



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:05 PM UTC

PDB ID : 3H4P / pdb_00003h4p
Title : Proteasome 20S core particle from Methanocaldococcus jannaschii
Authors : Jeffrey, P.D.; Zhang, F.; Hu, M.; Tian, G.; Zhang, P.; Finley, D.; Shi, Y.
Deposited on : 2009-04-20
Resolution : 4.10 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
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

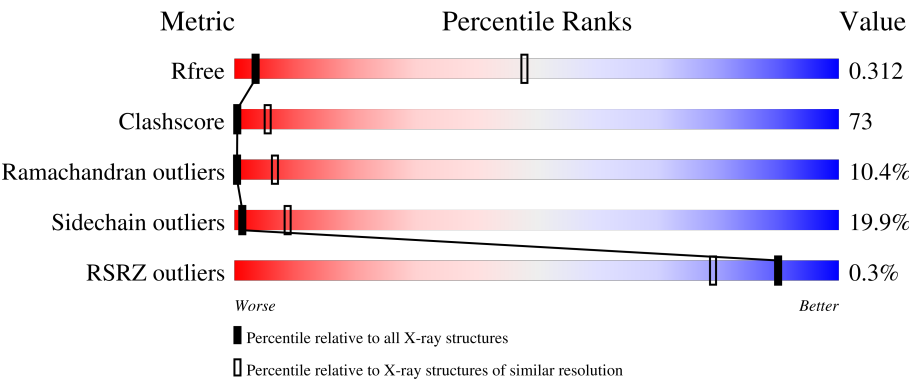
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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.



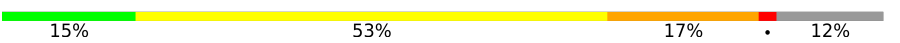
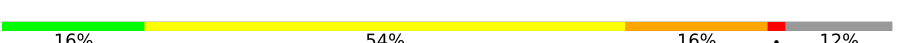
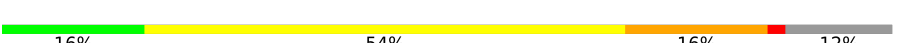
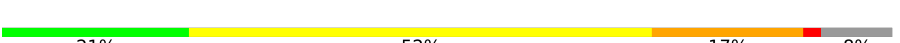
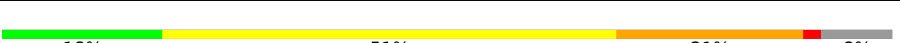
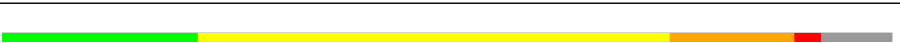
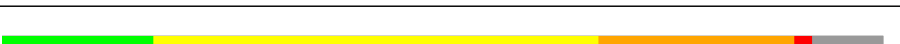
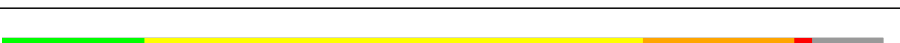
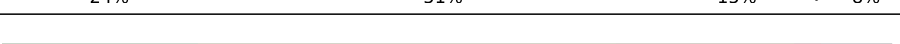
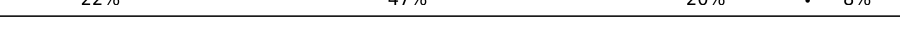
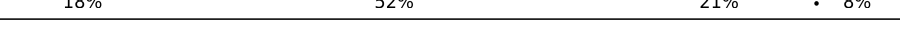
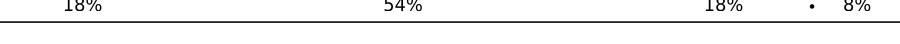
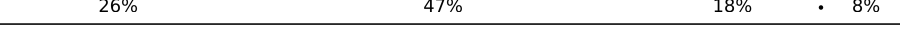
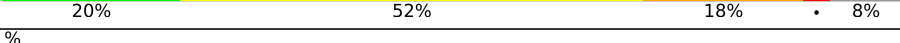
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	17%51%19%•12%
1	B	264	17%52%17%•12%
1	C	264	16%54%16%•12%
1	D	264	13%54%19%•12%
1	E	264	12%57%17%•12%

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Mol	Chain	Length	Quality of chain
1	F	264	
1	G	264	
1	H	264	
1	I	264	
1	J	264	
1	K	264	
1	L	264	
1	M	264	
1	N	264	
2	a	219	
2	b	219	
2	c	219	
2	d	219	
2	e	219	
2	f	219	
2	g	219	
2	h	219	
2	i	219	
2	j	219	
2	k	219	
2	l	219	
2	m	219	
2	n	219	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 46648 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
1	A	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	B	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	C	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	D	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	E	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	F	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	G	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	H	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	I	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	J	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	K	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	L	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	M	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	N	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q60177

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q60177
A	0	HIS	-	expression tag	UNP Q60177
B	-2	GLY	-	expression tag	UNP Q60177
B	-1	SER	-	expression tag	UNP Q60177
B	0	HIS	-	expression tag	UNP Q60177
C	-2	GLY	-	expression tag	UNP Q60177
C	-1	SER	-	expression tag	UNP Q60177
C	0	HIS	-	expression tag	UNP Q60177
D	-2	GLY	-	expression tag	UNP Q60177
D	-1	SER	-	expression tag	UNP Q60177
D	0	HIS	-	expression tag	UNP Q60177
E	-2	GLY	-	expression tag	UNP Q60177
E	-1	SER	-	expression tag	UNP Q60177
E	0	HIS	-	expression tag	UNP Q60177
F	-2	GLY	-	expression tag	UNP Q60177
F	-1	SER	-	expression tag	UNP Q60177
F	0	HIS	-	expression tag	UNP Q60177
G	-2	GLY	-	expression tag	UNP Q60177
G	-1	SER	-	expression tag	UNP Q60177
G	0	HIS	-	expression tag	UNP Q60177
H	-2	GLY	-	expression tag	UNP Q60177
H	-1	SER	-	expression tag	UNP Q60177
H	0	HIS	-	expression tag	UNP Q60177
I	-2	GLY	-	expression tag	UNP Q60177
I	-1	SER	-	expression tag	UNP Q60177
I	0	HIS	-	expression tag	UNP Q60177
J	-2	GLY	-	expression tag	UNP Q60177
J	-1	SER	-	expression tag	UNP Q60177
J	0	HIS	-	expression tag	UNP Q60177
K	-2	GLY	-	expression tag	UNP Q60177
K	-1	SER	-	expression tag	UNP Q60177
K	0	HIS	-	expression tag	UNP Q60177
L	-2	GLY	-	expression tag	UNP Q60177
L	-1	SER	-	expression tag	UNP Q60177
L	0	HIS	-	expression tag	UNP Q60177
M	-2	GLY	-	expression tag	UNP Q60177
M	-1	SER	-	expression tag	UNP Q60177
M	0	HIS	-	expression tag	UNP Q60177
N	-2	GLY	-	expression tag	UNP Q60177
N	-1	SER	-	expression tag	UNP Q60177
N	0	HIS	-	expression tag	UNP Q60177

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	b	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	c	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	d	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	e	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	f	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	g	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	h	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	i	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	j	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	k	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	l	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	m	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	n	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	6	MET	-	expression tag	UNP Q58634
b	6	MET	-	expression tag	UNP Q58634
c	6	MET	-	expression tag	UNP Q58634
d	6	MET	-	expression tag	UNP Q58634
e	6	MET	-	expression tag	UNP Q58634
f	6	MET	-	expression tag	UNP Q58634
g	6	MET	-	expression tag	UNP Q58634
h	6	MET	-	expression tag	UNP Q58634
i	6	MET	-	expression tag	UNP Q58634
j	6	MET	-	expression tag	UNP Q58634
k	6	MET	-	expression tag	UNP Q58634
l	6	MET	-	expression tag	UNP Q58634

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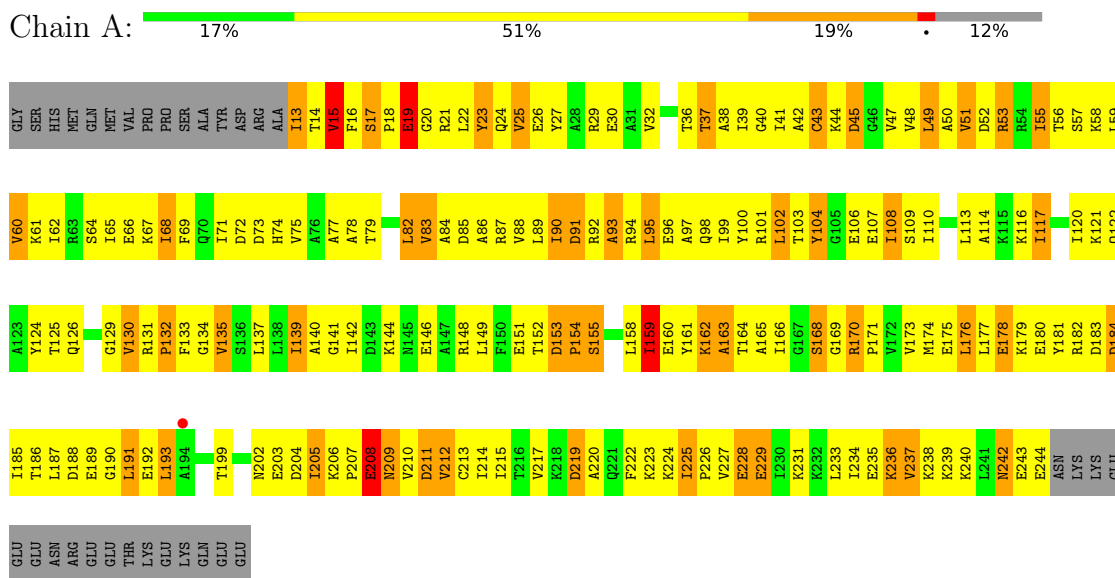
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Chain	Residue	Modelled	Actual	Comment	Reference
m	6	MET	-	expression tag	UNP Q58634
n	6	MET	-	expression tag	UNP Q58634

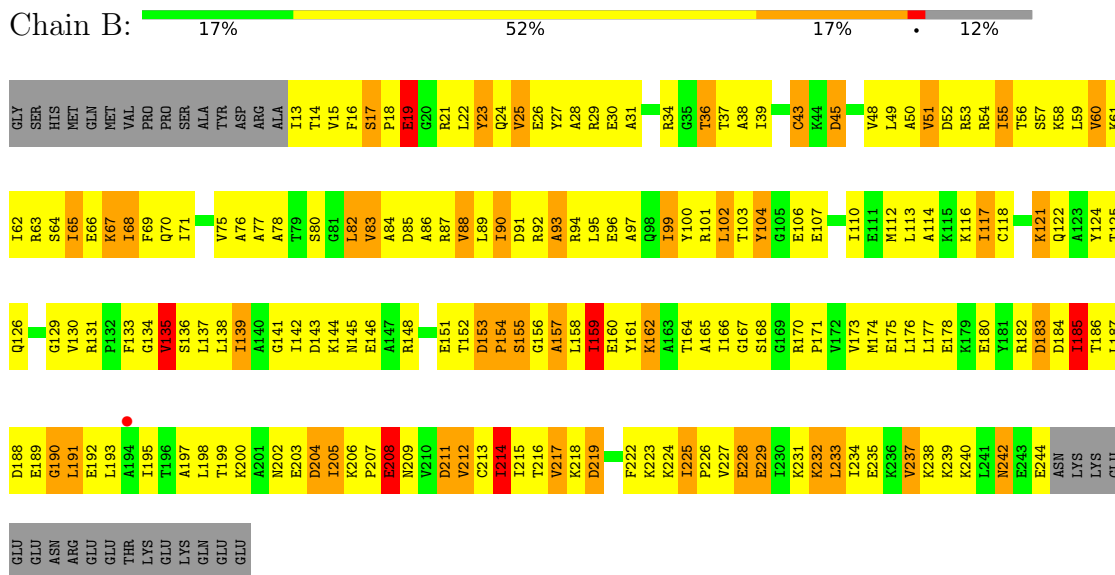
3 Residue-property plots

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.

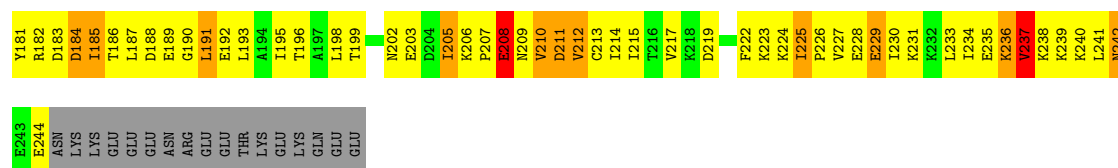
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

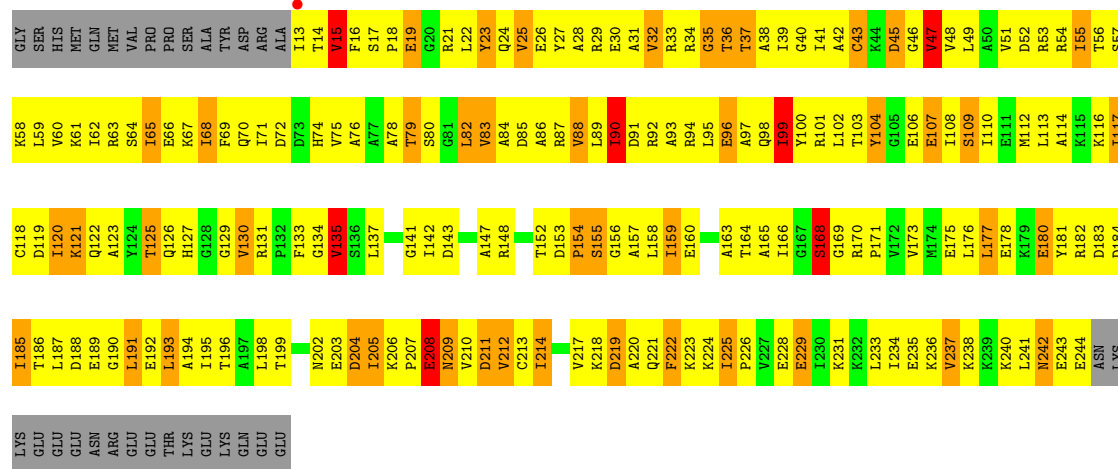


[illegible][illegible][illegible]



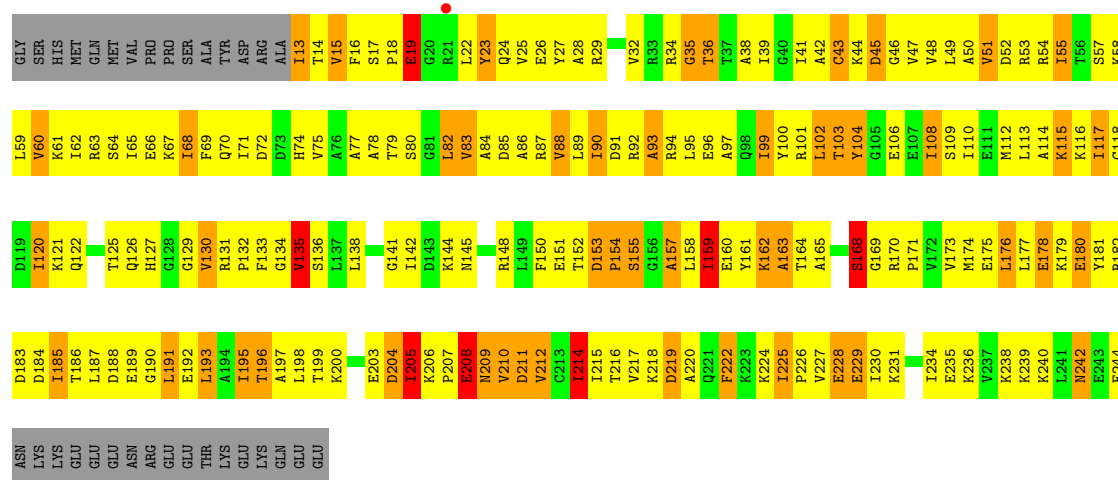
• Molecule 1: Proteasome subunit alpha

Chain F: 14% 54% 17% 12%



• Molecule 1: Proteasome subunit alpha

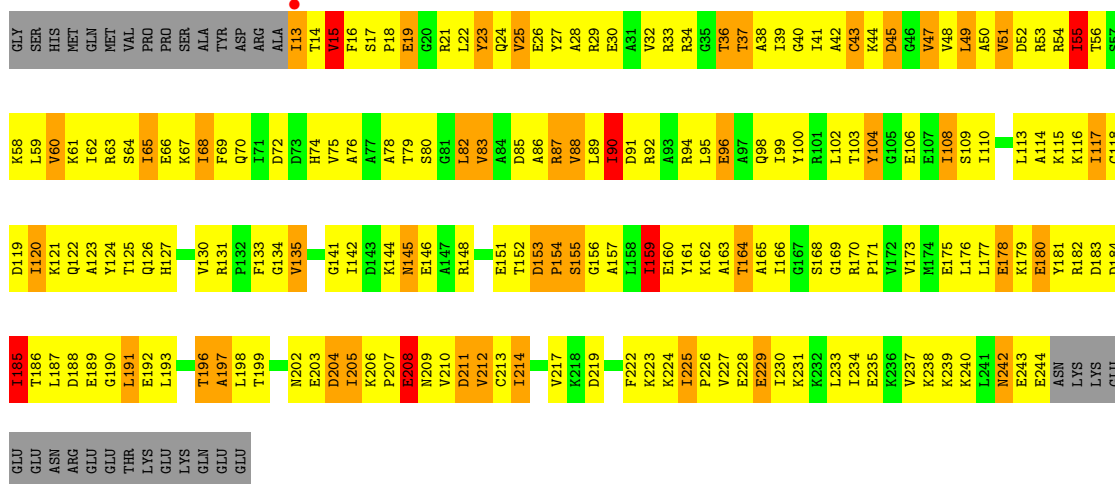
Chain G: 16% 51% 19% 12%



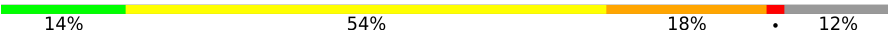
• Molecule 1: Proteasome subunit alpha

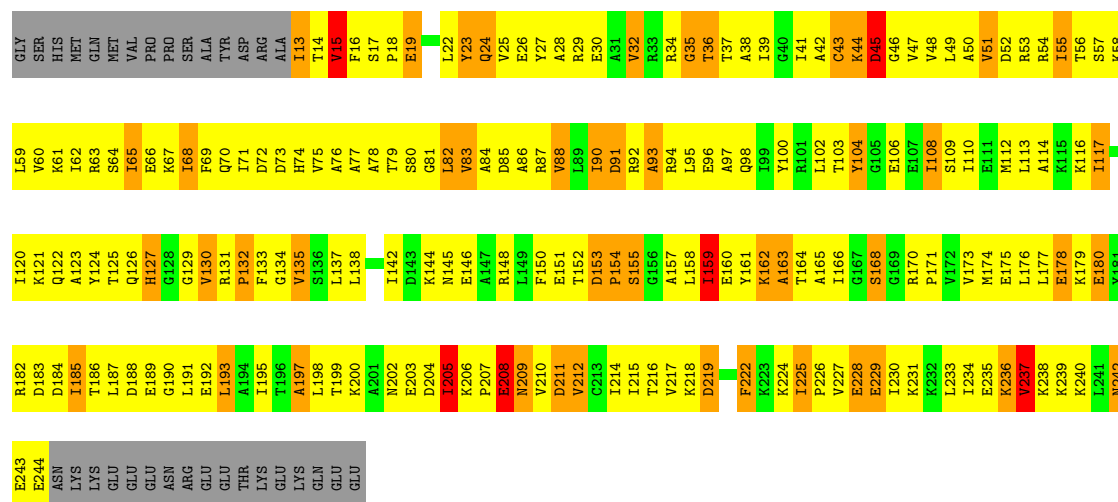
Chain H: 13% 54% 19% 12%

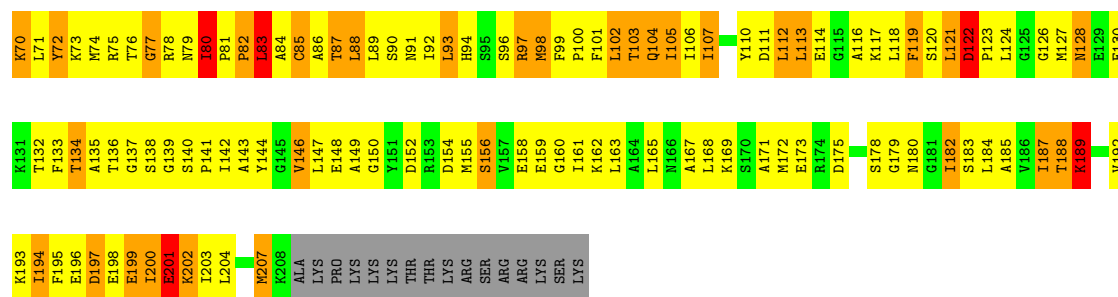




• Molecule 1: Proteasome subunit alpha

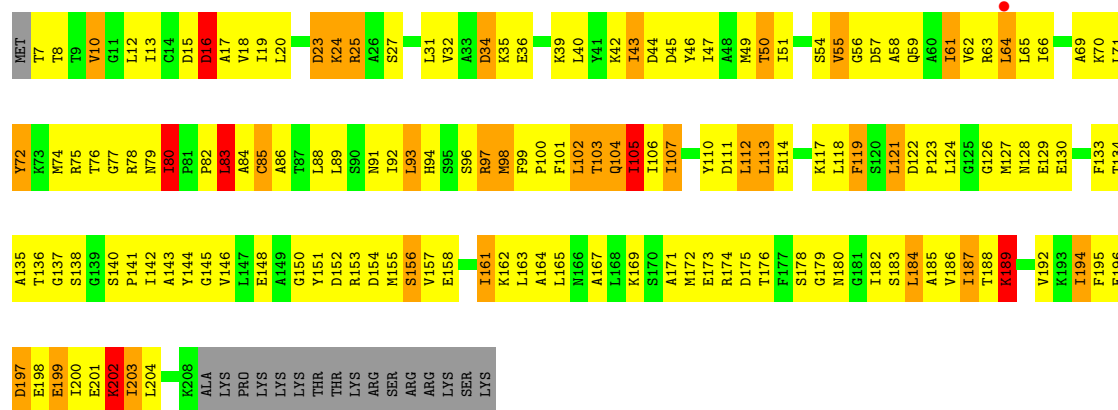
Chain K: 





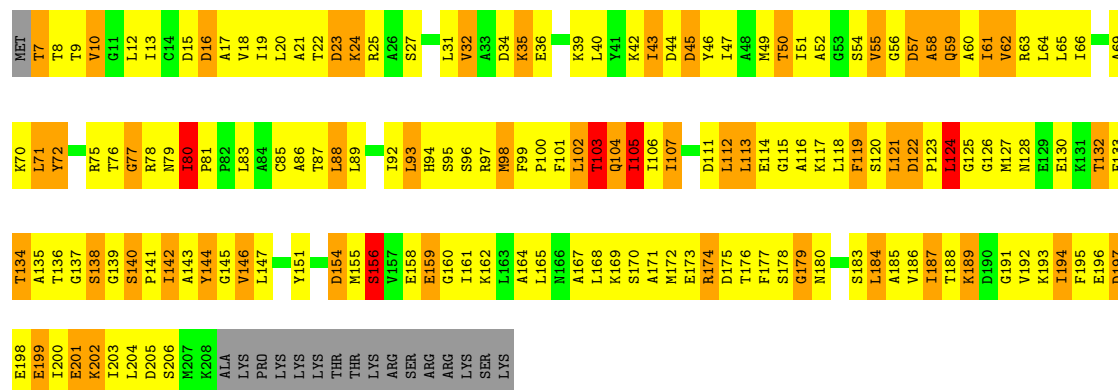
• Molecule 2: Proteasome subunit beta

Chain c: 22% 53% 14% 8%



• Molecule 2: Proteasome subunit beta

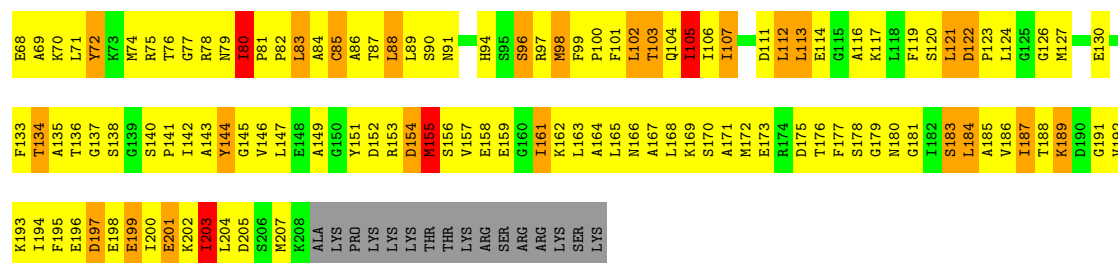
Chain d: 17% 50% 22% 8%



• Molecule 2: Proteasome subunit beta

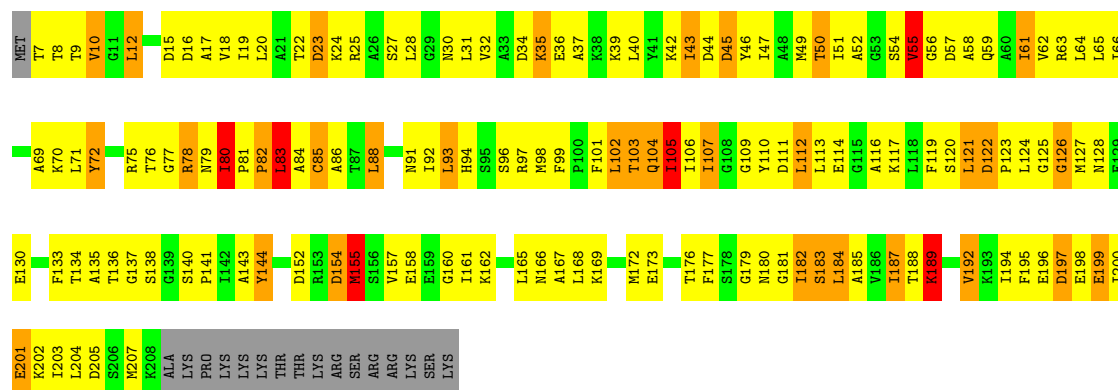
Chain e: 16% 56% 17% 8%





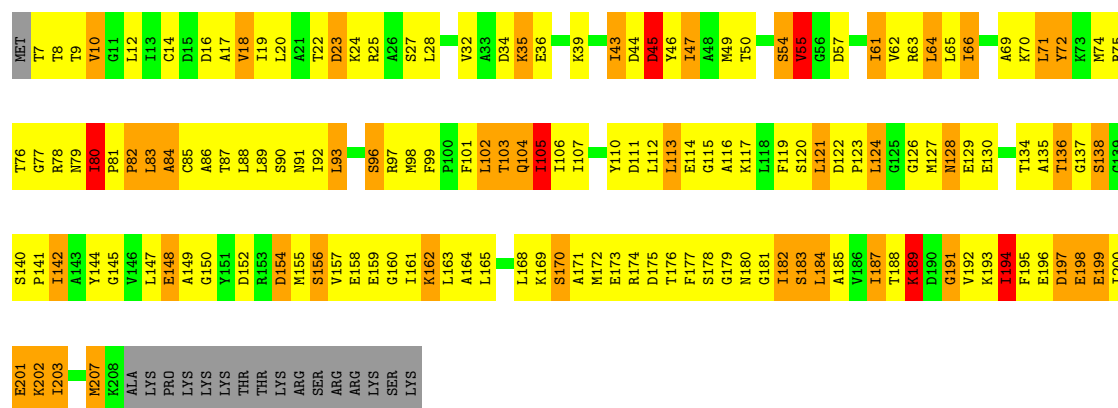
• Molecule 2: Proteasome subunit beta

Chain f: 24% 51% 15% 8%



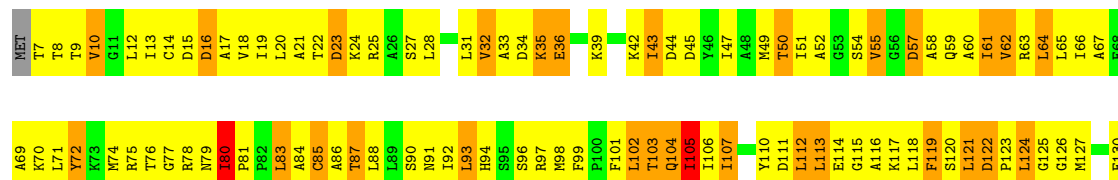
• Molecule 2: Proteasome subunit beta

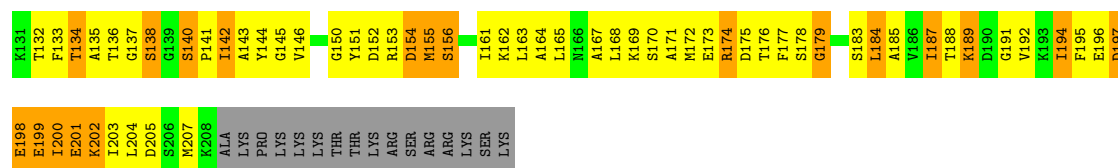
Chain g: 22% 47% 20% 8%



• Molecule 2: Proteasome subunit beta

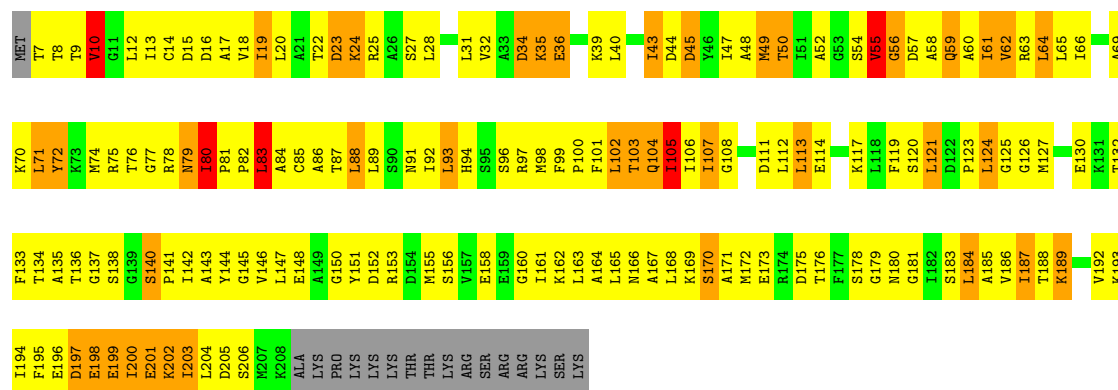
Chain h: 18% 52% 21% 8%





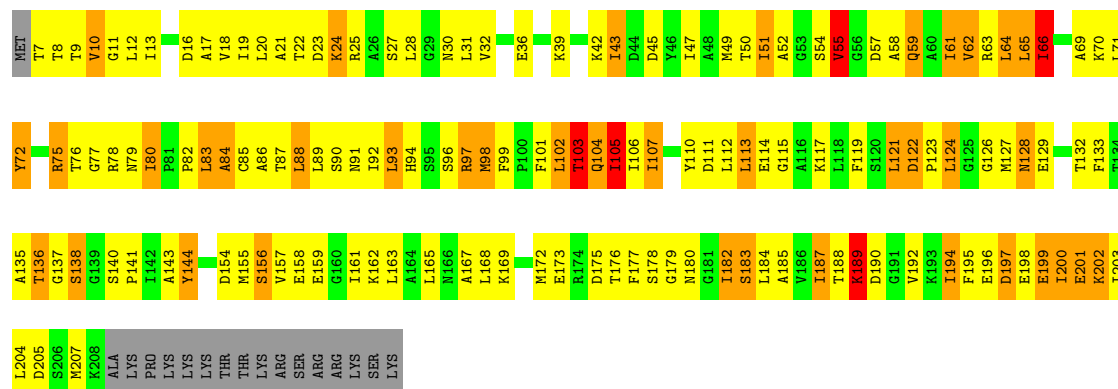
• Molecule 2: Proteasome subunit beta

Chain i: 18% 54% 18% 8%



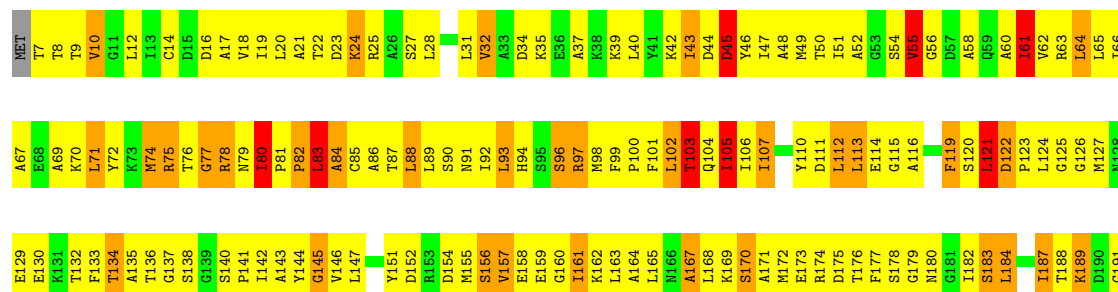
• Molecule 2: Proteasome subunit beta

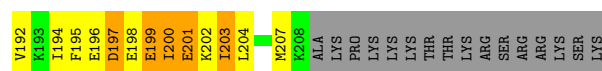
Chain j: 26% 47% 18% 8%



• Molecule 2: Proteasome subunit beta

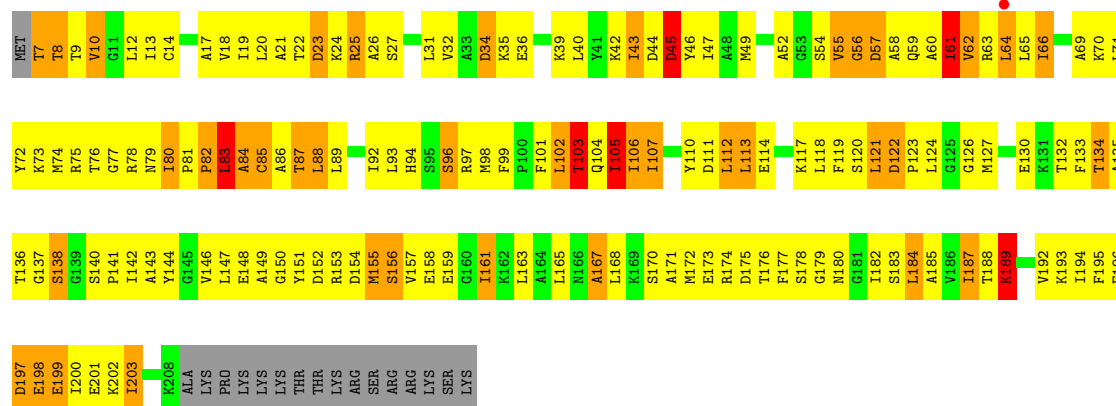
Chain k: 16% 55% 17% 8%





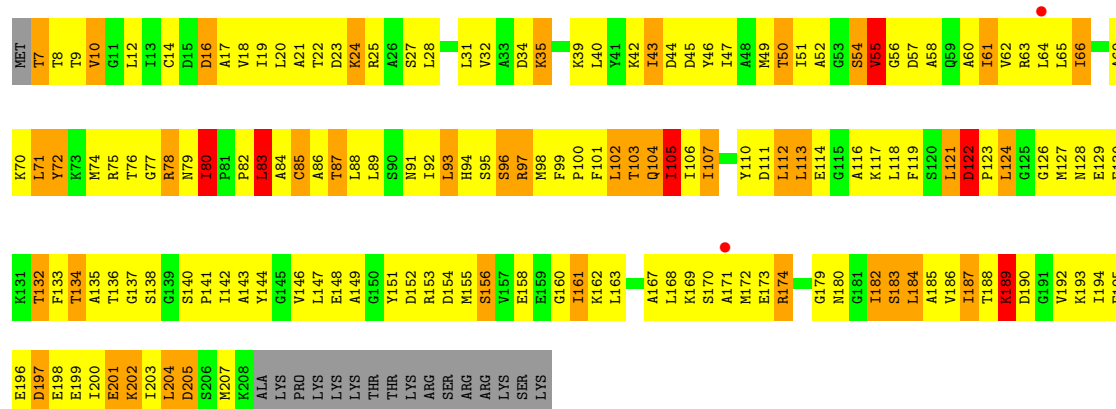
• Molecule 2: Proteasome subunit beta

Chain l: 20% 52% 18% 8%



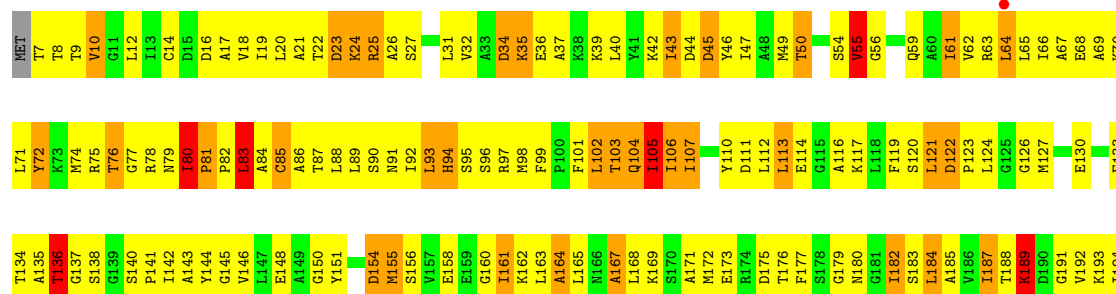
• Molecule 2: Proteasome subunit beta

Chain m: 19% 53% 18% 8%



• Molecule 2: Proteasome subunit beta

Chain n: 21% 51% 17% 8%



F195	E196	D197	E198	E199	I200	E201	K202	I203	L204	K208	ALA	LYS	PRO	LYS	LYS	LYS	THR	THR	LYS	ARG	SER	ARG	ARG	LYS	SER	LYS
------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	206.72Å 219.54Å 149.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 4.10 49.98 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.98-4.10) 99.8 (49.98-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.254 , 0.325 0.246 , 0.312	Depositor DCC
R_{free} test set	2740 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	118.1	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 203.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	46648	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6646e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

5.1 Standard geometry ⓘ

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	0.64	0/1832	1.00	7/2468 (0.3%)
1	B	0.61	0/1832	1.03	8/2468 (0.3%)
1	C	0.67	0/1832	1.07	6/2468 (0.2%)
1	D	0.72	0/1832	1.13	9/2468 (0.4%)
1	E	0.64	0/1832	1.04	6/2468 (0.2%)
1	F	0.74	0/1832	1.08	9/2468 (0.4%)
1	G	0.71	0/1832	1.09	10/2468 (0.4%)
1	H	0.66	0/1832	1.03	9/2468 (0.4%)
1	I	0.68	1/1832 (0.1%)	1.07	14/2468 (0.6%)
1	J	0.69	1/1832 (0.1%)	1.03	8/2468 (0.3%)
1	K	0.65	0/1832	1.05	12/2468 (0.5%)
1	L	0.68	0/1832	1.07	12/2468 (0.5%)
1	M	0.64	0/1832	1.01	7/2468 (0.3%)
1	N	0.63	0/1832	1.00	7/2468 (0.3%)
2	a	0.70	0/1536	1.02	4/2070 (0.2%)
2	b	0.66	0/1536	1.01	6/2070 (0.3%)
2	c	0.67	0/1536	0.98	4/2070 (0.2%)
2	d	0.70	0/1536	1.09	9/2070 (0.4%)
2	e	0.76	0/1536	1.05	6/2070 (0.3%)
2	f	0.81	0/1536	1.10	4/2070 (0.2%)
2	g	0.78	0/1536	1.05	5/2070 (0.2%)
2	h	0.71	0/1536	1.03	6/2070 (0.3%)
2	i	0.77	0/1536	1.03	3/2070 (0.1%)
2	j	0.80	0/1536	1.16	8/2070 (0.4%)
2	k	0.76	0/1536	1.10	10/2070 (0.5%)
2	l	0.71	0/1536	1.07	8/2070 (0.4%)
2	m	0.66	0/1536	1.07	7/2070 (0.3%)
2	n	0.68	0/1536	1.01	9/2070 (0.4%)
All	All	0.70	2/47152 (0.0%)	1.05	213/63532 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	90	ILE	CA-C	5.23	1.59	1.52
1	I	90	ILE	CA-C	5.05	1.58	1.52

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	229	GLU	N-CA-C	-9.42	101.01	111.28
1	L	229	GLU	N-CA-C	-9.23	101.20	111.07
1	C	93	ALA	N-CA-C	-9.11	101.31	111.14
1	E	229	GLU	N-CA-C	-8.95	101.47	111.14
1	G	93	ALA	N-CA-C	-8.75	101.69	111.14

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	1813	0	1899	276	0
1	B	1813	0	1899	278	2
1	C	1813	0	1899	281	0
1	D	1813	0	1899	326	0
1	E	1813	0	1899	329	1
1	F	1813	0	1899	279	1
1	G	1813	0	1899	299	0
1	H	1813	0	1899	285	0
1	I	1813	0	1899	284	1
1	J	1813	0	1899	278	0
1	K	1813	0	1899	299	0
1	L	1813	0	1899	275	0
1	M	1813	0	1899	269	2
1	N	1813	0	1899	278	0
2	a	1519	0	1567	230	0
2	b	1519	0	1567	248	0
2	c	1519	0	1567	240	2
2	d	1519	0	1567	239	0
2	e	1519	0	1567	243	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	f	1519	0	1567	223	1
2	g	1519	0	1567	230	0
2	h	1519	0	1567	240	0
2	i	1519	0	1567	238	2
2	j	1519	0	1567	224	0
2	k	1519	0	1567	248	0
2	l	1519	0	1567	229	0
2	m	1519	0	1567	243	1
2	n	1519	0	1567	233	0
All	All	46648	0	48524	6920	7

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 73.

The worst 5 of 6920 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:49:MET:HE2	2:j:62:VAL:HG13	1.27	1.16
2:m:18:VAL:HB	2:m:187:ILE:HD11	1.27	1.14
2:g:130:GLU:HG2	2:g:134:THR:HB	1.30	1.13
2:i:18:VAL:HB	2:i:187:ILE:HD11	1.31	1.12
1:J:178:GLU:HA	1:K:59:LEU:HD11	1.19	1.12

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:O	2:c:110:TYR:OH[2_565]	1.88	0.32
1:I:242:ASN:O	2:m:205:ASP:OD1[4_555]	2.00	0.20
1:M:243:GLU:N	2:i:205:ASP:OD1[4_455]	2.03	0.17
1:E:180:GLU:O	1:E:182:ARG:NH2[2_665]	2.09	0.11
1:B:231:LYS:NZ	2:c:15:ASP:OD1[2_565]	2.17	0.03

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	230/264 (87%)	163 (71%)	43 (19%)	24 (10%)	0	7
1	B	230/264 (87%)	162 (70%)	46 (20%)	22 (10%)	0	8
1	C	230/264 (87%)	155 (67%)	51 (22%)	24 (10%)	0	7
1	D	230/264 (87%)	158 (69%)	47 (20%)	25 (11%)	0	6
1	E	230/264 (87%)	158 (69%)	47 (20%)	25 (11%)	0	6
1	F	230/264 (87%)	152 (66%)	53 (23%)	25 (11%)	0	6
1	G	230/264 (87%)	156 (68%)	51 (22%)	23 (10%)	0	8
1	H	230/264 (87%)	153 (66%)	49 (21%)	28 (12%)	0	4
1	I	230/264 (87%)	159 (69%)	44 (19%)	27 (12%)	0	4
1	J	230/264 (87%)	161 (70%)	45 (20%)	24 (10%)	0	7
1	K	230/264 (87%)	151 (66%)	51 (22%)	28 (12%)	0	4
1	L	230/264 (87%)	162 (70%)	39 (17%)	29 (13%)	0	4
1	M	230/264 (87%)	159 (69%)	45 (20%)	26 (11%)	0	5
1	N	230/264 (87%)	159 (69%)	48 (21%)	23 (10%)	0	8
2	a	200/219 (91%)	135 (68%)	45 (22%)	20 (10%)	0	8
2	b	200/219 (91%)	129 (64%)	53 (26%)	18 (9%)	0	10
2	c	200/219 (91%)	140 (70%)	45 (22%)	15 (8%)	1	12
2	d	200/219 (91%)	132 (66%)	46 (23%)	22 (11%)	0	6
2	e	200/219 (91%)	136 (68%)	46 (23%)	18 (9%)	0	10
2	f	200/219 (91%)	142 (71%)	42 (21%)	16 (8%)	1	11
2	g	200/219 (91%)	132 (66%)	43 (22%)	25 (12%)	0	4
2	h	200/219 (91%)	136 (68%)	44 (22%)	20 (10%)	0	8
2	i	200/219 (91%)	130 (65%)	46 (23%)	24 (12%)	0	4
2	j	200/219 (91%)	145 (72%)	39 (20%)	16 (8%)	1	11
2	k	200/219 (91%)	126 (63%)	50 (25%)	24 (12%)	0	4
2	l	200/219 (91%)	143 (72%)	37 (18%)	20 (10%)	0	8
2	m	200/219 (91%)	139 (70%)	43 (22%)	18 (9%)	0	10
2	n	200/219 (91%)	136 (68%)	46 (23%)	18 (9%)	0	10
All	All	6020/6762 (89%)	4109 (68%)	1284 (21%)	627 (10%)	0	7

5 of 627 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	TYR
1	A	43	CYS
1	A	132	PRO
1	A	155	SER
1	A	168	SER

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	195/224 (87%)	162 (83%)	33 (17%)	2	12
1	B	195/224 (87%)	162 (83%)	33 (17%)	2	12
1	C	195/224 (87%)	157 (80%)	38 (20%)	1	9
1	D	195/224 (87%)	160 (82%)	35 (18%)	2	11
1	E	195/224 (87%)	157 (80%)	38 (20%)	1	9
1	F	195/224 (87%)	156 (80%)	39 (20%)	1	9
1	G	195/224 (87%)	158 (81%)	37 (19%)	1	10
1	H	195/224 (87%)	159 (82%)	36 (18%)	1	10
1	I	195/224 (87%)	160 (82%)	35 (18%)	2	11
1	J	195/224 (87%)	159 (82%)	36 (18%)	1	10
1	K	195/224 (87%)	163 (84%)	32 (16%)	2	13
1	L	195/224 (87%)	158 (81%)	37 (19%)	1	10
1	M	195/224 (87%)	163 (84%)	32 (16%)	2	13
1	N	195/224 (87%)	162 (83%)	33 (17%)	2	12
2	a	163/179 (91%)	131 (80%)	32 (20%)	1	9
2	b	163/179 (91%)	125 (77%)	38 (23%)	1	5
2	c	163/179 (91%)	130 (80%)	33 (20%)	1	8
2	d	163/179 (91%)	121 (74%)	42 (26%)	0	4
2	e	163/179 (91%)	124 (76%)	39 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	f	163/179 (91%)	128 (78%)	35 (22%)	1	6
2	g	163/179 (91%)	129 (79%)	34 (21%)	1	7
2	h	163/179 (91%)	129 (79%)	34 (21%)	1	7
2	i	163/179 (91%)	129 (79%)	34 (21%)	1	7
2	j	163/179 (91%)	126 (77%)	37 (23%)	1	6
2	k	163/179 (91%)	130 (80%)	33 (20%)	1	8
2	l	163/179 (91%)	127 (78%)	36 (22%)	1	6
2	m	163/179 (91%)	122 (75%)	41 (25%)	0	4
2	n	163/179 (91%)	128 (78%)	35 (22%)	1	6
All	All	5012/5642 (89%)	4015 (80%)	997 (20%)	1	9

5 of 997 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	f	154	ASP
2	l	10	VAL
1	I	225	ILE
2	k	161	ILE
2	m	122	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	g	128	ASN
1	I	126	GLN
2	k	79	ASN
1	L	98	GLN
1	N	98	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	232/264 (87%)	-0.06	1 (0%) 88 76	127, 157, 221, 336	0
1	B	232/264 (87%)	0.03	1 (0%) 88 76	118, 151, 270, 519	0
1	C	232/264 (87%)	-0.12	0 100 100	114, 132, 205, 333	0
1	D	232/264 (87%)	-0.14	0 100 100	59, 134, 205, 245	0
1	E	232/264 (87%)	-0.01	1 (0%) 88 76	82, 139, 252, 355	0
1	F	232/264 (87%)	-0.04	1 (0%) 88 76	92, 116, 204, 346	0
1	G	232/264 (87%)	-0.14	1 (0%) 88 76	106, 128, 215, 284	0
1	H	232/264 (87%)	-0.07	0 100 100	131, 148, 187, 271	0
1	I	232/264 (87%)	-0.10	1 (0%) 88 76	90, 136, 212, 299	0
1	J	232/264 (87%)	0.03	1 (0%) 88 76	81, 141, 259, 366	0
1	K	232/264 (87%)	-0.06	0 100 100	112, 139, 220, 291	0
1	L	232/264 (87%)	-0.05	1 (0%) 88 76	113, 135, 208, 253	0
1	M	232/264 (87%)	-0.07	1 (0%) 88 76	126, 143, 253, 507	0
1	N	232/264 (87%)	-0.03	1 (0%) 88 76	130, 147, 186, 303	0
2	a	202/219 (92%)	-0.14	1 (0%) 87 74	118, 138, 170, 185	0
2	b	202/219 (92%)	-0.13	0 100 100	113, 131, 161, 180	0
2	c	202/219 (92%)	-0.18	1 (0%) 87 74	101, 119, 195, 251	0
2	d	202/219 (92%)	-0.19	0 100 100	107, 124, 162, 194	0
2	e	202/219 (92%)	-0.17	0 100 100	93, 111, 159, 203	0
2	f	202/219 (92%)	-0.16	0 100 100	100, 115, 150, 175	0
2	g	202/219 (92%)	-0.13	0 100 100	110, 125, 149, 171	0
2	h	202/219 (92%)	-0.17	0 100 100	123, 139, 174, 186	0
2	i	202/219 (92%)	-0.10	0 100 100	110, 123, 155, 170	0
2	j	202/219 (92%)	-0.26	0 100 100	72, 87, 159, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	k	202/219 (92%)	-0.12	0 100 100	80, 102, 177, 209	0
2	l	202/219 (92%)	-0.16	1 (0%) 87 74	104, 120, 160, 193	0
2	m	202/219 (92%)	-0.10	2 (0%) 79 62	102, 122, 213, 254	0
2	n	202/219 (92%)	0.04	1 (0%) 87 74	122, 148, 181, 195	0
All	All	6076/6762 (89%)	-0.10	16 (0%) 90 79	59, 134, 207, 519	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	207	PRO	3.2
1	J	13	ILE	3.1
1	N	79	THR	3.0
1	B	194	ALA	3.0
2	n	64	LEU	2.5

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.