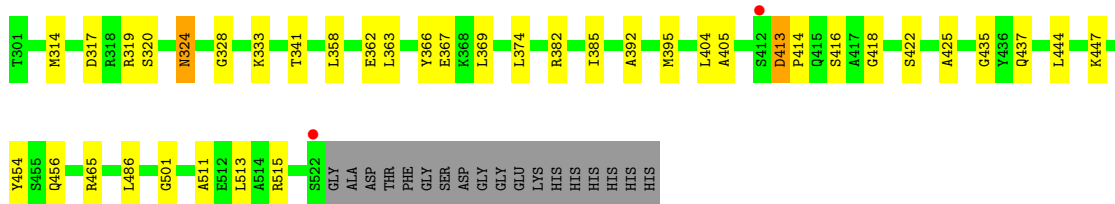
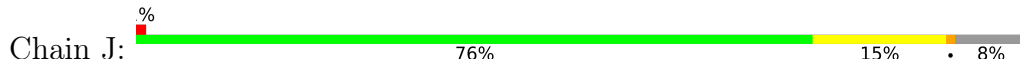




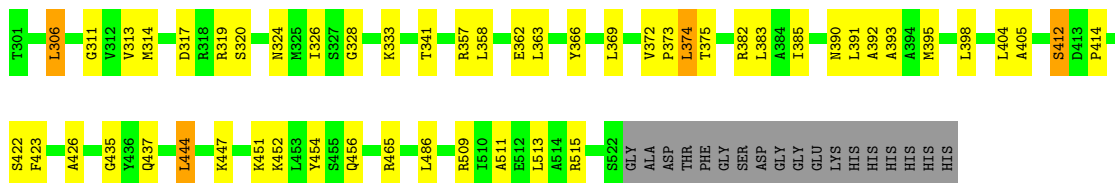
• Molecule 2: Proteasome subunit beta



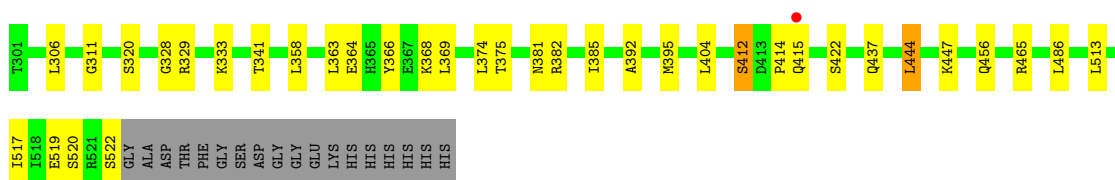
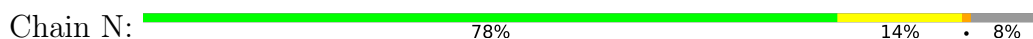
• Molecule 2: Proteasome subunit beta



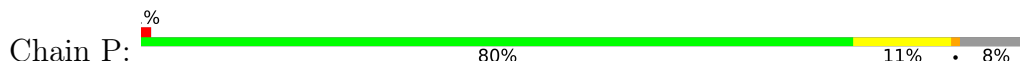
• Molecule 2: Proteasome subunit beta

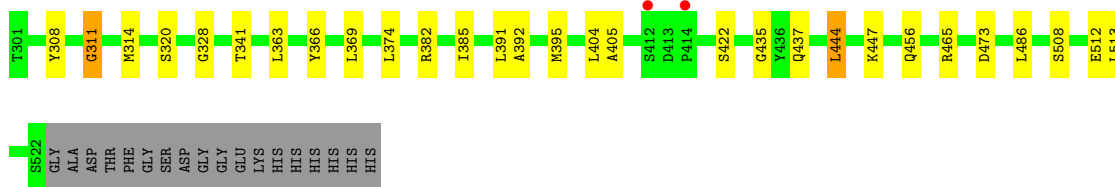


• Molecule 2: Proteasome subunit beta

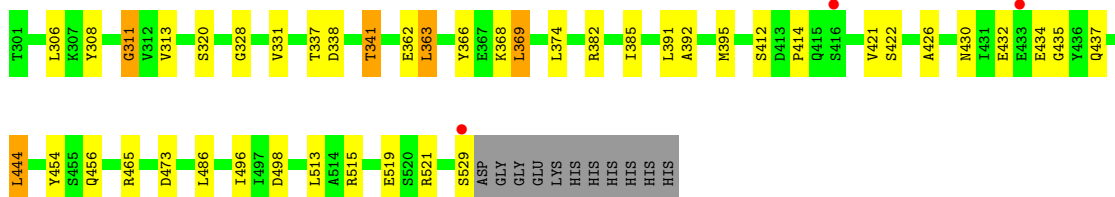
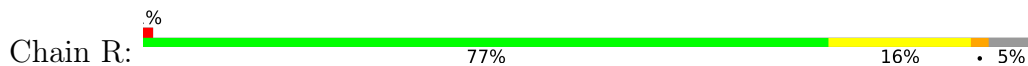


• Molecule 2: Proteasome subunit beta

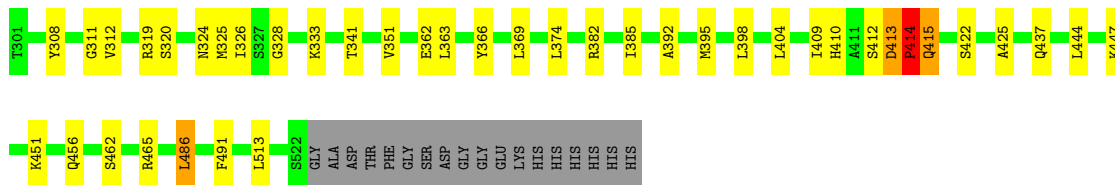




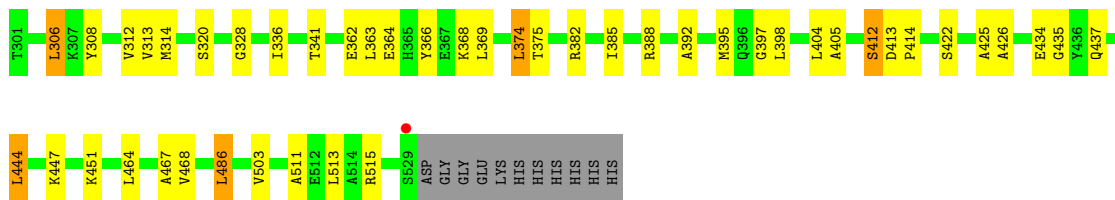
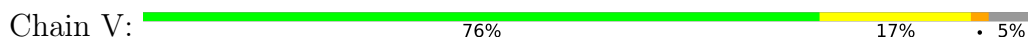
• Molecule 2: Proteasome subunit beta



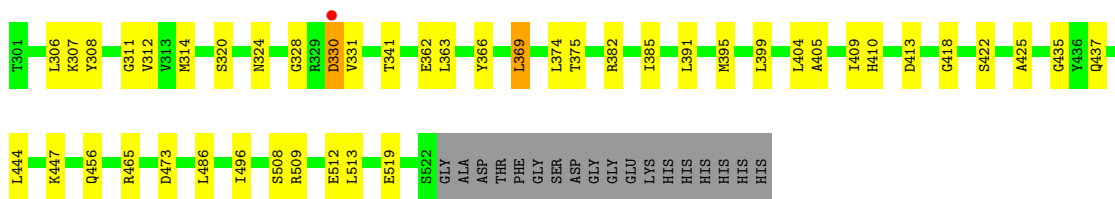
• Molecule 2: Proteasome subunit beta



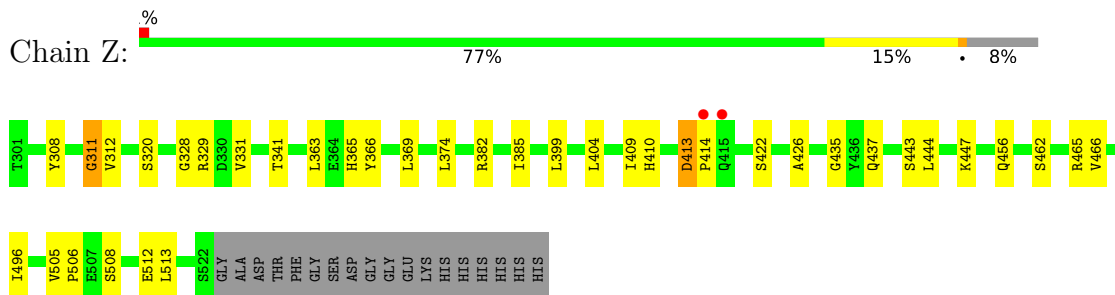
• Molecule 2: Proteasome subunit beta



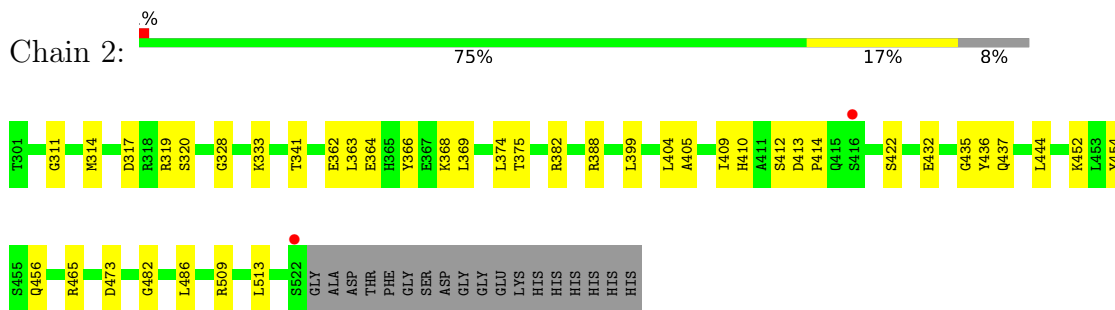
• Molecule 2: Proteasome subunit beta



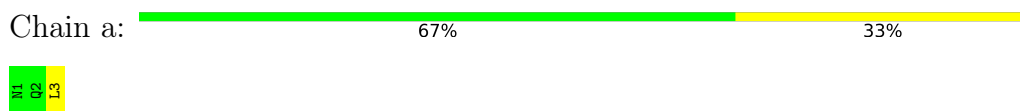
• Molecule 2: Proteasome subunit beta



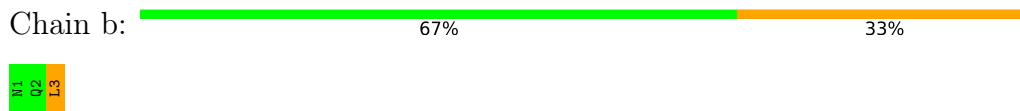
• Molecule 2: Proteasome subunit beta



• Molecule 3: Fellutamide B



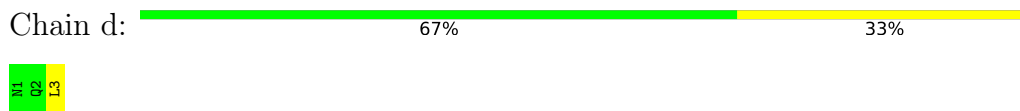
• Molecule 3: Fellutamide B



• Molecule 3: Fellutamide B



• Molecule 3: Fellutamide B



• Molecule 3: Fellutamide B



• Molecule 3: Fellutamide B

Chain f:  67% 33%



● Molecule 3: Fellutamide B

Chain g:  67% 33%



● Molecule 3: Fellutamide B

Chain h:  67% 33%



● Molecule 3: Fellutamide B

Chain i:  67% 33%



● Molecule 3: Fellutamide B

Chain j:  67% 33%



● Molecule 3: Fellutamide B

Chain k:  67% 33%



● Molecule 3: Fellutamide B

Chain l:  67% 33%



● Molecule 3: Fellutamide B

Chain m:  67% 33%



● Molecule 3: Fellutamide B

Chain n:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	170.19Å 118.10Å 194.35Å 90.00° 112.62° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (25.00-2.50) 96.5 (25.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.50Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.229 0.207 , 0.226	Depositor DCC
R_{free} test set	12081 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtrriage
Anisotropy	0.279	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	48828	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1	1.06	0/1679	1.11	11/2268 (0.5%)
1	A	0.88	2/1675 (0.1%)	1.03	8/2263 (0.4%)
1	B	0.78	0/1667	1.00	9/2252 (0.4%)
1	D	0.83	0/1671	1.17	16/2258 (0.7%)
1	F	0.95	0/1686	1.06	8/2278 (0.4%)
1	I	0.90	1/1679 (0.1%)	1.07	10/2268 (0.4%)
1	K	0.96	0/1679	1.08	8/2268 (0.4%)
1	M	0.84	1/1675 (0.1%)	1.05	9/2263 (0.4%)
1	O	0.94	0/1675	1.07	7/2263 (0.3%)
1	Q	0.89	0/1675	1.04	7/2263 (0.3%)
1	S	0.85	1/1682 (0.1%)	1.08	8/2273 (0.4%)
1	U	0.85	0/1675	1.05	12/2263 (0.5%)
1	W	0.77	0/1679	1.06	12/2268 (0.5%)
1	Y	0.92	0/1686	1.11	12/2278 (0.5%)
2	2	0.94	1/1662 (0.1%)	1.00	6/2254 (0.3%)
2	C	0.88	0/1662	1.03	5/2254 (0.2%)
2	E	0.98	0/1662	1.04	4/2254 (0.2%)
2	G	0.88	2/1662 (0.1%)	0.99	5/2254 (0.2%)
2	H	0.94	0/1662	1.01	5/2254 (0.2%)
2	J	0.96	0/1662	1.03	5/2254 (0.2%)
2	L	0.97	1/1662 (0.1%)	1.01	4/2254 (0.2%)
2	N	0.85	1/1662 (0.1%)	0.97	2/2254 (0.1%)
2	P	0.94	1/1662 (0.1%)	0.99	3/2254 (0.1%)
2	R	1.01	0/1708	1.06	4/2316 (0.2%)
2	T	1.02	1/1662 (0.1%)	1.08	7/2254 (0.3%)
2	V	1.03	4/1708 (0.2%)	1.02	4/2316 (0.2%)
2	X	0.90	1/1662 (0.1%)	1.03	6/2254 (0.3%)
2	Z	0.82	0/1662	1.02	6/2254 (0.3%)
3	a	2.63	1/24 (4.2%)	1.76	0/30
3	b	2.58	1/24 (4.2%)	1.74	0/30
3	c	2.56	1/24 (4.2%)	1.85	0/30
3	d	2.66	1/24 (4.2%)	1.77	0/30

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	e	2.59	1/24 (4.2%)	1.93	0/30
3	f	2.70	1/24 (4.2%)	1.76	0/30
3	g	2.68	1/24 (4.2%)	1.66	0/30
3	h	2.64	1/24 (4.2%)	1.93	0/30
3	i	2.42	1/24 (4.2%)	1.74	0/30
3	j	2.59	1/24 (4.2%)	2.04	0/30
3	k	2.61	1/24 (4.2%)	1.62	0/30
3	l	2.56	1/24 (4.2%)	1.69	0/30
3	m	2.56	1/24 (4.2%)	1.72	0/30
3	n	2.58	1/24 (4.2%)	1.75	0/30
All	All	0.94	31/47179 (0.1%)	1.05	203/63826 (0.3%)

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	3	LEU	C-OXT	11.04	1.45	1.23
3	b	3	LEU	C-OXT	10.74	1.45	1.23
3	d	3	LEU	C-OXT	10.66	1.44	1.23
3	m	3	LEU	C-OXT	10.61	1.44	1.23
3	f	3	LEU	C-OXT	10.61	1.44	1.23

The worst 5 of 203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	190	ALA	N-CA-C	-9.38	100.15	112.34
1	S	183	ILE	CB-CA-C	-9.23	99.67	112.14
1	D	49	SER	N-CA-C	8.99	124.48	112.88
1	Q	183	ILE	CB-CA-C	-8.85	100.20	112.14
1	1	221	ALA	N-CA-C	8.54	120.67	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1654	0	1651	95	0
1	A	1650	0	1648	74	0
1	B	1642	0	1637	63	0
1	D	1646	0	1645	148	0
1	F	1661	0	1660	70	0
1	I	1654	0	1651	62	0
1	K	1654	0	1651	86	0
1	M	1650	0	1648	72	0
1	O	1650	0	1648	97	0
1	Q	1650	0	1648	90	0
1	S	1657	0	1657	100	0
1	U	1650	0	1648	64	0
1	W	1654	0	1651	90	0
1	Y	1661	0	1660	123	0
2	2	1638	0	1629	28	0
2	C	1638	0	1629	41	0
2	E	1638	0	1629	32	0
2	G	1638	0	1629	35	0
2	H	1638	0	1629	25	0
2	J	1638	0	1629	33	0
2	L	1638	0	1629	54	0
2	N	1638	0	1629	23	0
2	P	1638	0	1629	20	0
2	R	1683	0	1665	39	0
2	T	1638	0	1629	37	0
2	V	1683	0	1665	31	0
2	X	1638	0	1629	30	0
2	Z	1638	0	1629	23	0
3	a	25	0	24	0	0
3	b	25	0	24	1	0
3	c	25	0	24	3	0
3	d	25	0	24	0	0
3	e	25	0	24	0	0
3	f	25	0	24	1	0
3	g	25	0	24	1	0
3	h	25	0	24	0	0
3	i	25	0	24	1	0
3	j	25	0	24	1	0
3	k	25	0	24	0	0
3	l	25	0	24	1	0
3	m	25	0	24	1	0
3	n	25	0	24	1	0
4	a	7	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	b	7	0	6	1	0
4	c	7	0	6	0	0
4	d	7	0	6	0	0
4	e	7	0	6	1	0
4	f	7	0	6	0	0
4	g	7	0	6	1	0
4	h	7	0	6	2	0
4	i	7	0	6	2	0
4	j	7	0	6	1	0
4	k	7	0	6	0	0
4	l	7	0	6	1	0
4	m	7	0	6	1	0
4	n	7	0	6	1	0
5	1	55	0	0	2	0
5	2	118	0	0	6	0
5	A	32	0	0	3	0
5	B	42	0	0	3	0
5	C	131	0	0	10	0
5	D	25	0	0	3	0
5	E	130	0	0	7	0
5	F	41	0	0	6	0
5	G	113	0	0	8	0
5	H	126	0	0	6	0
5	I	38	0	0	6	0
5	J	122	0	0	3	0
5	K	33	0	0	6	0
5	L	132	0	0	9	0
5	M	42	0	0	0	0
5	N	121	0	0	3	0
5	O	39	0	0	6	0
5	P	111	0	0	2	0
5	Q	34	0	0	0	0
5	R	143	0	0	9	0
5	S	43	0	0	19	0
5	T	103	0	0	5	0
5	U	33	0	0	2	0
5	V	149	0	0	5	0
5	W	26	0	0	3	0
5	X	115	0	0	4	0
5	Y	22	0	0	3	0
5	Z	106	0	0	1	0
All	All	48828	0	46401	1557	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 1557 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:ARG:HB2	1:D:217:ARG:NH1	1.41	1.30
1:A:13:MET:CE	1:O:116:LYS:HD3	1.62	1.27
1:M:217:ARG:HD3	1:M:223:ARG:NH2	1.53	1.24
1:B:170:SER:OG	1:B:183:ILE:HG23	1.39	1.23
1:Y:229:ALA:O	1:Y:233:LEU:HD13	1.41	1.20

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	1	211/248 (85%)	199 (94%)	11 (5%)	1 (0%)	24	43
1	A	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
1	B	209/248 (84%)	203 (97%)	6 (3%)	0	100	100
1	D	209/248 (84%)	203 (97%)	6 (3%)	0	100	100
1	F	212/248 (86%)	208 (98%)	4 (2%)	0	100	100
1	I	211/248 (85%)	208 (99%)	3 (1%)	0	100	100
1	K	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	M	210/248 (85%)	204 (97%)	6 (3%)	0	100	100
1	O	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
1	Q	210/248 (85%)	202 (96%)	8 (4%)	0	100	100
1	S	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	U	210/248 (85%)	206 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
1	Y	212/248 (86%)	206 (97%)	6 (3%)	0	100	100
2	2	220/240 (92%)	220 (100%)	0	0	100	100
2	C	220/240 (92%)	220 (100%)	0	0	100	100
2	E	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	G	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	H	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	J	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	L	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	N	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	P	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	R	227/240 (95%)	224 (99%)	3 (1%)	0	100	100
2	T	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	V	227/240 (95%)	226 (100%)	1 (0%)	0	100	100
2	X	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	Z	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
3	a	1/3 (33%)	1 (100%)	0	0	100	100
3	b	1/3 (33%)	1 (100%)	0	0	100	100
3	c	1/3 (33%)	1 (100%)	0	0	100	100
3	d	1/3 (33%)	1 (100%)	0	0	100	100
3	e	1/3 (33%)	1 (100%)	0	0	100	100
3	f	1/3 (33%)	1 (100%)	0	0	100	100
3	g	1/3 (33%)	1 (100%)	0	0	100	100
3	h	1/3 (33%)	1 (100%)	0	0	100	100
3	i	1/3 (33%)	1 (100%)	0	0	100	100
3	j	1/3 (33%)	1 (100%)	0	0	100	100
3	k	1/3 (33%)	1 (100%)	0	0	100	100
3	l	1/3 (33%)	1 (100%)	0	0	100	100
3	m	1/3 (33%)	1 (100%)	0	0	100	100
3	n	1/3 (33%)	1 (100%)	0	0	100	100
All	All	6055/6874 (88%)	5942 (98%)	112 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	131	GLY

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	1	164/192 (85%)	151 (92%)	13 (8%)	11	24
1	A	164/192 (85%)	158 (96%)	6 (4%)	30	57
1	B	163/192 (85%)	158 (97%)	5 (3%)	35	62
1	D	164/192 (85%)	146 (89%)	18 (11%)	6	13
1	F	165/192 (86%)	151 (92%)	14 (8%)	10	22
1	I	164/192 (85%)	157 (96%)	7 (4%)	26	51
1	K	164/192 (85%)	155 (94%)	9 (6%)	19	40
1	M	164/192 (85%)	153 (93%)	11 (7%)	15	31
1	O	164/192 (85%)	150 (92%)	14 (8%)	10	22
1	Q	164/192 (85%)	151 (92%)	13 (8%)	11	24
1	S	165/192 (86%)	156 (94%)	9 (6%)	19	40
1	U	164/192 (85%)	158 (96%)	6 (4%)	30	57
1	W	164/192 (85%)	158 (96%)	6 (4%)	30	57
1	Y	165/192 (86%)	156 (94%)	9 (6%)	19	40
2	2	165/178 (93%)	160 (97%)	5 (3%)	36	64
2	C	165/178 (93%)	160 (97%)	5 (3%)	36	64
2	E	165/178 (93%)	159 (96%)	6 (4%)	31	58
2	G	165/178 (93%)	159 (96%)	6 (4%)	31	58
2	H	165/178 (93%)	157 (95%)	8 (5%)	23	46
2	J	165/178 (93%)	160 (97%)	5 (3%)	36	64
2	L	165/178 (93%)	157 (95%)	8 (5%)	23	46
2	N	165/178 (93%)	158 (96%)	7 (4%)	26	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	165/178 (93%)	160 (97%)	5 (3%)	36	64
2	R	169/178 (95%)	160 (95%)	9 (5%)	20	42
2	T	165/178 (93%)	157 (95%)	8 (5%)	23	46
2	V	169/178 (95%)	160 (95%)	9 (5%)	20	42
2	X	165/178 (93%)	157 (95%)	8 (5%)	23	46
2	Z	165/178 (93%)	159 (96%)	6 (4%)	31	58
3	a	3/3 (100%)	3 (100%)	0	100	100
3	b	3/3 (100%)	3 (100%)	0	100	100
3	c	3/3 (100%)	3 (100%)	0	100	100
3	d	3/3 (100%)	3 (100%)	0	100	100
3	e	3/3 (100%)	3 (100%)	0	100	100
3	f	3/3 (100%)	3 (100%)	0	100	100
3	g	3/3 (100%)	3 (100%)	0	100	100
3	h	3/3 (100%)	3 (100%)	0	100	100
3	i	3/3 (100%)	3 (100%)	0	100	100
3	j	3/3 (100%)	3 (100%)	0	100	100
3	k	3/3 (100%)	3 (100%)	0	100	100
3	l	3/3 (100%)	3 (100%)	0	100	100
3	m	3/3 (100%)	3 (100%)	0	100	100
3	n	3/3 (100%)	3 (100%)	0	100	100
All	All	4658/5222 (89%)	4423 (95%)	235 (5%)	22	44

5 of 235 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	15	GLU
1	1	160	THR
1	Q	169	GLU
1	1	155	VAL
2	X	496	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	69	ASN
1	Y	165	ASN
1	1	152	HIS
1	K	73	ASN
1	K	69	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](#)

14 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	$\# Z > 2$
4	HXD	c	4	3	5,6,14	1.21	1 (20%)	5,6,15	1.29	0
4	HXD	b	4	3	5,6,14	1.18	0	5,6,15	1.15	0
4	HXD	m	4	3	5,6,14	1.14	0	5,6,15	1.17	1 (20%)
4	HXD	n	4	3	5,6,14	1.13	0	5,6,15	1.34	1 (20%)
4	HXD	j	4	3	5,6,14	1.16	1 (20%)	5,6,15	1.29	0
4	HXD	e	4	3	5,6,14	1.10	0	5,6,15	1.29	1 (20%)
4	HXD	f	4	3	5,6,14	1.05	0	5,6,15	1.37	0
4	HXD	k	4	3	5,6,14	1.04	0	5,6,15	1.21	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HXD	a	4	3	5,6,14	1.01	0	5,6,15	1.32	1 (20%)
4	HXD	g	4	3	5,6,14	1.11	0	5,6,15	1.43	1 (20%)
4	HXD	l	4	3	5,6,14	1.33	1 (20%)	5,6,15	1.42	1 (20%)
4	HXD	h	4	3	5,6,14	1.41	1 (20%)	5,6,15	1.46	1 (20%)
4	HXD	i	4	3	5,6,14	1.28	1 (20%)	5,6,15	1.05	0
4	HXD	d	4	3	5,6,14	1.51	1 (20%)	5,6,15	1.39	1 (20%)

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
4	HXD	c	4	3	-	0/5/5/13	-
4	HXD	b	4	3	-	0/5/5/13	-
4	HXD	m	4	3	-	0/5/5/13	-
4	HXD	n	4	3	-	0/5/5/13	-
4	HXD	j	4	3	-	0/5/5/13	-
4	HXD	e	4	3	-	0/5/5/13	-
4	HXD	f	4	3	-	0/5/5/13	-
4	HXD	k	4	3	-	0/5/5/13	-
4	HXD	a	4	3	-	0/5/5/13	-
4	HXD	g	4	3	-	0/5/5/13	-
4	HXD	l	4	3	-	0/5/5/13	-
4	HXD	h	4	3	-	0/5/5/13	-
4	HXD	i	4	3	-	0/5/5/13	-
4	HXD	d	4	3	-	0/5/5/13	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	4	HXD	C2-C1	2.85	1.57	1.50
4	h	4	HXD	C2-C1	2.42	1.56	1.50
4	l	4	HXD	C2-C1	2.17	1.55	1.50
4	c	4	HXD	C2-C1	2.08	1.55	1.50
4	i	4	HXD	C2-C1	2.07	1.55	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	g	4	HXD	O8-C3-C2	-2.49	102.81	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	4	HXD	C3-C2-C1	2.46	116.90	112.70
4	d	4	HXD	C3-C2-C1	2.40	116.79	112.70
4	h	4	HXD	C3-C2-C1	2.40	116.79	112.70
4	l	4	HXD	C3-C2-C1	2.38	116.75	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	b	4	HXD	1	0
4	m	4	HXD	1	0
4	n	4	HXD	1	0
4	j	4	HXD	1	0
4	e	4	HXD	1	0
4	a	4	HXD	2	0
4	g	4	HXD	1	0
4	l	4	HXD	1	0
4	h	4	HXD	2	0
4	i	4	HXD	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	215/248 (86%)	0.55	8 (3%) 45 40	23, 51, 86, 94	0
1	A	214/248 (86%)	0.69	12 (5%) 30 26	24, 53, 88, 100	0
1	B	213/248 (85%)	0.76	22 (10%) 12 10	24, 52, 87, 94	0
1	D	213/248 (85%)	1.13	48 (22%) 2 2	25, 55, 93, 112	0
1	F	216/248 (87%)	0.71	13 (6%) 27 24	23, 53, 86, 93	0
1	I	215/248 (86%)	0.77	16 (7%) 20 18	24, 52, 87, 95	0
1	K	215/248 (86%)	0.71	18 (8%) 17 15	24, 53, 87, 95	0
1	M	214/248 (86%)	0.78	23 (10%) 11 9	23, 54, 88, 96	0
1	O	214/248 (86%)	0.70	20 (9%) 14 12	22, 53, 88, 95	0
1	Q	214/248 (86%)	0.75	17 (7%) 18 16	26, 52, 87, 95	0
1	S	215/248 (86%)	0.75	19 (8%) 15 14	24, 53, 89, 99	0
1	U	214/248 (86%)	0.76	20 (9%) 14 12	23, 53, 87, 95	0
1	W	215/248 (86%)	0.86	18 (8%) 17 15	24, 54, 93, 98	0
1	Y	216/248 (87%)	0.89	28 (12%) 7 6	26, 55, 90, 98	0
2	2	222/240 (92%)	-0.41	2 (0%) 81 78	12, 23, 41, 66	0
2	C	222/240 (92%)	-0.45	1 (0%) 87 85	12, 24, 41, 68	0
2	E	222/240 (92%)	-0.43	0 100 100	13, 24, 41, 65	0
2	G	222/240 (92%)	-0.39	3 (1%) 73 70	14, 24, 43, 68	0
2	H	222/240 (92%)	-0.43	0 100 100	11, 24, 42, 66	0
2	J	222/240 (92%)	-0.41	2 (0%) 81 78	12, 24, 43, 65	0
2	L	222/240 (92%)	-0.38	0 100 100	13, 24, 42, 65	0
2	N	222/240 (92%)	-0.45	1 (0%) 87 85	13, 24, 43, 67	0
2	P	222/240 (92%)	-0.41	2 (0%) 81 78	14, 24, 42, 67	0
2	R	229/240 (95%)	-0.45	3 (1%) 75 71	13, 24, 46, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	222/240 (92%)	-0.36	0 100 100	15, 25, 43, 67	0
2	V	229/240 (95%)	-0.44	1 (0%) 88 86	12, 23, 44, 67	0
2	X	222/240 (92%)	-0.40	1 (0%) 87 85	13, 25, 43, 67	0
2	Z	222/240 (92%)	-0.34	2 (0%) 81 78	13, 25, 43, 67	0
3	a	3/3 (100%)	-0.52	0 100 100	24, 24, 24, 26	0
3	b	3/3 (100%)	-0.41	0 100 100	20, 20, 22, 23	0
3	c	3/3 (100%)	-0.31	0 100 100	23, 23, 24, 28	0
3	d	3/3 (100%)	-0.67	0 100 100	22, 22, 25, 27	0
3	e	3/3 (100%)	-0.50	0 100 100	21, 21, 23, 24	0
3	f	3/3 (100%)	-0.13	0 100 100	21, 21, 24, 28	0
3	g	3/3 (100%)	-0.37	0 100 100	21, 21, 22, 28	0
3	h	3/3 (100%)	-0.47	0 100 100	23, 23, 28, 28	0
3	i	3/3 (100%)	-0.35	0 100 100	25, 25, 26, 27	0
3	j	3/3 (100%)	-0.41	0 100 100	26, 26, 27, 30	0
3	k	3/3 (100%)	-0.62	0 100 100	22, 22, 25, 28	0
3	l	3/3 (100%)	-0.20	0 100 100	23, 23, 27, 27	0
3	m	3/3 (100%)	-0.36	0 100 100	30, 30, 30, 31	0
3	n	3/3 (100%)	-0.45	0 100 100	25, 25, 27, 28	0
All	All	6167/6874 (89%)	0.16	300 (4%) 35 31	11, 35, 84, 112	0

The worst 5 of 300 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	172	ALA	4.9
1	D	233	LEU	4.6
1	B	205	VAL	4.6
1	Y	9	PRO	4.1
1	Y	235	VAL	4.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	HXD	d	4	7/15	0.80	0.14	23,30,34,38	0
4	HXD	m	4	7/15	0.80	0.15	28,33,37,37	0
4	HXD	j	4	7/15	0.82	0.14	25,30,33,37	0
4	HXD	e	4	7/15	0.84	0.14	18,28,37,38	0
4	HXD	i	4	7/15	0.84	0.14	25,31,38,40	0
4	HXD	k	4	7/15	0.85	0.12	30,33,36,37	0
4	HXD	g	4	7/15	0.85	0.12	28,29,32,33	0
4	HXD	c	4	7/15	0.86	0.13	29,29,33,34	0
4	HXD	h	4	7/15	0.86	0.13	32,34,37,37	0
4	HXD	l	4	7/15	0.86	0.14	26,28,30,32	0
4	HXD	f	4	7/15	0.86	0.12	23,29,32,35	0
4	HXD	n	4	7/15	0.86	0.12	24,28,29,30	0
4	HXD	b	4	7/15	0.88	0.14	22,28,36,37	0
4	HXD	a	4	7/15	0.91	0.10	23,26,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.