



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2025 – 11:19 am BST

PDB ID : 9QBE / pdb_00009qbe
Title : Yeast 20S proteasome mutant: beta5_T3M in complex with ONX0914
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-03-02
Resolution : 2.80 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

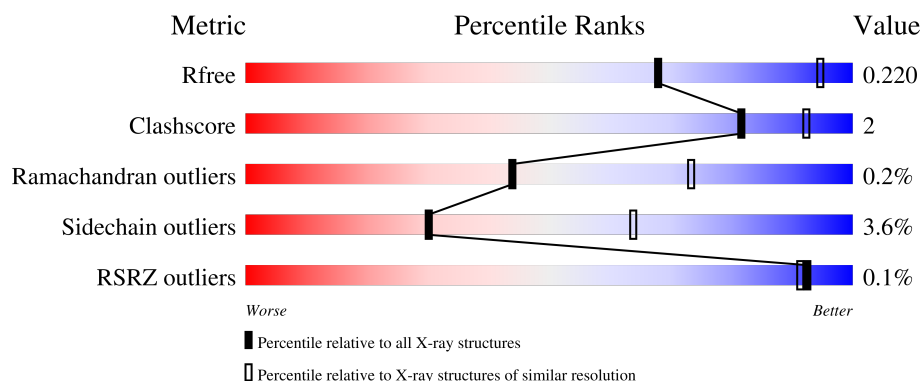
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.






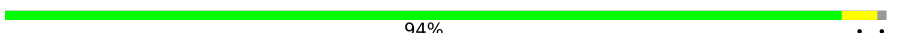














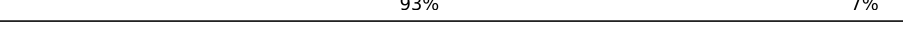






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	250	<div><div></div><div>95%</div><div>.</div></div>
1	O	250	<div><div></div><div>95%</div><div>5%</div></div>
2	B	258	<div><div></div><div>%</div><div>87%</div><div>7%</div><div>5%</div></div>
2	P	258	<div><div></div><div>89%</div><div>5%</div><div>5%</div></div>
3	C	254	<div><div></div><div>87%</div><div>5%</div><div>6%</div></div>

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Mol	Chain	Length	Quality of chain
3	Q	254	 89% . . 6%
4	D	260	 82% 8% 10%
4	R	260	 84% 6% 10%
5	E	234	 94% . .
5	S	234	 94% . .
6	F	288	 81% . . 16%
6	T	288	 81% . . 16%
7	G	252	 89% 6% .
7	U	252	 90% 6% .
8	H	231	 88% 6% . .
8	V	231	 88% 6% . .
9	I	205	 91% 8% .
9	W	205	 90% 8% .
10	J	198	 % 90% 6% . .
10	X	198	 % 89% 8% . .
11	K	211	 83% 15% .
11	Y	211	 82% 16% .
12	L	222	 93% 7%
12	Z	222	 91% 9%
13	M	246	 87% 6% . 5%
13	a	246	 87% 7% 5%
14	N	195	 91% 9%
14	b	195	 91% 9%
15	e	4	 50% 50%
15	f	4	 25% 50% 25%

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Mol	Chain	Length	Quality of chain
15	g	4	
15	h	4	
15	i	4	
15	j	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	00E	e	1	-	-	X	-
15	0A1	e	3	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49833 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
			1638	1042	279	309	8			
11	Y	211	Total	C	N	O	S	0	0	0
			1638	1042	279	309	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	3	MET	THR	engineered mutation	UNP P30656
Y	3	MET	THR	engineered mutation	UNP P30656

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			
14	b	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			

- 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	e	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	f	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	g	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	h	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	i	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	j	4	Total	C	N	O	0	0	0
			49	35	5	9			

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

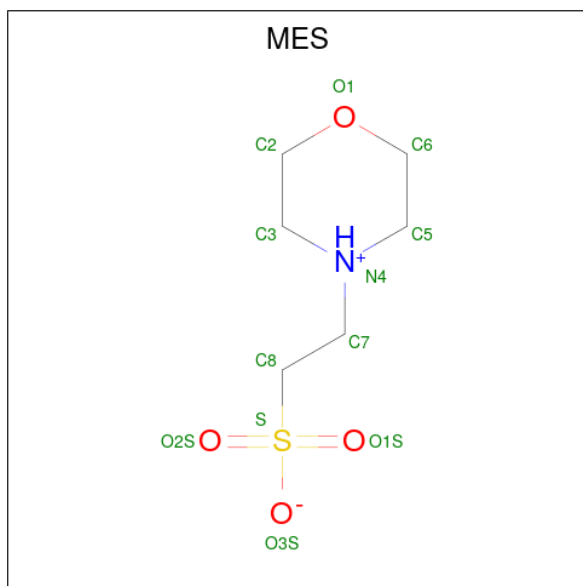
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	I	1	Total	Mg	0	0
			1	1		
16	K	2	Total	Mg	0	0
			2	2		
16	N	1	Total	Mg	0	0
			1	1		
16	V	1	Total	Mg	0	0
			1	1		
16	X	1	Total	Mg	0	0
			1	1		
16	Y	2	Total	Mg	0	0
			2	2		
16	Z	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total	Cl	0	0
			1	1		
17	U	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	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	h	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	7	Total	O	0	0
			7	7		
19	B	11	Total	O	0	0
			11	11		
19	C	8	Total	O	0	0
			8	8		
19	D	5	Total	O	0	0
			5	5		
19	E	6	Total	O	0	0
			6	6		
19	F	7	Total	O	0	0
			7	7		
19	G	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	H	11	Total O 11 11	0	0
19	I	4	Total O 4 4	0	0
19	J	15	Total O 15 15	0	0
19	K	5	Total O 5 5	0	0
19	L	12	Total O 12 12	0	0
19	M	13	Total O 13 13	0	0
19	N	8	Total O 8 8	0	0
19	O	5	Total O 5 5	0	0
19	P	7	Total O 7 7	0	0
19	Q	5	Total O 5 5	0	0
19	R	10	Total O 10 10	0	0
19	S	4	Total O 4 4	0	0
19	T	6	Total O 6 6	0	0
19	U	12	Total O 12 12	0	0
19	V	8	Total O 8 8	0	0
19	W	3	Total O 3 3	0	0
19	X	9	Total O 9 9	0	0
19	Y	2	Total O 2 2	0	0
19	Z	7	Total O 7 7	0	0
19	a	8	Total O 8 8	0	0
19	b	9	Total O 9 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	g	2	Total	O	0	0
			2	2		
19	j	2	Total	O	0	0
			2	2		

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:  95%




- Molecule 1: Proteasome subunit alpha type-2

Chain O:  95%




- Molecule 2: Proteasome subunit alpha type-3

Chain B:  87% 7% 5%



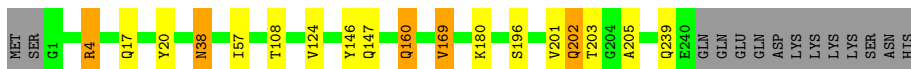
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  89% 5% 5%



- Molecule 3: Proteasome subunit alpha type-4

Chain C:  87% 5% 6%



- Molecule 3: Proteasome subunit alpha type-4

[illegible]

- | | |
|-----|------|
| GLU | MET |
| GLU | PHE |
| ALA | LEU |
| ASP | THR |
| VAL | ARG |
| GLI | SER |
| MET | GLU |
| SER | TRP |
| | D1 |
| | R2 |
| | L20 |
| | K24 |
| | L40 |
| | L51 |
| | V60 |
| | A88 |
| | H91 |
| | I99 |
| | L104 |
| | L113 |
| | E117 |
| | GLY |
| | ALA |
| | SER |
| | GLY |
| | GLU |
| | GLU |
| | ARG |
| | L125 |
| | N160 |
| | S166 |
| | L176 |
| | W179 |
| | L193 |
| | K197 |
| | T214 |
| | K236 |
| | E242 |
| | SER |

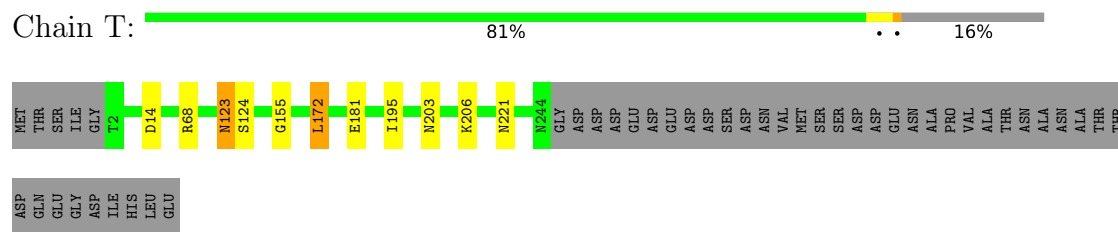
- [illegible]

-
- Sequence logo for the 12th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis lists amino acids: MET, PHE, ARG, N3, T9, L25, K29, E54, L71, A77, P78, L87, F98, A107, L188, and I233. MET, PHE, and ARG are greyed out. N3, T9, L25, K29, E54, L71, A77, P78, L87, F98, A107, L188, and I233 are yellow. L71 is highlighted in orange.

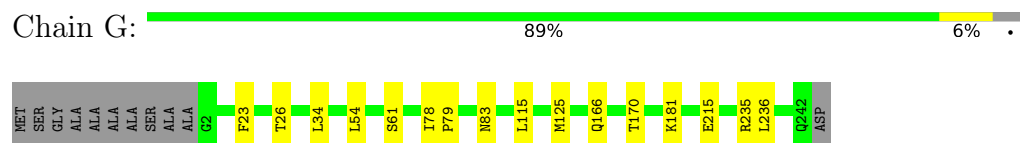
-
- | Amino Acid | Relative Abundance (%) |
|------------|------------------------|
| MET | 100 |
| PHE | 100 |
| ARG | 100 |
| N3 | 25 |
| T9 | 100 |
| L25 | 100 |
| K29 | 100 |
| E54 | 100 |
| L71 | 75 |
| A77 | 100 |
| P78 | 100 |
| L87 | 100 |
| F98 | 100 |
| A107 | 100 |
| L188 | 100 |
| I233 | 100 |

- [illegible]

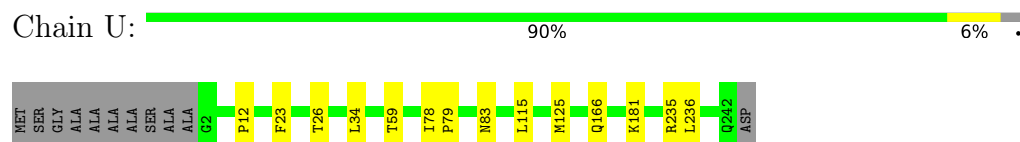
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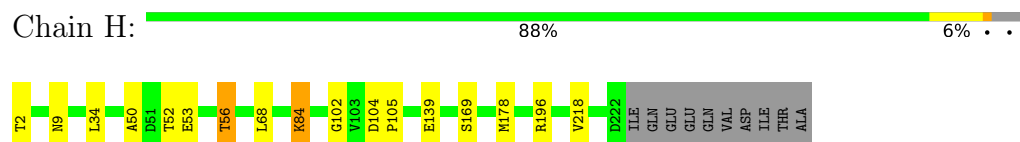
- Molecule 7: Proteasome subunit alpha type-1



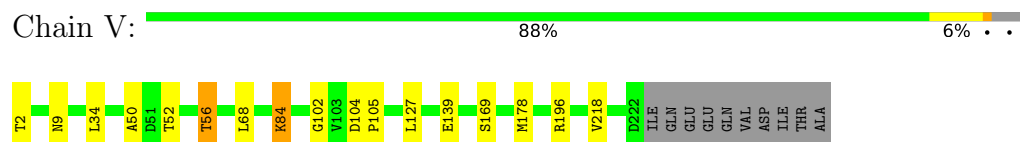
- Molecule 7: Proteasome subunit alpha type-1



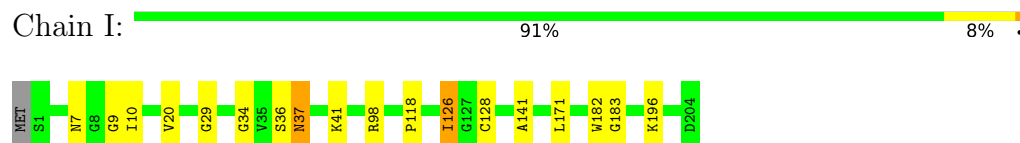
- Molecule 8: Proteasome subunit beta type-2



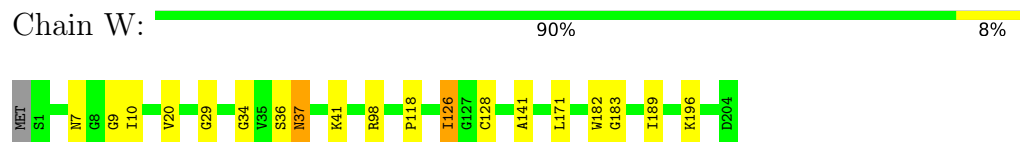
- Molecule 8: Proteasome subunit beta type-2



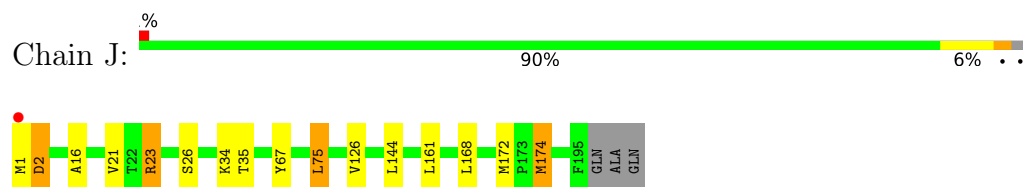
- Molecule 9: Proteasome subunit beta type-3



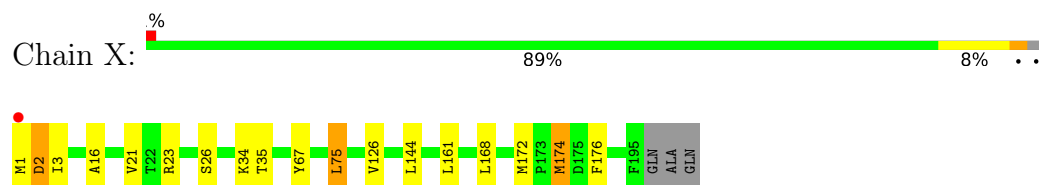
- Molecule 9: Proteasome subunit beta type-3



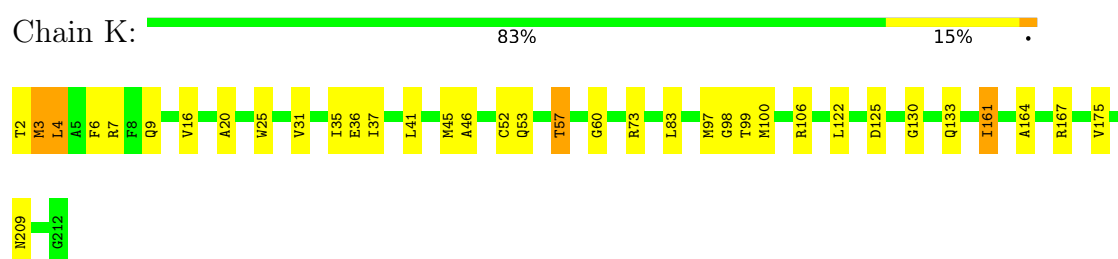
- Molecule 10: Proteasome subunit beta type-4



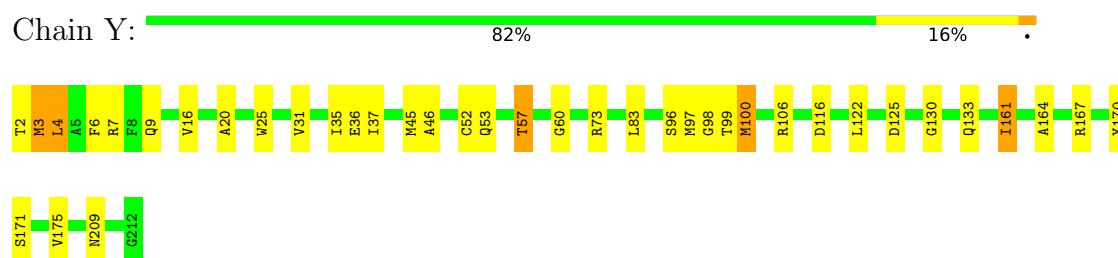
- Molecule 10: Proteasome subunit beta type-4



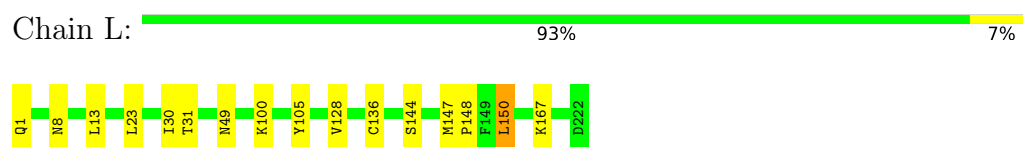
- Molecule 11: Proteasome subunit beta type-5



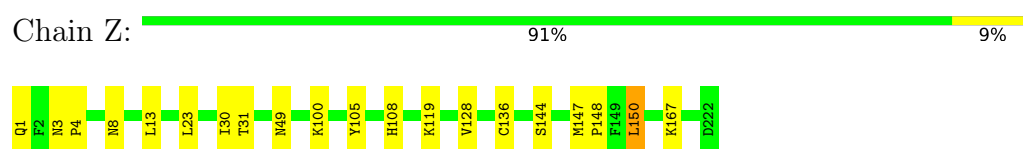
- Molecule 11: Proteasome subunit beta type-5




- Molecule 12: Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6




- Molecule 13: Proteasome subunit beta type-7

Chain M:  87% 6% • 5%



- Molecule 13: Proteasome subunit beta type-7

Chain a:  87% 7% 5%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  91% 9%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  91% 9%



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

Chain e:  50% 50%




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

Chain f:  25% 50% 25%




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

Chain g:  25% 25% 50%



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

Chain h:  25% 25% 50%



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

Chain i:  25% 50% 25%



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

Chain j:  25% 50% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.08Å 299.85Å 145.33Å 90.00° 113.14° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.7 (15.00-2.80) 94.7 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.175 , 0.211 0.172 , 0.220	Depositor DCC
R_{free} test set	12407 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	49833	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: A1I44, MES, 0A1, 00E, MG, CL

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	1.00	0/1952	1.39	0/2642
1	O	1.01	0/1952	1.40	0/2642
2	B	1.00	0/1934	1.40	1/2618 (0.0%)
2	P	1.01	0/1934	1.41	0/2618
3	C	1.00	0/1910	1.43	0/2586
3	Q	1.01	0/1910	1.43	0/2586
4	D	1.01	0/1837	1.42	2/2475 (0.1%)
4	R	1.01	0/1837	1.43	0/2475
5	E	1.01	0/1800	1.41	0/2433
5	S	1.01	0/1800	1.40	0/2433
6	F	0.99	0/1932	1.41	0/2609
6	T	1.00	0/1932	1.41	0/2609
7	G	0.99	0/1945	1.38	0/2634
7	U	0.99	0/1945	1.39	0/2634
8	H	1.00	0/1708	1.36	0/2316
8	V	1.00	0/1708	1.37	0/2316
9	I	0.97	0/1611	1.37	1/2174 (0.0%)
9	W	0.98	0/1611	1.38	1/2174 (0.0%)
10	J	0.98	0/1589	1.38	0/2142
10	X	0.98	0/1589	1.38	0/2142
11	K	0.97	0/1675	1.42	0/2264
11	Y	0.98	0/1675	1.41	0/2264
12	L	0.96	0/1795	1.35	0/2420
12	Z	0.97	0/1795	1.36	2/2420 (0.1%)
13	M	0.98	0/1855	1.37	3/2514 (0.1%)
13	a	0.98	0/1855	1.36	1/2514 (0.0%)
14	N	0.97	0/1534	1.38	0/2077
14	b	0.98	0/1534	1.38	0/2077
15	e	0.95	0/4	1.22	0/4
15	f	0.42	0/4	0.85	0/4
15	g	0.62	0/4	1.22	0/4
15	h	0.65	0/4	1.18	0/4

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	i	0.61	0/4	1.25	0/4
15	j	1.06	0/4	1.83	0/4
All	All	0.99	0/50178	1.39	11/67832 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	35	ARG	N-CA-C	7.04	118.75	111.14
13	M	35	ARG	N-CA-C	6.78	118.32	111.07
9	W	183	GLY	CA-C-O	-5.99	118.33	122.22
9	I	183	GLY	CA-C-O	-5.84	118.42	122.22
12	Z	119	LYS	CA-C-N	5.52	125.22	119.92
12	Z	119	LYS	C-N-CA	5.52	125.22	119.92
2	B	217	LYS	N-CA-C	-5.28	107.38	112.97
13	M	34	LEU	CA-C-N	5.07	127.03	120.44
13	M	34	LEU	C-N-CA	5.07	127.03	120.44
4	D	2	ARG	CA-C-N	5.01	124.86	120.10
4	D	2	ARG	C-N-CA	5.01	124.86	120.10

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	6	0
1	O	1915	0	1929	7	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	13	0
3	Q	1881	0	1895	9	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1773	0	1775	4	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	5	0
8	H	1677	0	1678	9	0
8	V	1677	0	1678	9	0
9	I	1581	0	1574	11	0
9	W	1581	0	1574	12	0
10	J	1561	0	1569	12	0
10	X	1561	0	1569	11	0
11	K	1638	0	1587	29	0
11	Y	1638	0	1587	30	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	8	0
13	M	1824	0	1832	10	0
13	a	1824	0	1832	8	0
14	N	1505	0	1471	9	0
14	b	1505	0	1471	11	0
15	e	49	0	25	6	0
15	f	49	0	25	5	0
15	g	49	0	25	3	0
15	h	49	0	25	2	0
15	i	49	0	25	8	0
15	j	49	0	25	3	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	K	2	0	0	0	0
16	N	1	0	0	0	0
16	V	1	0	0	0	0
16	X	1	0	0	0	0
16	Y	2	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	U	1	0	0	0	0
18	H	12	0	13	0	0
18	K	12	0	13	4	0
18	Y	12	0	13	3	0
18	h	12	0	13	1	0
19	A	7	0	0	0	0
19	B	11	0	0	0	0
19	C	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	5	0	0	0	0
19	E	6	0	0	0	0
19	F	7	0	0	0	0
19	G	12	0	0	0	0
19	H	11	0	0	0	0
19	I	4	0	0	0	0
19	J	15	0	0	0	0
19	K	5	0	0	0	0
19	L	12	0	0	0	0
19	M	13	0	0	1	0
19	N	8	0	0	0	0
19	O	5	0	0	0	0
19	P	7	0	0	0	0
19	Q	5	0	0	0	0
19	R	10	0	0	0	0
19	S	4	0	0	0	0
19	T	6	0	0	0	0
19	U	12	0	0	0	0
19	V	8	0	0	0	0
19	W	3	0	0	0	0
19	X	9	0	0	0	0
19	Y	2	0	0	0	0
19	Z	7	0	0	1	0
19	a	8	0	0	0	0
19	b	9	0	0	0	0
19	g	2	0	0	0	0
19	j	2	0	0	0	0
All	All	49833	0	49214	234	0

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

All (234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.49	0.78
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.49	0.77
11:Y:45:MET:HB3	11:Y:52:CYS:HB3	1.65	0.77
11:K:45:MET:HB3	11:K:52:CYS:HB3	1.66	0.75
15:e:1:00E:HD1A	15:e:3:0A1:CE2	2.21	0.71
15:e:1:00E:HD1A	15:e:3:0A1:HE2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:152:VAL:HA	14:b:175:MET:HE1	1.73	0.69
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.75	0.68
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.75	0.68
14:N:152:VAL:HA	14:N:175:MET:HE1	1.75	0.67
11:K:3:MET:HB2	11:K:16:VAL:HG12	1.76	0.67
8:V:2:THR:HG1	8:V:169:SER:HG	1.38	0.67
11:Y:3:MET:HB2	11:Y:16:VAL:HG12	1.76	0.66
15:f:2:ALA:C	15:f:3:0A1:HD2	2.22	0.65
11:Y:98:GLY:HA3	18:Y:303:MES:H62	1.79	0.64
10:X:1:MET:O	10:X:2:ASP:HB2	1.98	0.63
10:J:1:MET:O	10:J:2:ASP:HB2	1.98	0.62
7:U:23:PHE:O	7:U:26:THR:HB	2.02	0.60
7:G:23:PHE:O	7:G:26:THR:HB	2.02	0.59
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.28	0.58
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.86	0.58
11:K:4:LEU:HD22	11:K:4:LEU:C	2.29	0.57
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.85	0.57
11:Y:130:GLY:HA3	15:i:4:A1I44:O	2.05	0.56
15:e:1:00E:CD1	15:e:3:0A1:HE2	2.36	0.56
12:L:8:ASN:HA	12:L:30:ILE:O	2.06	0.56
13:M:35:ARG:HG2	13:M:36:PHE:CE2	2.41	0.56
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.71	0.55
15:g:3:0A1:C	15:g:4:A1I44:C12	2.84	0.55
15:f:3:0A1:C	15:f:4:A1I44:C12	2.85	0.55
11:K:83:LEU:HD11	11:K:97:MET:HE1	1.89	0.55
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.89	0.55
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.89	0.54
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.42	0.54
15:j:3:0A1:C	15:j:4:A1I44:C12	2.85	0.54
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.42	0.54
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.07	0.54
15:i:3:0A1:C	15:i:4:A1I44:C12	2.86	0.54
3:C:38:ASN:C	3:C:38:ASN:HD22	2.16	0.54
3:Q:38:ASN:C	3:Q:38:ASN:HD22	2.16	0.54
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.90	0.54
11:K:53:GLN:O	11:K:57:THR:OG1	2.25	0.54
15:i:1:00E:HD1A	15:i:1:00E:O	2.06	0.54
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.90	0.54
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.90	0.53
11:K:2:THR:HG21	11:K:164:ALA:CB	2.39	0.53
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:83:LEU:HD11	11:Y:97:MET:HE1	1.90	0.53
11:K:98:GLY:HA3	18:K:303:MES:H62	1.89	0.53
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.44	0.53
15:e:1:00E:CE1	15:e:3:0A1:HE2	2.39	0.53
15:j:4:A1I44:C12	15:j:4:A1I44:N22	2.72	0.52
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.44	0.52
11:Y:53:GLN:O	11:Y:57:THR:OG1	2.26	0.52
6:T:123:ASN:C	6:T:123:ASN:HD22	2.17	0.52
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.91	0.51
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.45	0.51
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.26	0.51
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.76	0.51
6:F:123:ASN:C	6:F:123:ASN:HD22	2.18	0.51
11:Y:2:THR:HG21	11:Y:164:ALA:CB	2.41	0.51
8:H:139:GLU:OE1	13:a:187:ARG:NH1	2.41	0.50
12:L:147:MET:N	12:L:148:PRO:HD2	2.25	0.50
10:J:23:ARG:NH2	18:K:303:MES:O1	2.44	0.50
13:M:104:ARG:NH2	19:M:301:HOH:O	2.44	0.50
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.94	0.50
10:J:174:MET:HA	10:X:174:MET:HA	1.93	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.50
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.94	0.49
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.39	0.49
13:M:228:TYR:HE2	14:b:35:THR:HG21	1.78	0.49
8:H:2:THR:OG1	8:H:169:SER:OG	2.29	0.49
11:K:3:MET:HE1	11:K:45:MET:O	2.13	0.49
11:K:130:GLY:HA2	18:K:303:MES:H81	1.95	0.49
18:Y:303:MES:O3S	15:i:4:A1I44:O21	2.30	0.49
15:g:4:A1I44:C12	15:g:4:A1I44:N22	2.76	0.49
7:G:78:ILE:N	7:G:79:PRO:CD	2.76	0.49
15:f:2:ALA:C	15:f:3:0A1:CD2	2.85	0.49
7:U:78:ILE:N	7:U:79:PRO:CD	2.76	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.95	0.48
14:b:49:ALA:O	14:b:53:GLN:HB2	2.13	0.48
11:Y:96:SER:CB	15:i:3:0A1:HMC3	2.42	0.48
11:K:3:MET:HE1	11:K:45:MET:C	2.38	0.48
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.48
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.95	0.48
15:e:1:00E:CE1	15:e:3:0A1:CE2	2.92	0.48
2:B:6:ASP:OD2	3:C:4:ARG:HG3	2.14	0.48
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:98:GLY:CA	18:Y:303:MES:H62	2.43	0.48
11:K:98:GLY:CA	18:K:303:MES:H62	2.44	0.48
11:Y:3:MET:HE1	11:Y:45:MET:C	2.38	0.48
14:N:49:ALA:O	14:N:53:GLN:HB2	2.13	0.47
1:O:119:GLN:O	1:O:122:THR:HB	2.13	0.47
1:O:12:PHE:H	2:P:20:GLN:HE22	1.61	0.47
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.49	0.47
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.96	0.47
11:Y:96:SER:HB2	15:i:3:0A1:HMC3	1.96	0.47
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.94	0.47
11:Y:3:MET:HE1	11:Y:45:MET:O	2.14	0.47
2:P:6:ASP:OD2	3:Q:4:ARG:HG3	2.14	0.47
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.97	0.47
5:E:98:PHE:O	13:M:91:TYR:HA	2.15	0.47
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.95	0.47
15:h:1:00E:HE1	15:h:3:0A1:HMC3	1.96	0.47
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.80	0.47
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.97	0.46
8:H:52:THR:O	8:H:56:THR:HB	2.15	0.46
15:e:1:00E:CD1	15:e:3:0A1:CE2	2.92	0.46
9:I:34:GLY:O	11:Y:167:ARG:NH1	2.48	0.46
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.46
11:K:2:THR:HG21	11:K:164:ALA:HB3	1.97	0.46
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.97	0.46
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.81	0.46
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.46	0.46
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.97	0.46
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.50	0.46
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.98	0.46
9:I:98:ARG:O	9:I:126:ILE:HD11	2.16	0.46
13:M:26:ASN:HA	13:M:39:VAL:O	2.16	0.46
14:N:44:CYS:HB2	14:N:98:ILE:HB	1.96	0.46
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.50	0.46
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.89	0.46
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.49	0.45
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.31	0.45
14:b:44:CYS:HB2	14:b:98:ILE:HB	1.98	0.45
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.51	0.45
3:C:201:VAL:HG13	3:C:202:GLN:N	2.31	0.45
8:V:52:THR:O	8:V:56:THR:HB	2.17	0.45
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.64	0.45
5:S:98:PHE:O	13:a:91:TYR:HA	2.16	0.45
11:K:130:GLY:HA3	15:f:4:A1I44:O	2.16	0.45
1:A:119:GLN:O	1:A:122:THR:HB	2.16	0.45
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.98	0.45
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.98	0.45
9:W:98:ARG:O	9:W:126:ILE:HD11	2.16	0.45
11:Y:73:ARG:HG2	11:Y:73:ARG:HH11	1.82	0.45
3:C:108:THR:HG21	3:C:146:TYR:HB3	1.98	0.45
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.98	0.45
11:K:3:MET:CE	11:K:46:ALA:HB2	2.47	0.45
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.98	0.45
7:G:34:LEU:C	7:G:34:LEU:HD23	2.42	0.45
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.48	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.98	0.44
11:K:73:ARG:HG2	11:K:73:ARG:HH11	1.81	0.44
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.99	0.44
11:K:25:TRP:CH2	12:L:144:SER:HA	2.53	0.44
11:Y:3:MET:CE	11:Y:46:ALA:HB2	2.47	0.44
7:G:61:SER:OG	7:G:215:GLU:OE2	2.34	0.44
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.52	0.44
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.83	0.44
1:A:149:GLN:O	1:A:156:TYR:HA	2.18	0.44
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.98	0.44
11:K:4:LEU:C	11:K:4:LEU:CD2	2.89	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.61	0.44
10:X:26:SER:CB	11:Y:133:GLN:NE2	2.80	0.44
10:X:168:LEU:O	10:X:172:MET:HB2	2.17	0.44
13:a:26:ASN:HA	13:a:39:VAL:O	2.17	0.44
1:A:12:PHE:H	2:B:20:GLN:HE22	1.65	0.44
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.98	0.44
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.48	0.44
5:S:77:ALA:N	5:S:78:PRO:CD	2.81	0.44
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.48	0.44
10:X:26:SER:HB2	11:Y:133:GLN:NE2	2.33	0.43
1:O:149:GLN:O	1:O:156:TYR:HA	2.18	0.43
15:g:1:00E:HE1	15:g:3:0A1:HMC2	2.00	0.43
8:V:84:LYS:HE3	14:b:57:ASP:OD2	2.19	0.43
11:Y:170:TYR:O	15:i:4:A1I44:C11	2.66	0.43
2:B:50:LYS:O	2:B:51:VAL:C	2.61	0.43
13:M:96:LEU:O	13:M:100:MET:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:53:GLU:O	8:H:56:THR:HG22	2.19	0.43
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.00	0.43
10:J:168:LEU:O	10:J:172:MET:HB2	2.18	0.43
11:K:6:PHE:HA	11:K:125:ASP:O	2.19	0.43
15:h:4:A1I44:O13	18:h:101:MES:O1S	2.37	0.43
5:E:77:ALA:N	5:E:78:PRO:CD	2.82	0.42
11:K:209:ASN:O	9:W:37:ASN:ND2	2.52	0.42
3:C:201:VAL:O	3:C:202:GLN:CB	2.67	0.42
7:U:34:LEU:C	7:U:34:LEU:HD23	2.43	0.42
9:W:7:ASN:HA	9:W:29:GLY:O	2.19	0.42
11:Y:161:ILE:CG2	11:Y:175:VAL:HG22	2.50	0.42
14:b:3:ILE:HD12	14:b:44:CYS:HB3	2.01	0.42
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.67	0.42
9:I:126:ILE:HD12	9:I:126:ILE:HA	1.86	0.42
6:T:123:ASN:HD22	6:T:124:SER:N	2.18	0.42
10:X:1:MET:HA	10:X:34:LYS:CE	2.50	0.42
12:Z:108:HIS:HB3	19:Z:405:HOH:O	2.18	0.42
13:a:96:LEU:O	13:a:100:MET:HG2	2.19	0.42
15:i:4:A1I44:C12	15:i:4:A1I44:N22	2.83	0.42
11:K:161:ILE:CG2	11:K:175:VAL:HG22	2.49	0.42
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.01	0.42
2:B:12:PHE:H	3:C:17:GLN:HE22	1.68	0.42
14:b:128:GLY:HA3	15:j:4:A1I44:O	2.19	0.42
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.02	0.42
2:B:148:TYR:OH	3:C:57:ILE:HB	2.20	0.42
9:I:7:ASN:HA	9:I:29:GLY:O	2.19	0.42
10:J:26:SER:CB	11:K:133:GLN:NE2	2.83	0.42
15:f:4:A1I44:C12	15:f:4:A1I44:N22	2.79	0.42
8:H:102:GLY:HA2	8:H:178:MET:SD	2.60	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.02	0.42
11:K:167:ARG:NH1	9:W:34:GLY:O	2.51	0.42
14:N:4:MET:HB3	14:N:126:ILE:HG22	2.02	0.42
5:S:71:LEU:C	5:S:71:LEU:CD2	2.93	0.42
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.20	0.42
14:b:4:MET:HB3	14:b:126:ILE:HG22	2.01	0.41
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.03	0.41
11:K:161:ILE:HD13	11:K:161:ILE:HA	1.87	0.41
8:V:2:THR:HG1	8:V:169:SER:CB	2.32	0.41
4:D:113:LEU:HD12	5:E:78:PRO:HB2	2.03	0.41
6:F:123:ASN:HD22	6:F:124:SER:N	2.19	0.41
10:J:1:MET:HA	10:J:34:LYS:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:75:LEU:HD12	10:J:75:LEU:HA	1.87	0.41
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.23	0.41
1:A:115:ALA:HB1	1:A:154:GLY:O	2.20	0.41
8:V:102:GLY:HA2	8:V:178:MET:SD	2.60	0.41
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.56	0.41
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.50	0.41
11:Y:100:MET:HE2	11:Y:100:MET:HB2	1.97	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.03	0.41
5:E:71:LEU:C	5:E:71:LEU:CD2	2.94	0.41
8:H:84:LYS:HE3	14:N:57:ASP:OD2	2.21	0.41
9:W:126:ILE:HD12	9:W:126:ILE:HA	1.86	0.41
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.86	0.41
10:J:26:SER:HB2	11:K:133:GLN:NE2	2.36	0.41
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.56	0.41
11:K:161:ILE:HG22	11:K:175:VAL:HG22	2.03	0.40
1:O:115:ALA:HB1	1:O:154:GLY:O	2.20	0.40
11:Y:97:MET:O	11:Y:116:ASP:HA	2.21	0.40
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.03	0.40
6:F:158:GLY:O	7:G:54:LEU:HB3	2.22	0.40
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.51	0.40
11:K:41:LEU:HD23	11:K:41:LEU:HA	1.94	0.40
4:D:24:LYS:O	4:D:166:SER:HA	2.22	0.40
11:Y:2:THR:OG1	11:Y:171:SER:OG	2.23	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%)	239 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	30	61
2	P	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	30	61
3	C	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	10	32
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	10	32
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	239/252 (95%)	233 (98%)	6 (2%)	0	100	100
7	U	239/252 (95%)	233 (98%)	6 (2%)	0	100	100
8	H	219/231 (95%)	216 (99%)	2 (1%)	1 (0%)	25	56
8	V	219/231 (95%)	216 (99%)	2 (1%)	1 (0%)	25	56
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%)	190 (98%)	2 (1%)	1 (0%)	25	56
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	25	56
11	K	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
11	Y	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	222 (96%)	8 (4%)	1 (0%)	30	61
13	a	231/246 (94%)	222 (96%)	8 (4%)	1 (0%)	30	61
14	N	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
14	b	193/195 (99%)	186 (96%)	7 (4%)	0	100	100
15	e	1/4 (25%)	1 (100%)	0	0	100	100
15	f	1/4 (25%)	1 (100%)	0	0	100	100
15	g	1/4 (25%)	1 (100%)	0	0	100	100
15	h	1/4 (25%)	1 (100%)	0	0	100	100
15	i	1/4 (25%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	j	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6276/6632 (95%)	6095 (97%)	167 (3%)	14 (0%)	44	73

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
3	C	205	ALA
3	Q	205	ALA
8	H	9	ASN
8	V	9	ASN
3	C	239	GLN
3	Q	239	GLN
13	M	229	GLY
13	a	229	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%)	44	77
1	O	209/209 (100%)	204 (98%)	5 (2%)	44	77
2	B	203/216 (94%)	194 (96%)	9 (4%)	24	56
2	P	203/216 (94%)	194 (96%)	9 (4%)	24	56
3	C	212/226 (94%)	205 (97%)	7 (3%)	33	67
3	Q	212/226 (94%)	205 (97%)	7 (3%)	33	67
4	D	194/215 (90%)	182 (94%)	12 (6%)	15	43
4	R	194/215 (90%)	182 (94%)	12 (6%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	68
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	68
6	F	201/239 (84%)	194 (96%)	7 (4%)	31	65
6	T	201/239 (84%)	193 (96%)	8 (4%)	27	60
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	66
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	66
8	H	180/189 (95%)	175 (97%)	5 (3%)	38	72
8	V	180/189 (95%)	174 (97%)	6 (3%)	33	67
9	I	172/173 (99%)	168 (98%)	4 (2%)	45	78
9	W	172/173 (99%)	168 (98%)	4 (2%)	45	78
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	71
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	71
11	K	168/168 (100%)	157 (94%)	11 (6%)	14	40
11	Y	168/168 (100%)	157 (94%)	11 (6%)	14	40
12	L	185/185 (100%)	177 (96%)	8 (4%)	25	57
12	Z	185/185 (100%)	177 (96%)	8 (4%)	25	57
13	M	199/208 (96%)	194 (98%)	5 (2%)	42	75
13	a	199/208 (96%)	194 (98%)	5 (2%)	42	75
14	N	161/161 (100%)	157 (98%)	4 (2%)	42	75
14	b	161/161 (100%)	158 (98%)	3 (2%)	52	82
All	All	5306/5534 (96%)	5115 (96%)	191 (4%)	30	64

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	29	LYS
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU

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Mol	Chain	Res	Type
2	B	102	ASN
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
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	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	188	LEU
6	F	68	ARG
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG

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Mol	Chain	Res	Type
7	G	236	LEU
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	84	LYS
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	144	LEU
10	J	174	MET
11	K	3	MET
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	35	ILE
11	K	36	GLU
11	K	57	THR
11	K	99	THR
11	K	100	MET
11	K	106	ARG
11	K	161	ILE
12	L	1	GLN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	128	VAL
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
14	N	2	SER
14	N	9	LYS
14	N	36	ARG

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Mol	Chain	Res	Type
14	N	119	VAL
1	O	17	LYS
1	O	29	LYS
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	102	ASN
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
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	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	188	LEU
6	T	14	ASP
6	T	68	ARG

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Mol	Chain	Res	Type
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	221	ASN
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	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	84	LYS
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
9	W	182	TRP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	144	LEU
10	X	174	MET
11	Y	3	MET
11	Y	4	LEU
11	Y	7	ARG
11	Y	9	GLN
11	Y	35	ILE
11	Y	36	GLU
11	Y	57	THR
11	Y	99	THR
11	Y	100	MET
11	Y	106	ARG
11	Y	161	ILE
12	Z	1	GLN
12	Z	23	LEU
12	Z	31	THR

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Mol	Chain	Res	Type
12	Z	49	ASN
12	Z	128	VAL
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
14	b	2	SER
14	b	9	LYS
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	176	GLN
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
3	C	233	GLN
4	D	15	GLN
4	D	91	HIS
4	D	106	GLN
4	D	160	ASN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN

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Mol	Chain	Res	Type
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	184	ASN
6	F	86	ASN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	6	HIS
7	G	30	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	212	ASN
8	H	22	GLN
8	H	86	HIS
8	H	165	ASN
8	H	172	ASN
8	H	200	GLN
9	I	37	ASN
9	I	44	HIS
9	I	63	ASN
9	I	88	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
10	J	147	HIS
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	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN

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Mol	Chain	Res	Type
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	69	GLN
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
2	P	232	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	106	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN
5	S	165	GLN
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN

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Mol	Chain	Res	Type
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	212	ASN
8	V	22	GLN
8	V	86	HIS
8	V	165	ASN
8	V	172	ASN
8	V	200	GLN
9	W	37	ASN
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	146	HIS
10	X	147	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	69	GLN
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
15	00E	g	1	15	9,9,10	0.65	0	10,10,12	1.91	4 (40%)
15	00E	h	1	15	9,9,10	0.67	0	10,10,12	1.40	1 (10%)
15	0A1	j	3	15	12,13,14	1.74	1 (8%)	13,16,18	1.15	2 (15%)
15	0A1	f	3	15	12,13,14	1.88	1 (8%)	13,16,18	1.71	2 (15%)
15	00E	f	1	15	9,9,10	0.59	0	10,10,12	1.10	0
15	0A1	g	3	15	12,13,14	1.62	1 (8%)	13,16,18	1.03	1 (7%)
15	00E	j	1	15	9,9,10	0.81	0	10,10,12	1.62	1 (10%)
15	00E	e	1	15	9,9,10	0.59	0	10,10,12	1.43	1 (10%)
15	0A1	h	3	15	12,13,14	1.77	1 (8%)	13,16,18	1.51	2 (15%)
15	0A1	e	3	15	12,13,14	1.80	1 (8%)	13,16,18	1.56	1 (7%)
15	0A1	i	3	15	12,13,14	1.66	1 (8%)	13,16,18	1.28	1 (7%)
15	00E	i	1	15	9,9,10	0.45	0	10,10,12	0.90	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
15	00E	g	1	15	-	2/2/11/12	0/1/1/1
15	00E	h	1	15	-	1/2/11/12	0/1/1/1
15	0A1	j	3	15	-	2/7/8/10	0/1/1/1
15	0A1	f	3	15	-	4/7/8/10	0/1/1/1
15	00E	f	1	15	-	0/2/11/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	0A1	g	3	15	-	2/7/8/10	0/1/1/1
15	00E	j	1	15	-	2/2/11/12	0/1/1/1
15	00E	e	1	15	-	2/2/11/12	0/1/1/1
15	0A1	h	3	15	-	4/7/8/10	0/1/1/1
15	0A1	e	3	15	-	4/7/8/10	0/1/1/1
15	0A1	i	3	15	-	4/7/8/10	0/1/1/1
15	00E	i	1	15	-	0/2/11/12	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	3	0A1	CB-CG	-6.14	1.36	1.51
15	e	3	0A1	CB-CG	-5.79	1.37	1.51
15	j	3	0A1	CB-CG	-5.76	1.37	1.51
15	h	3	0A1	CB-CG	-5.72	1.37	1.51
15	i	3	0A1	CB-CG	-5.49	1.38	1.51
15	g	3	0A1	CB-CG	-5.42	1.38	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	e	3	0A1	CM-OH-CZ	-5.12	106.39	117.51
15	h	3	0A1	CM-OH-CZ	-4.76	107.18	117.51
15	f	3	0A1	CM-OH-CZ	-4.24	108.32	117.51
15	f	3	0A1	CG-CB-CA	-3.68	106.65	114.10
15	i	3	0A1	CM-OH-CZ	-3.60	109.70	117.51
15	g	1	00E	C-CA-NB	-3.46	105.89	112.84
15	j	1	00E	C-CA-NB	-3.30	106.22	112.84
15	h	1	00E	C-CA-NB	-3.08	106.66	112.84
15	g	1	00E	CA-NB-CD2	2.96	113.78	110.48
15	j	3	0A1	CG-CB-CA	-2.69	108.66	114.10
15	g	1	00E	O-C-CA	-2.33	119.35	126.39
15	e	1	00E	CA-NB-CD2	-2.31	107.90	110.48
15	g	3	0A1	CM-OH-CZ	-2.22	112.69	117.51
15	g	1	00E	OZ-CE1-CD1	-2.11	107.14	111.80
15	h	3	0A1	CG-CB-CA	-2.10	109.85	114.10
15	j	3	0A1	CM-OH-CZ	-2.07	113.02	117.51

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	e	1	00E	C-CA-NB-CD1
15	g	1	00E	C-CA-NB-CD1
15	g	1	00E	C-CA-NB-CD2
15	j	1	00E	C-CA-NB-CD1
15	j	1	00E	C-CA-NB-CD2
15	g	3	0A1	C-CA-CB-CG
15	j	3	0A1	C-CA-CB-CG
15	e	3	0A1	CE1-CZ-OH-CM
15	e	3	0A1	CE2-CZ-OH-CM
15	f	3	0A1	CE2-CZ-OH-CM
15	f	3	0A1	CE1-CZ-OH-CM
15	h	3	0A1	CE1-CZ-OH-CM
15	h	3	0A1	CE2-CZ-OH-CM
15	i	3	0A1	CE2-CZ-OH-CM
15	i	3	0A1	CE1-CZ-OH-CM
15	e	3	0A1	N-CA-CB-CG
15	f	3	0A1	N-CA-CB-CG
15	h	3	0A1	N-CA-CB-CG
15	i	3	0A1	N-CA-CB-CG
15	j	3	0A1	N-CA-CB-CG
15	e	1	00E	C-CA-NB-CD2
15	h	1	00E	C-CA-NB-CD1
15	g	3	0A1	N-CA-CB-CG
15	e	3	0A1	C-CA-CB-CG
15	f	3	0A1	C-CA-CB-CG
15	h	3	0A1	C-CA-CB-CG
15	i	3	0A1	C-CA-CB-CG

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	g	1	00E	1	0
15	h	1	00E	1	0
15	j	3	0A1	1	0
15	f	3	0A1	3	0
15	g	3	0A1	2	0
15	e	1	00E	6	0
15	h	3	0A1	1	0
15	e	3	0A1	6	0
15	i	3	0A1	3	0
15	i	1	00E	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	$\# Z > 2$
18	MES	H	301	-	12,12,12	0.71	0	14,16,16	0.42	0
18	MES	K	303	-	12,12,12	0.73	0	14,16,16	0.39	0
18	MES	h	101	-	12,12,12	0.75	0	14,16,16	0.39	0
18	MES	Y	303	-	12,12,12	0.74	0	14,16,16	0.35	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	H	301	-	-	3/6/14/14	0/1/1/1
18	MES	K	303	-	-	5/6/14/14	0/1/1/1
18	MES	h	101	-	-	1/6/14/14	0/1/1/1
18	MES	Y	303	-	-	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 (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	K	303	MES	N4-C7-C8-S
18	Y	303	MES	N4-C7-C8-S

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Mol	Chain	Res	Type	Atoms
18	h	101	MES	N4-C7-C8-S
18	K	303	MES	C7-C8-S-O3S
18	H	301	MES	C7-C8-S-O3S
18	H	301	MES	C7-C8-S-O1S
18	H	301	MES	C7-C8-S-O2S
18	K	303	MES	C7-C8-S-O1S
18	K	303	MES	C7-C8-S-O2S
18	K	303	MES	C8-C7-N4-C5

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	K	303	MES	4	0
18	h	101	MES	1	0
18	Y	303	MES	3	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	A	250/250 (100%)	-1.00	1 (0%) 89 85	56, 72, 102, 161	0
1	O	250/250 (100%)	-0.96	0 100 100	60, 80, 115, 170	0
2	B	244/258 (94%)	-0.88	2 (0%) 82 77	58, 77, 123, 169	0
2	P	244/258 (94%)	-0.88	0 100 100	61, 82, 122, 158	0
3	C	240/254 (94%)	-0.92	0 100 100	60, 84, 141, 158	0
3	Q	240/254 (94%)	-0.86	1 (0%) 89 85	65, 93, 154, 177	0
4	D	235/260 (90%)	-0.96	0 100 100	65, 84, 111, 140	0
4	R	235/260 (90%)	-0.94	0 100 100	62, 86, 117, 143	0
5	E	231/234 (98%)	-0.87	0 100 100	65, 86, 118, 145	0
5	S	231/234 (98%)	-0.81	0 100 100	66, 90, 126, 148	0
6	F	243/288 (84%)	-0.96	0 100 100	56, 78, 117, 145	0
6	T	243/288 (84%)	-0.93	0 100 100	57, 83, 126, 147	0
7	G	241/252 (95%)	-1.01	0 100 100	52, 70, 106, 150	0
7	U	241/252 (95%)	-1.04	0 100 100	58, 73, 103, 127	0
8	H	221/231 (95%)	-0.99	0 100 100	56, 71, 103, 130	0
8	V	221/231 (95%)	-0.96	0 100 100	59, 73, 103, 135	0
9	I	204/205 (99%)	-1.04	0 100 100	55, 73, 99, 121	0
9	W	204/205 (99%)	-1.05	0 100 100	58, 76, 105, 128	0
10	J	195/198 (98%)	-1.02	1 (0%) 87 83	54, 72, 98, 135	0
10	X	195/198 (98%)	-1.04	1 (0%) 87 83	59, 75, 97, 157	0
11	K	211/211 (100%)	-0.81	0 100 100	67, 83, 110, 127	0
11	Y	211/211 (100%)	-0.78	0 100 100	66, 83, 112, 135	0
12	L	222/222 (100%)	-0.93	0 100 100	61, 78, 118, 138	0
12	Z	222/222 (100%)	-0.89	0 100 100	59, 76, 110, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.98	0 100 100	56, 72, 108, 124	0
13	a	233/246 (94%)	-1.00	1 (0%) 89 85	54, 71, 102, 131	0
14	N	195/195 (100%)	-1.06	0 100 100	56, 66, 94, 117	0
14	b	195/195 (100%)	-1.01	0 100 100	53, 67, 93, 116	0
15	e	1/4 (25%)	0.75	0 100 100	80, 80, 80, 80	0
15	f	1/4 (25%)	0.75	0 100 100	100, 100, 100, 100	0
15	g	1/4 (25%)	0.70	0 100 100	93, 93, 93, 93	0
15	h	1/4 (25%)	1.01	0 100 100	85, 85, 85, 85	0
15	i	1/4 (25%)	0.61	0 100 100	111, 111, 111, 111	0
15	j	1/4 (25%)	-0.11	0 100 100	91, 91, 91, 91	0
All	All	6336/6632 (95%)	-0.95	7 (0%) 92 91	52, 78, 117, 177	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	a	1	THR	2.5
10	X	1	MET	2.4
3	Q	50	LEU	2.3
2	B	219	ALA	2.2
2	B	51	VAL	2.2
10	J	1	MET	2.1
1	A	1	MET	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
15	00E	i	1	9/10	0.78	0.13	109,111,117,117	0
15	0A1	f	3	13/14	0.80	0.12	93,97,106,109	0
15	00E	e	1	9/10	0.89	0.10	92,110,113,114	0
15	0A1	e	3	13/14	0.89	0.10	78,82,86,89	0
15	00E	h	1	9/10	0.89	0.09	92,102,105,107	0
15	0A1	j	3	13/14	0.89	0.11	83,87,99,100	0
15	0A1	i	3	13/14	0.90	0.08	99,102,107,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	0A1	h	3	13/14	0.90	0.09	77,83,88,88	0
15	00E	g	1	9/10	0.91	0.10	97,114,120,120	0
15	00E	j	1	9/10	0.92	0.12	90,118,127,127	0
15	00E	f	1	9/10	0.92	0.11	100,108,112,115	0
15	0A1	g	3	13/14	0.93	0.08	81,86,91,92	0

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(\AA^2)	Q<0.9
18	MES	K	303	12/12	0.89	0.11	104,107,113,118	0
18	MES	h	101	12/12	0.93	0.09	109,112,119,119	0
18	MES	Y	303	12/12	0.94	0.10	100,109,114,117	0
18	MES	H	301	12/12	0.94	0.09	99,107,111,112	0
16	MG	Z	301	1/1	0.95	0.07	86,86,86,86	0
16	MG	I	301	1/1	0.96	0.12	83,83,83,83	0
16	MG	Y	302	1/1	0.97	0.11	69,69,69,69	0
16	MG	Y	301	1/1	0.97	0.04	80,80,80,80	0
16	MG	K	302	1/1	0.98	0.15	63,63,63,63	0
16	MG	G	301	1/1	0.98	0.04	70,70,70,70	0
17	CL	G	302	1/1	0.99	0.06	57,57,57,57	0
17	CL	U	301	1/1	0.99	0.06	62,62,62,62	0
16	MG	X	201	1/1	0.99	0.08	53,53,53,53	0
16	MG	K	301	1/1	0.99	0.06	80,80,80,80	0
16	MG	N	201	1/1	0.99	0.03	63,63,63,63	0
16	MG	V	301	1/1	0.99	0.06	97,97,97,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.