



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:37 AM UTC

PDB ID : 9QDF / pdb_00009qdf
Title : Yeast 20S proteasome mutant: beta1_G128V (b1-propeptide deleted) in complex with Bortezomib
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-03-06
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

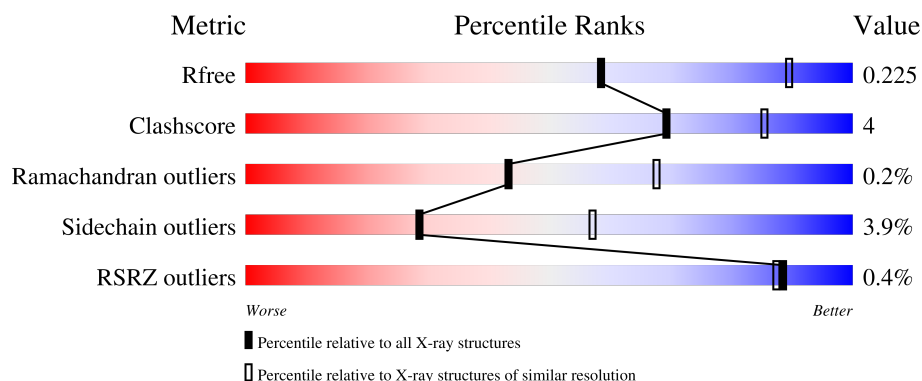
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	250	96%
1	O	250	% 95%
2	B	258	% 88% 5% • 5%
2	P	258	% 88% 5% • 5%
3	C	254	88% • • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 2% 89% 6%
4	D	260	 84% 6% 10%
4	R	260	 85% 5% 10%
5	E	234	 91% 7%
5	S	234	 92% 6%
6	F	288	 80% 16%
6	T	288	 80% 16%
7	G	252	 87% 8%
7	U	252	 87% 8%
8	H	231	 87% 8%
8	V	231	 89% 6%
9	I	205	 94% 5%
9	W	205	 92% 7%
10	J	198	 1% 87% 10%
10	X	198	 1% 85% 12%
11	K	211	 82% 14%
11	Y	211	 1% 80% 16%
12	L	222	 90% 9%
12	Z	222	 91% 9%
13	M	246	 82% 11% 5%
13	a	246	 81% 12% 5%
14	N	195	 1% 84% 12%
14	b	195	 1% 84% 14%
15	d	3	 67% 33%
15	e	3	 33% 67%

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Mol	Chain	Length	Quality of chain
15	f	3	67% 33%
15	g	3	67% 33%
15	h	3	33% 67%
15	i	3	33% 67%

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49860 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			
8	V	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	1	0
			1767	1121	306	336	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	195	Total	C	N	O	S	0	0	0
			1508	954	249	298	7			
14	b	195	Total	C	N	O	S	0	0	0
			1508	954	249	298	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	128	VAL	GLY	engineered mutation	UNP P38624
b	128	VAL	GLY	engineered mutation	UNP P38624

- Molecule 15 is a protein called 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C]PYRAZ

OLE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	d	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	e	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	f	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	g	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	h	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	i	3	Total	C	N	O	0	0	0
			35	24	5	6			

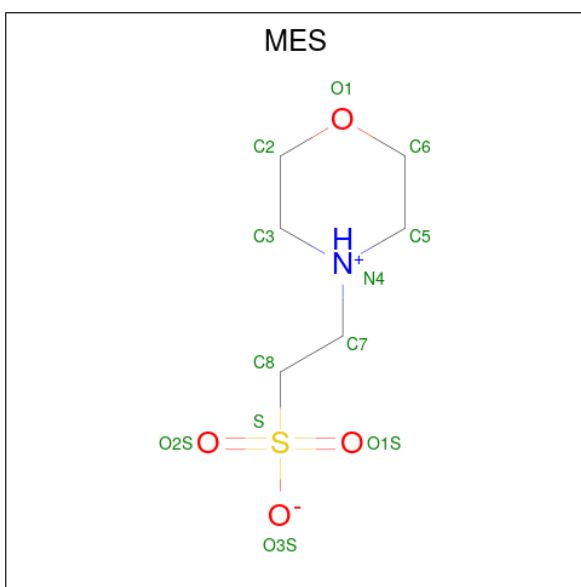
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	I	1	Total	Mg	0	0
			1	1		
16	V	1	Total	Mg	0	0
			1	1		
16	Z	1	Total	Mg	0	0
			1	1		

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

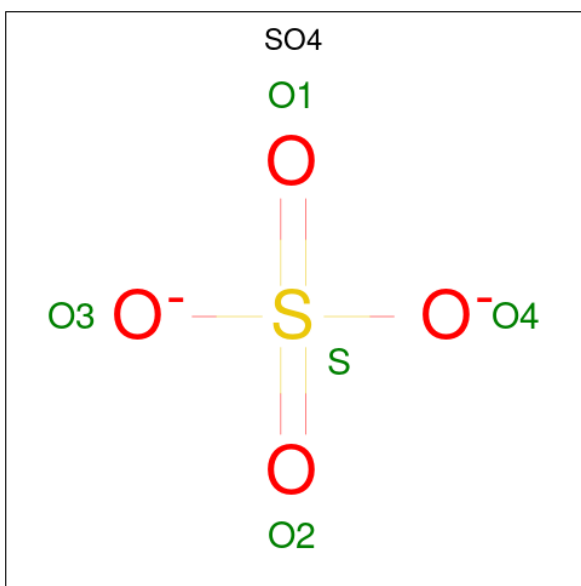
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	2	Total	Cl	0	0
			2	2		
17	N	1	Total	Cl	0	0
			1	1		
17	U	1	Total	Cl	0	0
			1	1		
17	b	1	Total	Cl	0	0
			1	1		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	a	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	d	1	Total	O	S	0	0
			5	4	1		
19	g	1	Total	O	S	0	0
			5	4	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	14	Total O 14 14	0	0
20	B	13	Total O 13 13	0	0
20	C	6	Total O 6 6	0	0
20	D	6	Total O 6 6	0	0
20	E	6	Total O 6 6	0	0
20	F	15	Total O 15 15	0	0
20	G	15	Total O 15 15	0	0
20	H	16	Total O 16 16	0	0
20	I	16	Total O 16 16	0	0
20	J	17	Total O 17 17	0	0
20	K	8	Total O 8 8	0	0
20	L	19	Total O 19 19	0	0
20	M	16	Total O 16 16	0	0
20	N	8	Total O 8 8	0	0
20	O	8	Total O 8 8	0	0
20	P	11	Total O 11 11	0	0
20	Q	12	Total O 12 12	0	0
20	R	11	Total O 11 11	0	0
20	S	4	Total O 4 4	0	0
20	T	14	Total O 14 14	0	0
20	U	17	Total O 17 17	0	0
20	V	20	Total O 20 20	0	0

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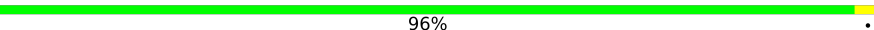
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	W	9	Total 9	O 9	0	0
20	X	10	Total 10	O 10	0	0
20	Y	12	Total 12	O 12	0	0
20	Z	15	Total 15	O 15	0	0
20	a	18	Total 18	O 18	0	0
20	b	11	Total 11	O 11	0	0
20	d	1	Total 1	O 1	0	0
20	f	1	Total 1	O 1	0	0

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.

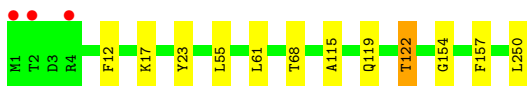
- Molecule 1: Proteasome subunit alpha type-2

Chain A:  96%



- Molecule 1: Proteasome subunit alpha type-2

Chain O:  95%



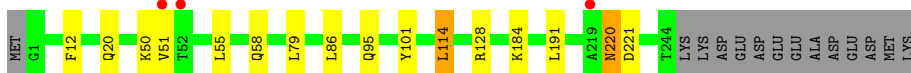
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  88% 5% 5%



- Molecule 2: Proteasome subunit alpha type-3

Chain P:  88% 5% 5%

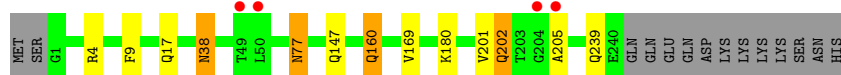
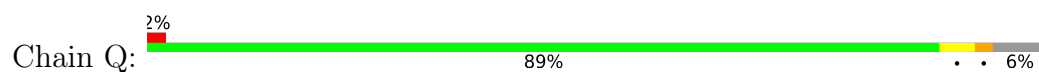


- Molecule 3: Proteasome subunit alpha type-4

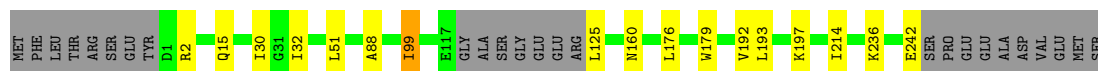
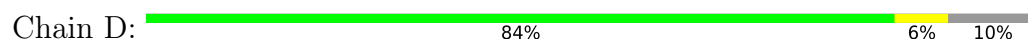
Chain C:  88% 6% 6%



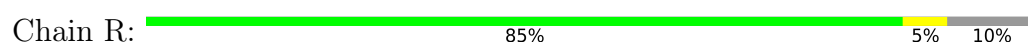
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



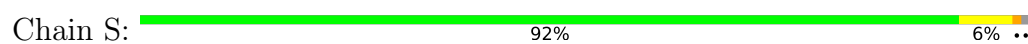
- Molecule 4: Proteasome subunit alpha type-5



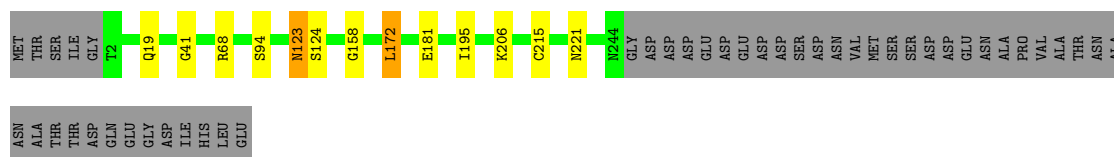
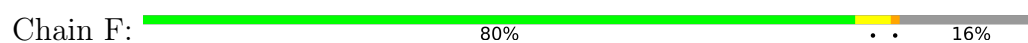
- Molecule 5: Proteasome subunit alpha type-6



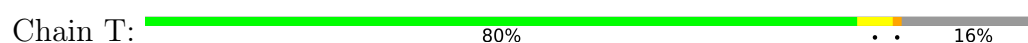
- Molecule 5: Proteasome subunit alpha type-6

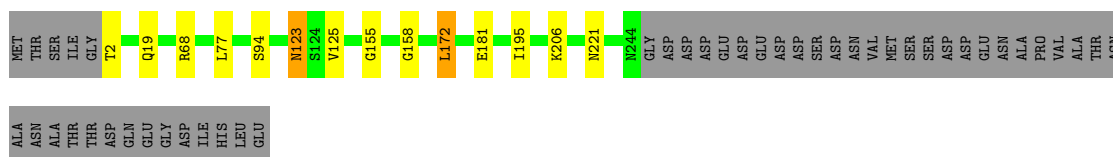


- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7





- Molecule 7: Proteasome subunit alpha type-1

Chain G: 87% 8% . .



- Molecule 7: Proteasome subunit alpha type-1

Chain U: 87% 8% . .



- Molecule 8: Proteasome subunit beta type-2

Chain H: 87% 8% .



- Molecule 8: Proteasome subunit beta type-2

Chain V: 89% 6% .



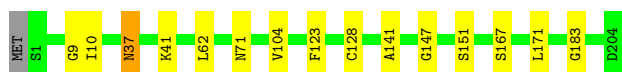
- Molecule 9: Proteasome subunit beta type-3

Chain I: 94% 5%

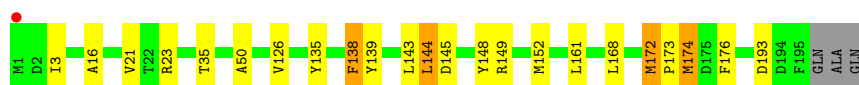
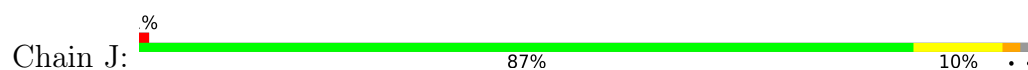


- Molecule 9: Proteasome subunit beta type-3

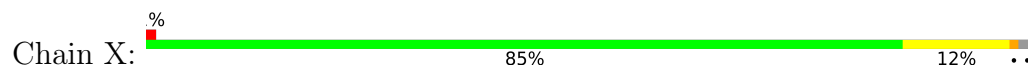
Chain W: 92% 7%



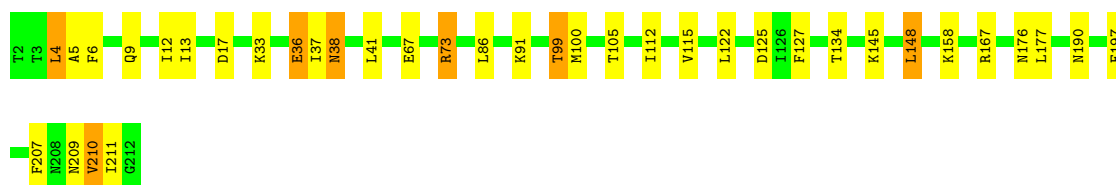
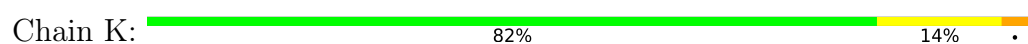
- Molecule 10: Proteasome subunit beta type-4



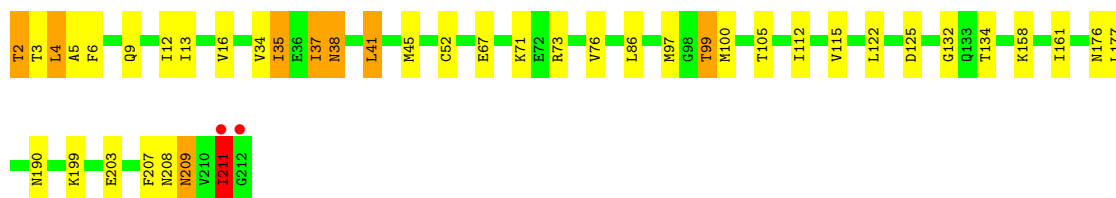
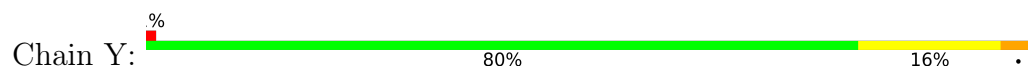
- Molecule 10: Proteasome subunit beta type-4



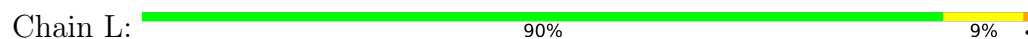
- Molecule 11: Proteasome subunit beta type-5



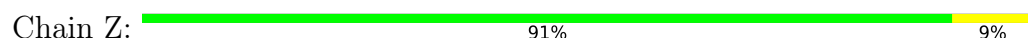
- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7

[illegible]

- | | | | | | | | | |
|------|----|-----|-----|------|------|------|------|------|
| V159 | T1 | S10 | L27 | N48 | I157 | I114 | L127 | V159 |
| I165 | Q2 | S29 | Q28 | I137 | I163 | I128 | R128 | I166 |
| P166 | Q3 | S10 | S29 | N48 | I170 | I129 | V130 | |
| N179 | | | S29 | N48 | I170 | I129 | V130 | |
| R182 | | | S29 | N48 | I170 | I129 | V130 | |
| R187 | | | S29 | N48 | I170 | I129 | V130 | |
| S192 | | | S29 | N48 | I170 | I129 | V130 | |
| W219 | | | S29 | N48 | I170 | I129 | V130 | |
| I233 | | | S29 | N48 | I170 | I129 | V130 | |

- | Category | Value | Color |
|----------|-------|--------|
| S2 | 13 | Orange |
| K9 | 13 | Yellow |
| I13 | 13 | Orange |
| L14 | 13 | Orange |
| T22 | 13 | Orange |
| R36 | 13 | Yellow |
| W42 | 13 | Yellow |
| S46 | 13 | Orange |
| L65 | 13 | Yellow |
| Q69 | 13 | Yellow |
| K83 | 13 | Orange |
| N89 | 13 | Yellow |
| L93 | 13 | Orange |
| T94 | 13 | Orange |
| A100 | 13 | Orange |
| V119 | 13 | Orange |
| Y124 | 13 | Yellow |
| V128 | 13 | Orange |
| S129 | 13 | Orange |
| F133 | 13 | Orange |
| I134 | 13 | Green |
| Y135 | 13 | Yellow |
| G136 | 13 | Orange |
| D139 | 13 | Orange |
| K140 | 13 | Orange |
| K148 | 13 | Yellow |
| I155 | 13 | Orange |
| W165 | 13 | Red |
| G171 | 13 | Yellow |
| M175 | 13 | Orange |
| L178 | 13 | Orange |
| E184 | 13 | Orange |
| T196 | 13 | Green |

- | Category | Item | Value |
|----------|------|-------|
| S2 | S2 | 100 |
| | K9 | 100 |
| | I13 | 100 |
| | L14 | 100 |
| | D17 | 100 |
| | T22 | 100 |
| | R36 | 100 |
| | W42 | 100 |
| | L65 | 100 |
| | Q69 | 100 |
| K83 | K83 | 100 |
| | N89 | 100 |
| | L93 | 100 |
| | T94 | 100 |
| | A100 | 100 |
| | G116 | 100 |
| | V119 | 100 |
| | Y124 | 100 |
| | S129 | 100 |
| | G130 | 100 |
| Y135 | S131 | 100 |
| | Y135 | 100 |
| | G136 | 100 |
| | Y137 | 100 |
| | C138 | 100 |
| | K139 | 100 |
| | K140 | 100 |
| | K148 | 100 |
| | I155 | 100 |
| | W165 | 100 |
| G171 | G171 | 100 |
| | M175 | 100 |
| | L178 | 100 |
| | E184 | 100 |
| | T195 | 100 |

- VGL1
F2
A1I493

- | | |
|------|--------|
| VGL1 | |
| F2 | A1I493 |

- 

Chain f:  67% 33%

VGL1
F2
A11493

- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C.]PYRAZOLE

Chain g:  67% 33%

VGL1
F2
A11493

- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C.]PYRAZOLE

Chain h:  33% 67%

VGL1
F2
A11493

- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C.]PYRAZOLE

Chain i:  33% 67%

VGL1
F2
A11493

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.95Å 300.39Å 145.30Å 90.00° 113.18° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (15.00-2.70) 96.4 (15.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.179 , 0.217 0.180 , 0.225	Depositor DCC
R_{free} test set	14184 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	1.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	49860	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MES, A1I49, MG, CL, SO4, VGL

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	1.04	0/1952	1.42	0/2642
1	O	1.04	1/1952 (0.1%)	1.43	0/2642
2	B	1.02	0/1934	1.43	0/2618
2	P	1.03	0/1934	1.43	0/2618
3	C	1.03	0/1910	1.46	0/2586
3	Q	1.04	0/1910	1.47	0/2586
4	D	1.04	0/1837	1.48	4/2475 (0.2%)
4	R	1.04	0/1837	1.48	2/2475 (0.1%)
5	E	1.04	0/1800	1.44	0/2433
5	S	1.04	0/1800	1.45	0/2433
6	F	1.02	0/1932	1.45	0/2609
6	T	1.03	0/1932	1.45	2/2609 (0.1%)
7	G	1.01	0/1945	1.42	0/2634
7	U	1.02	0/1945	1.43	0/2634
8	H	1.04	0/1708	1.41	2/2316 (0.1%)
8	V	1.03	0/1708	1.42	2/2316 (0.1%)
9	I	1.01	0/1611	1.41	1/2174 (0.0%)
9	W	1.01	0/1611	1.41	1/2174 (0.0%)
10	J	1.00	0/1589	1.40	1/2142 (0.0%)
10	X	1.01	0/1589	1.40	0/2142
11	K	1.00	0/1674	1.44	1/2264 (0.0%)
11	Y	1.01	0/1674	1.43	1/2264 (0.0%)
12	L	1.01	0/1795	1.39	0/2420
12	Z	1.00	0/1806	1.38	0/2435
13	M	1.01	0/1855	1.39	0/2514
13	a	1.01	0/1855	1.40	0/2514
14	N	1.02	0/1537	1.44	1/2082 (0.0%)
14	b	1.01	0/1537	1.43	1/2082 (0.0%)
15	d	2.02	1/11 (9.1%)	1.13	0/13
15	e	2.05	1/11 (9.1%)	1.07	0/13
15	f	2.39	1/11 (9.1%)	3.23	1/13 (7.7%)
15	g	1.83	1/11 (9.1%)	0.89	0/13

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	h	1.82	1/11 (9.1%)	0.95	0/13
15	i	2.25	1/11 (9.1%)	3.27	1/13 (7.7%)
All	All	1.02	7/50235 (0.0%)	1.43	21/67911 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	2	PHE	CB-CG	-7.30	1.33	1.50
15	i	2	PHE	CB-CG	-6.68	1.35	1.50
15	e	2	PHE	CB-CG	-6.16	1.36	1.50
15	d	2	PHE	CB-CG	-5.99	1.36	1.50
15	g	2	PHE	CB-CG	-5.71	1.37	1.50
15	h	2	PHE	CB-CG	-5.39	1.38	1.50
1	O	68	THR	N-CA	5.09	1.49	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	2	PHE	CA-CB-CG	-10.55	103.25	113.80
15	i	2	PHE	CA-CB-CG	-9.98	103.82	113.80
14	N	94	THR	CB-CA-C	6.30	120.52	111.82
14	b	94	THR	CB-CA-C	6.28	120.48	111.82
9	I	183	GLY	CA-C-O	-6.20	118.19	122.22
9	W	183	GLY	CA-C-O	-6.12	118.24	122.22
8	H	4	VAL	CA-C-N	6.00	125.73	121.65
8	H	4	VAL	C-N-CA	6.00	125.73	121.65
8	V	4	VAL	CA-C-N	5.67	125.50	121.65
8	V	4	VAL	C-N-CA	5.67	125.50	121.65
10	J	138	PHE	CB-CA-C	5.37	119.70	110.79
11	K	36	GLU	CA-C-O	-5.35	114.75	120.42
4	R	2	ARG	CA-C-N	5.32	125.15	120.10
4	R	2	ARG	C-N-CA	5.32	125.15	120.10
4	D	2	ARG	CA-C-N	5.30	125.13	120.10
4	D	2	ARG	C-N-CA	5.30	125.13	120.10
4	D	30	ILE	CA-C-N	5.27	125.23	121.65
4	D	30	ILE	C-N-CA	5.27	125.23	121.65
6	T	77	LEU	CA-C-N	5.23	124.52	120.33
6	T	77	LEU	C-N-CA	5.23	124.52	120.33
11	Y	2	THR	CA-CB-OG1	-5.00	102.09	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	4	0
1	O	1915	0	1929	6	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	12	0
3	Q	1881	0	1895	8	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	13	0
5	S	1773	0	1775	13	0
6	F	1892	0	1883	6	0
6	T	1892	0	1883	7	0
7	G	1907	0	1901	11	0
7	U	1907	0	1901	12	0
8	H	1677	0	1678	16	0
8	V	1677	0	1678	7	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	10	0
10	J	1561	0	1569	16	0
10	X	1561	0	1569	21	0
11	K	1637	0	1585	47	0
11	Y	1637	0	1585	50	0
12	L	1757	0	1711	15	0
12	Z	1767	0	1717	13	0
13	M	1824	0	1832	27	0
13	a	1824	0	1832	23	0
14	N	1508	0	1477	29	0
14	b	1508	0	1477	28	0
15	d	35	0	11	0	0
15	e	35	0	11	2	0
15	f	35	0	11	4	0
15	g	35	0	11	4	0
15	h	35	0	11	1	0
15	i	35	0	11	2	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Z	1	0	0	0	0
17	G	2	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	b	1	0	0	0	0
18	a	12	0	13	0	0
19	d	5	0	0	0	0
19	g	5	0	0	0	0
20	A	14	0	0	0	0
20	B	13	0	0	0	0
20	C	6	0	0	0	0
20	D	6	0	0	0	0
20	E	6	0	0	0	0
20	F	15	0	0	0	0
20	G	15	0	0	0	0
20	H	16	0	0	1	0
20	I	16	0	0	0	0
20	J	17	0	0	1	0
20	K	8	0	0	0	0
20	L	19	0	0	0	0
20	M	16	0	0	0	0
20	N	8	0	0	0	0
20	O	8	0	0	0	0
20	P	11	0	0	0	0
20	Q	12	0	0	0	0
20	R	11	0	0	0	0
20	S	4	0	0	0	0
20	T	14	0	0	1	0
20	U	17	0	0	0	0
20	V	20	0	0	0	0
20	W	9	0	0	0	0
20	X	10	0	0	0	0
20	Y	12	0	0	0	0
20	Z	15	0	0	0	0
20	a	18	0	0	1	0
20	b	11	0	0	0	0
20	d	1	0	0	0	0
20	f	1	0	0	0	0
All	All	49860	0	49105	349	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 4.

All (349) 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)
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.30	1.10
11:K:197:PHE:CE1	11:K:207:PHE:CE1	2.43	1.06
13:a:37:ASN:HB3	14:b:135:TYR:HE2	1.20	1.06
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.38	1.04
11:K:134:THR:HG22	10:X:139:TYR:CE1	1.94	1.03
13:M:37:ASN:HB3	14:N:135:TYR:HE2	1.27	1.00
8:H:213:LEU:HD13	11:Y:211:ILE:CG1	1.94	0.96
13:a:37:ASN:CB	14:b:135:TYR:HE2	1.81	0.93
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.36	0.90
13:a:37:ASN:HB3	14:b:135:TYR:CE2	2.05	0.90
11:K:197:PHE:CE1	11:K:207:PHE:CD1	2.60	0.89
13:M:37:ASN:CB	14:N:135:TYR:HE2	1.85	0.89
11:K:197:PHE:CD1	11:K:207:PHE:HE1	1.91	0.89
8:H:213:LEU:HD13	11:Y:211:ILE:HG13	1.56	0.87
15:h:3:A1I49:O28	15:h:3:A1I49:N	2.08	0.87
14:b:135:TYR:HD1	14:b:136:GLY:N	1.73	0.87
14:N:135:TYR:HD1	14:N:136:GLY:N	1.73	0.86
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.40	0.86
13:M:37:ASN:HB3	14:N:135:TYR:CE2	2.11	0.86
13:M:30:TYR:HB2	13:M:34:LEU:HB2	1.58	0.85
11:K:167:ARG:NH2	10:X:141:PHE:HD1	1.75	0.84
11:K:5:ALA:HB3	11:K:100:MET:CE	2.08	0.84
8:H:213:LEU:CD1	11:Y:211:ILE:HD11	2.09	0.82
11:K:5:ALA:N	11:K:100:MET:HE1	1.93	0.82
14:b:129:SER:OG	14:b:130:GLY:N	2.12	0.81
11:K:197:PHE:CE1	11:K:207:PHE:HE1	1.99	0.81
11:K:167:ARG:CZ	10:X:141:PHE:CD1	2.65	0.80
11:Y:209:ASN:HD22	11:Y:209:ASN:H	1.29	0.79
11:K:197:PHE:CZ	11:K:207:PHE:CD1	2.70	0.79
11:K:167:ARG:CZ	10:X:141:PHE:HD1	1.97	0.77
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.67	0.77
14:b:135:TYR:HD1	14:b:135:TYR:C	1.91	0.76
14:N:135:TYR:HD1	14:N:135:TYR:C	1.92	0.76
13:a:37:ASN:CB	14:b:135:TYR:CE2	2.65	0.76
11:Y:73:ARG:HH21	11:Y:73:ARG:HB3	1.51	0.76
11:K:5:ALA:CB	11:K:100:MET:HE2	2.15	0.75
14:b:135:TYR:C	14:b:135:TYR:CD1	2.65	0.74
14:b:135:TYR:CD1	14:b:136:GLY:N	2.55	0.74
11:K:197:PHE:CZ	11:K:207:PHE:HD1	2.05	0.74
13:M:37:ASN:CB	14:N:135:TYR:CE2	2.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:135:TYR:C	14:N:135:TYR:CD1	2.66	0.73
14:N:135:TYR:CD1	14:N:136:GLY:N	2.55	0.73
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.35	0.73
14:N:22:THR:OG1	15:f:1:VGL:H3	1.88	0.73
11:K:197:PHE:CD1	11:K:207:PHE:CE1	2.73	0.72
10:J:139:TYR:CE1	11:Y:134:THR:HG22	2.25	0.72
8:H:213:LEU:HD13	11:Y:211:ILE:CD1	2.20	0.71
14:N:14:LEU:CD1	14:N:100:ALA:HB3	2.15	0.71
1:O:12:PHE:H	2:P:20:GLN:HE22	1.39	0.71
11:K:33:LYS:NZ	15:e:3:A1I49:OG1	2.26	0.68
2:B:12:PHE:H	3:C:17:GLN:HE22	1.41	0.68
14:N:14:LEU:HD11	14:N:100:ALA:CB	2.16	0.68
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.42	0.68
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.41	0.68
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.42	0.67
7:U:23:PHE:O	7:U:26:THR:HB	1.95	0.67
3:C:9:PHE:H	4:D:15:GLN:HE22	1.42	0.66
5:S:12:PHE:H	6:T:19:GLN:HE22	1.44	0.66
7:G:23:PHE:O	7:G:26:THR:HB	1.96	0.65
8:H:213:LEU:HD13	11:Y:211:ILE:HD11	1.77	0.65
11:K:17:ASP:O	11:K:33:LYS:HD2	1.96	0.65
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.45	0.65
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.95	0.64
11:K:167:ARG:NH2	10:X:141:PHE:CD1	2.62	0.63
14:b:2:SER:N	14:b:17:ASP:OD1	2.31	0.63
5:E:12:PHE:H	6:F:19:GLN:HE22	1.46	0.63
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.96	0.62
11:K:73:ARG:HH21	11:K:73:ARG:HB3	1.64	0.62
8:H:52:THR:O	8:H:56:THR:HB	2.00	0.61
11:K:134:THR:HG22	10:X:139:TYR:CZ	2.35	0.60
11:Y:73:ARG:HB3	11:Y:73:ARG:NH2	2.15	0.60
13:a:30:TYR:HB2	13:a:34:LEU:HB2	1.84	0.59
13:M:30:TYR:OH	14:N:133:PHE:HB2	2.02	0.59
1:A:12:PHE:H	2:B:20:GLN:HE22	1.51	0.59
11:K:209:ASN:OD1	10:X:145:ASP:OD1	2.20	0.59
7:G:61:SER:OG	7:G:215:GLU:OE2	2.21	0.58
12:L:4:PRO:O	13:M:104:ARG:NH1	2.35	0.58
15:f:3:A1I49:N	15:f:3:A1I49:O28	2.36	0.57
11:K:4:LEU:HD22	11:K:4:LEU:C	2.29	0.57
8:V:52:THR:O	8:V:56:THR:HB	2.03	0.57
11:Y:5:ALA:N	11:Y:100:MET:HE1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:99:THR:HG22	11:K:115:VAL:HB	1.85	0.57
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.03	0.57
11:K:5:ALA:CB	11:K:100:MET:CE	2.81	0.57
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.03	0.57
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.02	0.56
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.30	0.56
8:H:213:LEU:CD1	11:Y:211:ILE:CG1	2.77	0.55
6:F:123:ASN:C	6:F:123:ASN:HD22	2.15	0.55
11:K:99:THR:HG22	11:K:115:VAL:O	2.06	0.55
14:N:155:ILE:HG21	14:N:175:MET:HE3	1.89	0.55
10:J:139:TYR:CZ	11:Y:134:THR:HG22	2.41	0.55
10:J:148:TYR:O	11:Y:208:ASN:OD1	2.25	0.55
11:K:5:ALA:H	11:K:100:MET:HE1	1.68	0.54
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.90	0.54
11:K:197:PHE:HZ	11:K:210:VAL:HG11	1.72	0.54
3:C:38:ASN:C	3:C:38:ASN:HD22	2.15	0.54
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.90	0.54
15:e:3:A1I49:O28	15:e:3:A1I49:N	2.40	0.54
8:H:213:LEU:CD1	11:Y:211:ILE:CD1	2.79	0.54
11:K:73:ARG:HB3	11:K:73:ARG:NH2	2.21	0.54
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.71	0.54
11:Y:3:THR:HG22	11:Y:16:VAL:HG12	1.89	0.54
13:M:37:ASN:HB2	14:N:135:TYR:CE2	2.43	0.54
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.90	0.54
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.37	0.54
14:b:155:ILE:HG21	14:b:175:MET:HE3	1.90	0.54
15:g:3:A1I49:O28	15:g:3:A1I49:N	2.42	0.53
6:T:123:ASN:C	6:T:123:ASN:HD22	2.16	0.53
13:M:27:LEU:HD12	13:M:36:PHE:O	2.08	0.53
10:X:3:ILE:HG12	10:X:136:SER:OG	2.09	0.53
14:b:14:LEU:HD11	14:b:100:ALA:HB3	1.91	0.53
13:a:37:ASN:HB2	14:b:135:TYR:CE2	2.41	0.53
6:T:2:THR:N	20:T:301:HOH:O	2.42	0.53
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.91	0.53
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.90	0.52
11:Y:209:ASN:HD22	11:Y:209:ASN:N	2.04	0.52
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.07	0.52
7:U:68:ARG:O	7:U:223:LYS:HA	2.10	0.52
12:Z:4:PRO:O	13:a:104:ARG:NH1	2.38	0.52
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.92	0.52
11:Y:73:ARG:NH2	11:Y:73:ARG:CB	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:38:ASN:C	3:Q:38:ASN:HD22	2.17	0.51
13:M:159:VAL:HG23	13:M:159:VAL:O	2.09	0.51
14:N:3:ILE:HD13	14:N:46:SER:HB3	1.92	0.51
11:K:209:ASN:OD1	10:X:130:TYR:OH	2.29	0.51
11:Y:35:ILE:HG23	11:Y:37:ILE:CG1	2.40	0.51
14:N:148:LYS:NZ	14:N:184:GLU:OE2	2.32	0.51
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.46	0.50
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.59	0.50
10:J:168:LEU:O	10:J:172:MET:HB2	2.10	0.50
13:a:159:VAL:HG23	13:a:159:VAL:O	2.11	0.50
11:Y:35:ILE:HG23	11:Y:37:ILE:HG13	1.93	0.50
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.42	0.50
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.27	0.50
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.57	0.50
14:b:148:LYS:NZ	14:b:184:GLU:OE2	2.34	0.50
12:L:8:ASN:HA	12:L:30:ILE:O	2.12	0.49
10:J:145:ASP:HB3	11:Y:207:PHE:CE2	2.47	0.49
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.94	0.49
13:a:36:PHE:HA	14:b:135:TYR:HB2	1.93	0.49
12:L:147:MET:N	12:L:148:PRO:HD2	2.27	0.49
7:U:78:ILE:N	7:U:79:PRO:CD	2.75	0.49
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.94	0.49
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.47	0.49
11:Y:99:THR:HG22	11:Y:115:VAL:HB	1.95	0.49
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.95	0.49
11:K:167:ARG:NH1	10:X:141:PHE:CD1	2.81	0.49
5:E:9:THR:HG21	5:E:119:THR:HA	1.95	0.49
7:G:78:ILE:N	7:G:79:PRO:CD	2.76	0.49
13:M:27:LEU:HB2	13:M:192:SER:HB3	1.95	0.49
8:V:49:ALA:HA	15:g:3:A1I49:C24	2.43	0.49
14:N:124:TYR:OH	14:N:136:GLY:O	2.24	0.48
1:O:55:LEU:HB3	7:U:159:ALA:O	2.13	0.48
13:a:27:LEU:HB2	13:a:192:SER:HB3	1.95	0.48
15:i:3:A1I49:N	15:i:3:A1I49:O28	2.45	0.48
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.95	0.48
5:S:9:THR:HG21	5:S:119:THR:HA	1.95	0.48
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.43	0.48
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.95	0.48
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.78	0.48
5:E:65:CYS:SG	5:E:71:LEU:CD1	3.02	0.48
7:U:83:ASN:C	7:U:83:ASN:HD22	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:168:LEU:O	10:X:172:MET:HB2	2.13	0.48
13:a:30:TYR:CB	13:a:34:LEU:HB2	2.43	0.48
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.62	0.48
10:J:149:ARG:NH1	20:J:203:HOH:O	2.47	0.48
11:Y:35:ILE:CG2	11:Y:37:ILE:HG13	2.44	0.48
13:M:48:ASN:H	13:M:48:ASN:HD22	1.59	0.48
14:N:2:SER:HB3	14:N:128:VAL:HG23	1.96	0.48
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.14	0.48
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.96	0.47
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.96	0.47
11:K:36:GLU:O	11:K:41:LEU:O	2.33	0.47
14:N:135:TYR:HD1	14:N:136:GLY:CA	2.27	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.14	0.47
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.96	0.47
10:J:135:TYR:HA	10:J:138:PHE:HD1	1.80	0.47
13:a:48:ASN:H	13:a:48:ASN:HD22	1.62	0.47
7:G:73:VAL:HG12	7:G:133:THR:HB	1.96	0.46
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.51	0.46
14:b:135:TYR:HD1	14:b:136:GLY:CA	2.27	0.46
7:G:34:LEU:C	7:G:34:LEU:HD23	2.40	0.46
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.96	0.46
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.96	0.46
8:V:22:GLN:HB2	15:g:1:VGL:H3	1.97	0.46
11:K:12:ILE:HG23	11:K:112:ILE:HD11	1.97	0.46
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.97	0.46
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.97	0.46
13:M:27:LEU:CD1	13:M:36:PHE:O	2.63	0.46
11:Y:35:ILE:CG2	11:Y:37:ILE:CG1	2.93	0.46
11:Y:45:MET:HB3	11:Y:52:CYS:HB3	1.98	0.46
14:b:2:SER:N	15:i:3:A1I49:CG2	2.79	0.46
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.51	0.46
11:K:6:PHE:HA	11:K:125:ASP:O	2.16	0.46
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.16	0.46
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.63	0.46
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.64	0.46
14:b:124:TYR:OH	14:b:136:GLY:O	2.24	0.46
2:P:101:TYR:CE1	10:X:75:LEU:HD21	2.51	0.45
2:P:86:LEU:HB3	2:P:114:LEU:HD21	1.98	0.45
7:U:78:ILE:HG22	7:U:79:PRO:HD3	1.99	0.45
11:Y:52:CYS:SG	11:Y:97:MET:HG2	2.56	0.45
20:a:404:HOH:O	14:b:116:GLY:HA3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.97	0.45
7:G:78:ILE:HG22	7:G:79:PRO:HD3	1.98	0.45
1:O:119:GLN:O	1:O:122:THR:HB	2.16	0.45
13:a:179:ASN:HD22	13:a:182:ARG:HH11	1.64	0.45
12:L:110:ILE:HD11	12:L:137:ARG:HG3	1.98	0.45
14:N:65:LEU:HG	14:N:69:GLN:HE21	1.81	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.45
10:X:174:MET:SD	10:X:174:MET:N	2.88	0.45
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.46	0.45
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.97	0.45
2:B:220:ASN:OD1	2:B:220:ASN:N	2.50	0.45
12:Z:54:ALA:C	12:Z:107:VAL:HG22	2.42	0.45
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.46	0.45
7:G:83:ASN:C	7:G:83:ASN:HD22	2.25	0.45
8:V:210:THR:HG21	9:W:167:SER:HB3	1.98	0.45
11:Y:12:ILE:HG23	11:Y:112:ILE:HD11	1.98	0.45
14:b:65:LEU:HG	14:b:69:GLN:HE21	1.82	0.45
6:T:158:GLY:O	7:U:54:LEU:HB3	2.17	0.45
11:Y:73:ARG:HH22	11:Y:105:THR:HG22	1.82	0.45
8:H:102:GLY:HA2	8:H:178:MET:SD	2.58	0.44
7:U:73:VAL:HG12	7:U:133:THR:HB	1.98	0.44
11:Y:209:ASN:H	11:Y:209:ASN:ND2	2.07	0.44
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.17	0.44
8:H:199:LYS:HE3	9:I:151:SER:O	2.17	0.44
14:N:140:LYS:HD2	14:N:140:LYS:HA	1.54	0.44
7:U:34:LEU:C	7:U:34:LEU:HD23	2.42	0.44
11:Y:73:ARG:HH21	11:Y:73:ARG:CB	2.26	0.44
13:a:63:ILE:HD13	13:a:114:ILE:HD11	1.99	0.44
13:a:37:ASN:HB2	14:b:135:TYR:HE2	1.73	0.44
15:f:2:PHE:N	15:f:2:PHE:CD1	2.85	0.44
6:F:158:GLY:O	7:G:54:LEU:HB3	2.18	0.44
2:B:86:LEU:HB3	2:B:114:LEU:HD21	1.99	0.44
11:K:4:LEU:C	11:K:4:LEU:CD2	2.91	0.44
14:N:3:ILE:CD1	14:N:46:SER:HB3	2.48	0.44
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.32	0.44
11:Y:2:THR:OG1	11:Y:132:GLY:HA3	2.18	0.43
3:C:201:VAL:O	3:C:202:GLN:CB	2.67	0.43
7:G:66:ILE:HG21	7:G:108:LEU:HD21	1.99	0.43
8:H:114:HIS:HB3	20:H:312:HOH:O	2.17	0.43
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.83	0.43
13:M:63:ILE:HD13	13:M:114:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.47	0.43
14:b:140:LYS:HD2	14:b:140:LYS:HA	1.54	0.43
10:J:174:MET:SD	10:J:174:MET:N	2.90	0.43
7:U:83:ASN:C	7:U:83:ASN:ND2	2.75	0.43
14:b:13:ILE:HG21	14:b:175:MET:HE2	2.00	0.43
3:C:201:VAL:HG13	3:C:202:GLN:N	2.33	0.43
12:Z:141:ALA:HB1	12:Z:195:HIS:NE2	2.33	0.43
14:N:3:ILE:HG23	15:f:3:A1I49:CG2	2.48	0.43
5:S:92:ASN:CG	12:Z:70:ASN:HD21	2.26	0.43
10:X:75:LEU:HD12	10:X:75:LEU:HA	1.91	0.43
7:G:83:ASN:C	7:G:83:ASN:ND2	2.77	0.43
2:P:220:ASN:OD1	2:P:220:ASN:N	2.51	0.43
9:W:123:PHE:HA	9:W:128:CYS:O	2.18	0.43
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	2.00	0.43
11:K:99:THR:CG2	11:K:115:VAL:HB	2.48	0.43
1:A:119:GLN:O	1:A:122:THR:HB	2.19	0.43
10:J:50:ALA:O	11:K:91:LYS:NZ	2.51	0.43
10:J:145:ASP:HB3	11:Y:207:PHE:CD2	2.53	0.43
12:L:141:ALA:HB1	12:L:195:HIS:NE2	2.33	0.43
11:Y:176:ASN:HD21	11:Y:190:ASN:HD22	1.66	0.43
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.54	0.42
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.54	0.42
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.92	0.42
14:b:165:TRP:O	14:b:165:TRP:CG	2.72	0.42
1:A:115:ALA:HB1	1:A:154:GLY:O	2.19	0.42
14:N:89:ASN:HB2	14:N:93:LEU:HD12	2.00	0.42
14:b:89:ASN:HB2	14:b:93:LEU:HD12	2.01	0.42
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.66	0.42
11:Y:35:ILE:HG22	11:Y:35:ILE:O	2.20	0.42
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.84	0.42
14:N:83:LYS:HB2	14:N:119:VAL:HG22	2.00	0.42
5:S:77:ALA:N	5:S:78:PRO:CD	2.82	0.42
8:V:21:THR:O	15:g:2:PHE:HB2	2.19	0.42
11:Y:4:LEU:C	11:Y:100:MET:HE1	2.43	0.42
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD3	2.02	0.42
11:K:4:LEU:HD22	11:K:4:LEU:O	2.19	0.42
5:S:65:CYS:SG	5:S:71:LEU:CD1	3.08	0.42
5:S:71:LEU:C	5:S:71:LEU:CD2	2.93	0.42
14:b:83:LYS:HB2	14:b:119:VAL:HG22	2.01	0.42
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:71:LEU:C	5:S:71:LEU:HD22	2.45	0.42
8:V:199:LYS:HE3	9:W:151:SER:O	2.20	0.42
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.45	0.42
3:C:156:SER:O	4:D:51:LEU:HD12	2.20	0.42
5:E:77:ALA:N	5:E:78:PRO:CD	2.83	0.42
12:L:1:GLN:HE21	13:M:1:THR:HG21	1.85	0.42
1:O:115:ALA:HB1	1:O:154:GLY:O	2.19	0.42
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.19	0.42
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.00	0.42
11:K:86:LEU:C	11:K:86:LEU:HD13	2.44	0.42
5:E:71:LEU:C	5:E:71:LEU:CD2	2.93	0.41
13:M:48:ASN:HD22	13:M:48:ASN:N	2.17	0.41
11:Y:199:LYS:O	11:Y:203:GLU:HG3	2.20	0.41
13:a:96:LEU:O	13:a:100:MET:HG2	2.19	0.41
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.02	0.41
5:E:71:LEU:C	5:E:71:LEU:HD22	2.45	0.41
8:H:106:THR:O	8:H:106:THR:HG22	2.20	0.41
13:M:30:TYR:HB3	13:M:31:GLY:H	1.54	0.41
13:M:37:ASN:HB2	14:N:135:TYR:HE2	1.73	0.41
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	2.02	0.41
12:Z:152:ASN:O	12:Z:156:PHE:HA	2.19	0.41
10:J:3:ILE:HD12	10:J:176:PHE:CD2	2.55	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.41
5:E:38:ARG:NH1	5:E:39:SER:O	2.53	0.41
11:K:158:LYS:HB2	11:K:177:LEU:HD11	2.02	0.41
13:M:96:LEU:O	13:M:100:MET:HG2	2.21	0.41
12:L:145:LEU:O	9:W:147:GLY:HA3	2.20	0.41
5:S:10:VAL:CG2	6:T:125:VAL:C	2.94	0.41
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.51	0.41
11:K:5:ALA:HA	11:K:13:ILE:O	2.21	0.41
11:Y:41:LEU:HD23	11:Y:41:LEU:HA	1.87	0.41
10:X:92:ILE:HD12	10:X:92:ILE:HA	1.97	0.41
3:C:161:THR:HG21	3:C:169:VAL:HG13	2.02	0.41
8:H:210:THR:HG21	9:I:167:SER:HB3	2.02	0.41
11:K:73:ARG:HH22	11:K:105:THR:HG22	1.85	0.41
11:K:209:ASN:O	9:W:37:ASN:ND2	2.53	0.41
12:L:152:ASN:O	12:L:156:PHE:HA	2.21	0.41
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.55	0.41
10:X:3:ILE:HD12	10:X:176:PHE:CD2	2.56	0.41
10:X:101:ASN:HB3	10:X:133:HIS:CD2	2.56	0.41
9:I:123:PHE:HA	9:I:128:CYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:38:ASN:OD1	11:K:38:ASN:C	2.64	0.41
11:Y:5:ALA:CB	11:Y:100:MET:CE	2.99	0.41
13:a:39:VAL:HG11	13:a:57:ILE:HD12	2.03	0.41
10:J:173:PRO:HD3	10:X:25:ILE:O	2.21	0.40
3:Q:77:ASN:HD22	3:Q:77:ASN:N	2.19	0.40
5:S:68:HIS:HE1	5:S:102:LEU:O	2.04	0.40
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.64	0.40
4:D:32:ILE:HD12	4:D:192:VAL:HG23	2.03	0.40
13:M:10:SER:HB3	13:M:147:GLY:H	1.87	0.40
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.56	0.40
13:a:129:TYR:O	13:a:136:THR:HA	2.22	0.40
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.55	0.40
5:E:68:HIS:HE1	5:E:102:LEU:O	2.04	0.40
6:F:123:ASN:HD22	6:F:124:SER:N	2.19	0.40
7:G:72:MET:HE3	7:G:74:VAL:CG2	2.52	0.40
10:J:144:LEU:HD12	10:J:144:LEU:HA	1.93	0.40
4:R:32:ILE:HD12	4:R:192:VAL:HG23	2.02	0.40
3:C:77:ASN:HD22	3:C:77:ASN:N	2.18	0.40
5:E:92:ASN:CG	12:L:70:ASN:HD21	2.30	0.40
6:F:41:GLY:HA3	6:F:215:CYS:O	2.21	0.40
13:M:119:VAL:HG23	13:M:200:ILE:HG22	2.03	0.40
11:Y:4:LEU:CD1	11:Y:161:ILE:HD11	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	240 (97%)	8 (3%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	16	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	16	37
3	C	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	25
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	25
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
7	G	239/252 (95%)	229 (96%)	10 (4%)	0	100	100
7	U	239/252 (95%)	229 (96%)	10 (4%)	0	100	100
8	H	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
8	V	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	209/211 (99%)	205 (98%)	3 (1%)	1 (0%)	24	48
11	Y	209/211 (99%)	205 (98%)	2 (1%)	2 (1%)	12	32
12	L	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
12	Z	221/222 (100%)	218 (99%)	3 (1%)	0	100	100
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	30	54
14	N	193/195 (99%)	185 (96%)	8 (4%)	0	100	100
14	b	193/195 (99%)	185 (96%)	8 (4%)	0	100	100
All	All	6271/6608 (95%)	6082 (97%)	175 (3%)	14 (0%)	43	68

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL

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Mol	Chain	Res	Type
3	Q	202	GLN
11	Y	211	ILE
3	C	205	ALA
3	Q	205	ALA
3	C	239	GLN
3	Q	239	GLN
11	Y	37	ILE
2	B	221	ASP
11	K	37	ILE
2	P	221	ASP
13	a	31	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	204 (98%)	5 (2%)	43	72
1	O	209/209 (100%)	204 (98%)	5 (2%)	43	72
2	B	203/216 (94%)	195 (96%)	8 (4%)	28	57
2	P	203/216 (94%)	195 (96%)	8 (4%)	28	57
3	C	212/226 (94%)	205 (97%)	7 (3%)	33	63
3	Q	212/226 (94%)	205 (97%)	7 (3%)	33	63
4	D	194/215 (90%)	186 (96%)	8 (4%)	27	56
4	R	194/215 (90%)	186 (96%)	8 (4%)	27	56
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	64
5	S	190/193 (98%)	185 (97%)	5 (3%)	40	70
6	F	201/239 (84%)	194 (96%)	7 (4%)	32	61
6	T	201/239 (84%)	194 (96%)	7 (4%)	32	61
7	G	206/210 (98%)	198 (96%)	8 (4%)	28	57
7	U	206/210 (98%)	195 (95%)	11 (5%)	20	46
8	H	180/189 (95%)	173 (96%)	7 (4%)	28	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	180/189 (95%)	173 (96%)	7 (4%)	28	57
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	84
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	84
10	J	173/175 (99%)	165 (95%)	8 (5%)	24	51
10	X	173/175 (99%)	165 (95%)	8 (5%)	24	51
11	K	168/168 (100%)	159 (95%)	9 (5%)	20	45
11	Y	168/168 (100%)	157 (94%)	11 (6%)	15	37
12	L	185/185 (100%)	178 (96%)	7 (4%)	29	58
12	Z	186/185 (100%)	179 (96%)	7 (4%)	29	58
13	M	199/208 (96%)	192 (96%)	7 (4%)	32	61
13	a	199/208 (96%)	189 (95%)	10 (5%)	22	48
14	N	162/162 (100%)	149 (92%)	13 (8%)	11	28
14	b	162/162 (100%)	152 (94%)	10 (6%)	16	39
15	d	1/1 (100%)	1 (100%)	0	100	100
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
15	g	1/1 (100%)	1 (100%)	0	100	100
15	h	1/1 (100%)	1 (100%)	0	100	100
15	i	1/1 (100%)	1 (100%)	0	100	100
All	All	5315/5542 (96%)	5107 (96%)	208 (4%)	28	57

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	114	LEU
2	B	184	LYS

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Mol	Chain	Res	Type
2	B	191	LEU
2	B	220	ASN
3	C	4	ARG
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	197	LYS
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	95	SER
5	E	188	LEU
6	F	68	ARG
6	F	94	SER
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	206	LYS
6	F	221	ASN
7	G	26	THR
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	7	LYS
8	H	34	LEU
8	H	38	SER
8	H	56	THR

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Mol	Chain	Res	Type
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	23	ARG
10	J	35	THR
10	J	126	VAL
10	J	143	LEU
10	J	144	LEU
10	J	172	MET
10	J	174	MET
10	J	193	ASP
11	K	4	LEU
11	K	9	GLN
11	K	38	ASN
11	K	67	GLU
11	K	73	ARG
11	K	99	THR
11	K	148	LEU
11	K	210	VAL
11	K	211	ILE
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	107	VAL
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
13	M	10	SER
13	M	29	SER
13	M	37	ASN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
14	N	2	SER
14	N	3	ILE
14	N	9	LYS
14	N	13	ILE
14	N	14	LEU
14	N	22	THR

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Mol	Chain	Res	Type
14	N	94	THR
14	N	119	VAL
14	N	129	SER
14	N	135	TYR
14	N	139	ASP
14	N	140	LYS
14	N	178	LEU
1	O	17	LYS
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
2	P	220	ASN
3	Q	4	ARG
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	197	LYS
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	188	LEU
6	T	68	ARG
6	T	94	SER

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Mol	Chain	Res	Type
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	206	LYS
6	T	221	ASN
7	U	26	THR
7	U	59	THR
7	U	63	ILE
7	U	67	SER
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	7	LYS
8	V	34	LEU
8	V	38	SER
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	23	ARG
10	X	35	THR
10	X	126	VAL
10	X	143	LEU
10	X	144	LEU
10	X	172	MET
10	X	174	MET
10	X	193	ASP
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	38	ASN
11	Y	41	LEU
11	Y	67	GLU
11	Y	71	LYS
11	Y	76	VAL
11	Y	99	THR

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Mol	Chain	Res	Type
11	Y	209	ASN
11	Y	211	ILE
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	130	SER
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	3	GLN
13	a	10	SER
13	a	29	SER
13	a	30	TYR
13	a	32	SER
13	a	37	ASN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
14	b	9	LYS
14	b	13	ILE
14	b	22	THR
14	b	94	THR
14	b	119	VAL
14	b	131	SER
14	b	135	TYR
14	b	139	ASP
14	b	140	LYS
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
2	B	20	GLN
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	176	GLN

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Mol	Chain	Res	Type
2	B	232	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	106	GLN
4	D	160	ASN
4	D	198	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	147	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	143	HIS
6	F	178	HIS
6	F	191	GLN
6	F	203	ASN
6	F	240	GLN
7	G	6	HIS
7	G	30	ASN
7	G	83	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	231	ASN
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS

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Mol	Chain	Res	Type
8	H	86	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	31	GLN
9	I	44	HIS
9	I	88	GLN
9	I	168	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	78	GLN
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	153	GLN
12	L	158	ASN
12	L	165	ASN
12	L	197	GLN
13	M	2	GLN
13	M	18	ASN
13	M	26	ASN
13	M	37	ASN
13	M	48	ASN
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	69	GLN
1	O	149	GLN
2	P	20	GLN
2	P	93	HIS
2	P	95	GLN

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Mol	Chain	Res	Type
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	160	ASN
4	R	198	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	147	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	143	HIS
6	T	178	HIS
6	T	191	GLN
6	T	203	ASN
6	T	240	GLN
7	U	6	HIS
7	U	30	ASN
7	U	83	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN

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Mol	Chain	Res	Type
7	U	175	ASN
7	U	231	ASN
8	V	30	ASN
8	V	57	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	31	GLN
9	W	37	ASN
9	W	44	HIS
9	W	88	GLN
9	W	168	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	133	HIS
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
11	Y	209	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	94	GLN
12	Z	153	GLN
12	Z	158	ASN
13	a	18	ASN
13	a	26	ASN
13	a	37	ASN
13	a	48	ASN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	69	GLN
14	b	145	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](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	SO4	g	101	-	4,4,4	0.32	0	6,6,6	0.08	0
18	MES	a	301	-	12,12,12	0.71	0	15,16,16	0.30	0
19	SO4	d	101	-	4,4,4	0.34	0	6,6,6	0.07	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
18	MES	a	301	-	-	1/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	a	301	MES	N4-C7-C8-S

There are no ring outliers.

No monomer is involved in short contacts.

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	250/250 (100%)	-0.56	1 (0%) 88 87	48, 62, 92, 148	0
1	O	250/250 (100%)	-0.53	3 (1%) 76 75	52, 69, 106, 141	0
2	B	244/258 (94%)	-0.41	3 (1%) 76 75	48, 67, 110, 155	0
2	P	244/258 (94%)	-0.36	3 (1%) 76 75	53, 71, 119, 159	0
3	C	240/254 (94%)	-0.46	1 (0%) 88 87	50, 72, 124, 147	0
3	Q	240/254 (94%)	-0.36	4 (1%) 69 67	53, 81, 141, 171	0
4	D	235/260 (90%)	-0.53	0 100 100	52, 72, 101, 125	0
4	R	235/260 (90%)	-0.48	1 (0%) 88 87	52, 73, 105, 134	0
5	E	231/234 (98%)	-0.42	0 100 100	54, 73, 104, 135	0
5	S	231/234 (98%)	-0.35	1 (0%) 88 87	54, 77, 114, 135	0
6	F	243/288 (84%)	-0.47	0 100 100	46, 67, 108, 132	0
6	T	243/288 (84%)	-0.46	0 100 100	46, 73, 117, 137	0
7	G	241/252 (95%)	-0.60	0 100 100	46, 62, 90, 120	0
7	U	241/252 (95%)	-0.58	0 100 100	50, 64, 95, 118	0
8	H	221/231 (95%)	-0.61	0 100 100	46, 57, 80, 104	0
8	V	221/231 (95%)	-0.60	0 100 100	47, 60, 81, 121	0
9	I	204/205 (99%)	-0.68	0 100 100	43, 58, 79, 111	0
9	W	204/205 (99%)	-0.71	0 100 100	44, 59, 86, 111	0
10	J	195/198 (98%)	-0.55	1 (0%) 87 86	44, 60, 84, 117	0
10	X	195/198 (98%)	-0.53	1 (0%) 87 86	47, 62, 83, 127	0
11	K	211/211 (100%)	-0.61	0 100 100	45, 59, 86, 166	0
11	Y	211/211 (100%)	-0.55	2 (0%) 81 80	46, 59, 91, 148	0
12	L	222/222 (100%)	-0.61	0 100 100	45, 60, 89, 106	0
12	Z	222/222 (100%)	-0.58	1 (0%) 87 86	38, 58, 86, 98	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.63	1 (0%) 88 87	44, 61, 83, 104	0
13	a	233/246 (94%)	-0.64	1 (0%) 88 87	43, 59, 79, 104	0
14	N	195/195 (100%)	-0.50	1 (0%) 87 86	42, 58, 109, 146	0
14	b	195/195 (100%)	-0.46	2 (1%) 79 78	46, 59, 104, 155	0
15	d	1/3 (33%)	-0.48	0 100 100	59, 59, 59, 59	0
15	e	1/3 (33%)	-1.21	0 100 100	50, 50, 50, 50	0
15	f	1/3 (33%)	0.87	0 100 100	72, 72, 72, 72	0
15	g	1/3 (33%)	-0.43	0 100 100	63, 63, 63, 63	0
15	h	1/3 (33%)	-0.68	0 100 100	57, 57, 57, 57	0
15	i	1/3 (33%)	1.02	0 100 100	77, 77, 77, 77	0
All	All	6336/6626 (95%)	-0.53	27 (0%) 88 87	38, 64, 105, 171	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	3.7
3	Q	50	LEU	3.6
3	Q	205	ALA	3.3
2	P	219	ALA	3.2
2	P	51	VAL	3.0
4	R	113	LEU	2.9
2	B	51	VAL	2.7
10	X	1	MET	2.7
3	Q	204	GLY	2.7
5	S	122	TYR	2.5
11	Y	211	ILE	2.5
3	Q	49	THR	2.5
1	O	2	THR	2.4
14	b	196	LEU	2.4
14	N	165	TRP	2.4
3	C	205	ALA	2.4
10	J	1	MET	2.3
11	Y	212	GLY	2.3
12	Z	108[A]	HIS	2.3
1	A	1	MET	2.2
2	P	52	THR	2.2
2	B	218	GLY	2.2
14	b	138	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	1	MET	2.1
13	M	69	ASP	2.1
13	a	36	PHE	2.1
1	O	4	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
16	MG	Z	301	1/1	0.75	0.35	173,173,173,173	0
17	CL	G	302	1/1	0.81	0.22	30,30,30,30	0
18	MES	a	301	12/12	0.87	0.16	133,143,149,153	0
17	CL	b	201	1/1	0.95	0.07	87,87,87,87	0
16	MG	V	301	1/1	0.95	0.10	120,120,120,120	0
16	MG	I	301	1/1	0.96	0.10	112,112,112,112	0
17	CL	N	201	1/1	0.96	0.09	76,76,76,76	0
16	MG	G	301	1/1	0.97	0.06	88,88,88,88	0
17	CL	U	301	1/1	0.97	0.04	73,73,73,73	0
19	SO4	g	101	5/5	0.97	0.16	94,101,109,111	0
19	SO4	d	101	5/5	0.98	0.13	101,102,106,107	0
17	CL	G	303	1/1	0.99	0.04	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.