



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:39 am GMT

PDB ID : 4R18  
Title : Ligand-induced Lys33-Thr1 crosslinking at subunit beta5 of the yeast 20S proteasome  
Authors : Dubiella, C.; Cui, H.; Gersch, M.; Brouwer, A.J.; Sieber, S.A.; Krueger, A.; Liskamp, R.; Groll, M.  
Deposited on : 2014-08-04  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

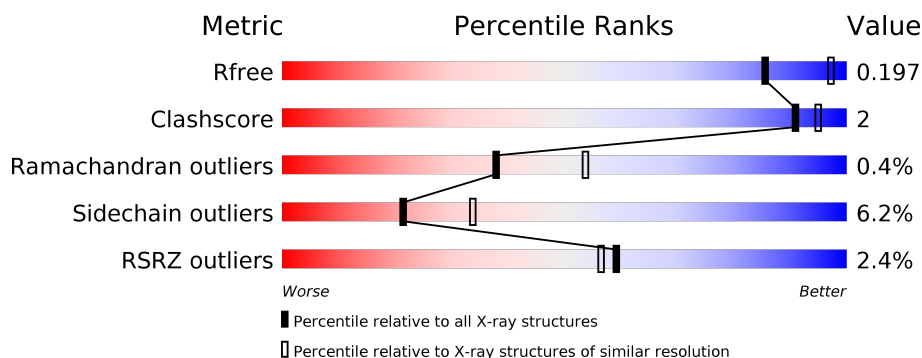
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.



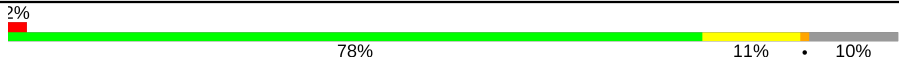
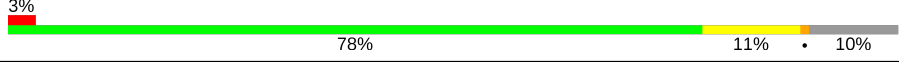



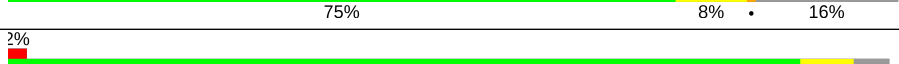
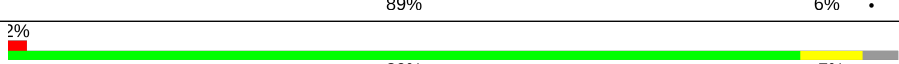
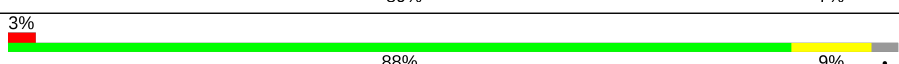
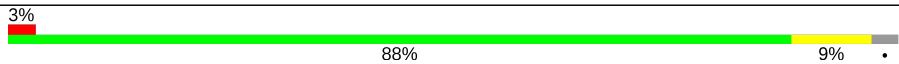
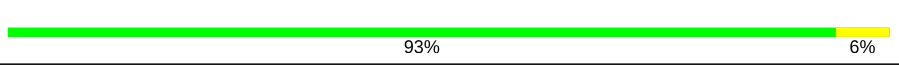
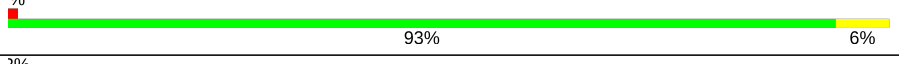
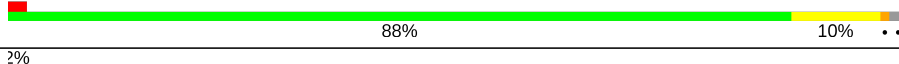

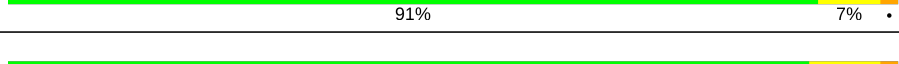
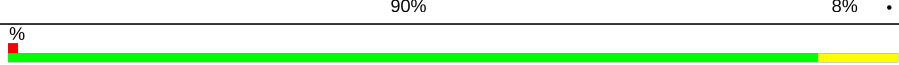
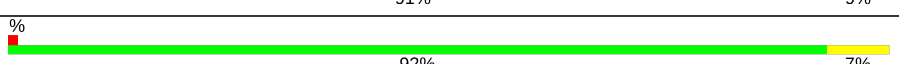

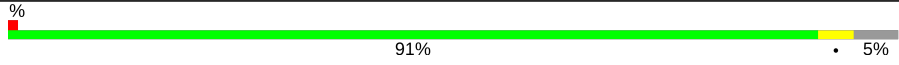
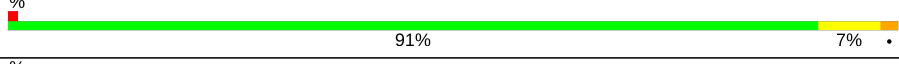
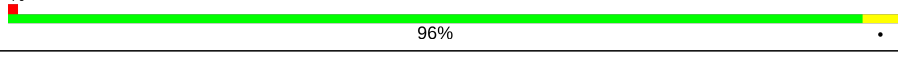


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>4%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	O	250	<div> <div>3%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
2	B	258	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>5%</div> </div> </div>
2	P	258	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>5%</div> </div> </div>
3	C	254	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>6%</div> </div> </div>
3	Q	254	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

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	MG	I	302	-	-	-	X
15	MG	J	201	-	-	-	X
15	MG	K	303	-	-	-	X
16	ABA	K	301	-	-	-	X

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 51115 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 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	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	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	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	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

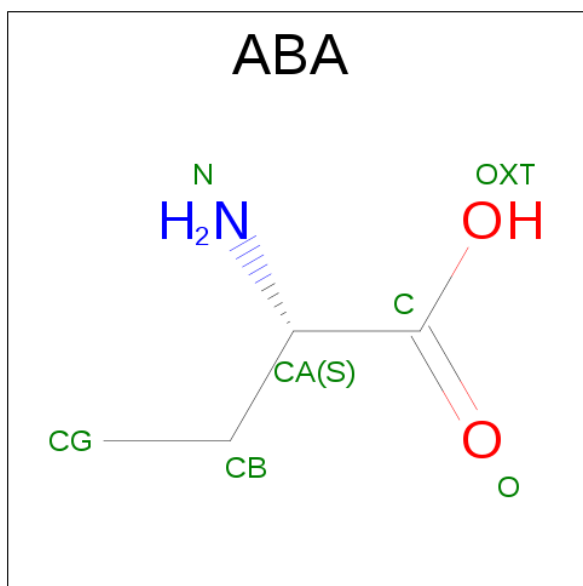
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	J	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	2	Total	Mg	0	0
			2	2		
15	H	1	Total	Mg	0	0
			1	1		
15	I	2	Total	Mg	0	0
			2	2		
15	V	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		

- Molecule 16 is ALPHA-AMINOBUTYRIC ACID (three-letter code: ABA) (formula:  $C_4H_9NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			6	4	1	1		
16	Y	1	Total	C	N	O	0	0
			6	4	1	1		

- Molecule 17 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	79	Total O 79 79	0	0
17	B	62	Total O 62 62	0	0
17	C	48	Total O 48 48	0	0
17	D	56	Total O 56 56	0	0
17	E	18	Total O 18 18	0	0
17	F	67	Total O 67 67	0	0
17	G	83	Total O 83 83	0	0
17	H	66	Total O 66 66	0	0
17	I	73	Total O 73 73	0	0
17	J	85	Total O 85 85	0	0
17	K	77	Total O 77 77	0	0
17	L	69	Total O 69 69	0	0
17	M	81	Total O 81 81	0	0
17	N	61	Total O 61 61	0	0
17	O	42	Total O 42 42	0	0
17	P	52	Total O 52 52	0	0
17	Q	31	Total O 31 31	0	0
17	R	50	Total O 50 50	0	0
17	S	24	Total O 24 24	0	0
17	T	62	Total O 62 62	0	0
17	U	62	Total O 62 62	0	0
17	V	58	Total O 58 58	0	0

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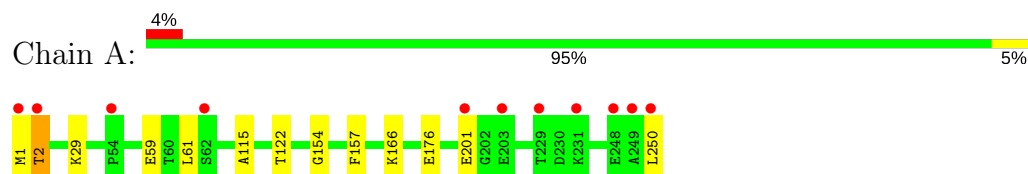
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	68	Total 68	O 68	0	0
17	X	66	Total 66	O 66	0	0
17	Y	69	Total 69	O 69	0	0
17	Z	81	Total 81	O 81	0	0
17	a	84	Total 84	O 84	0	0
17	b	66	Total 66	O 66	0	0

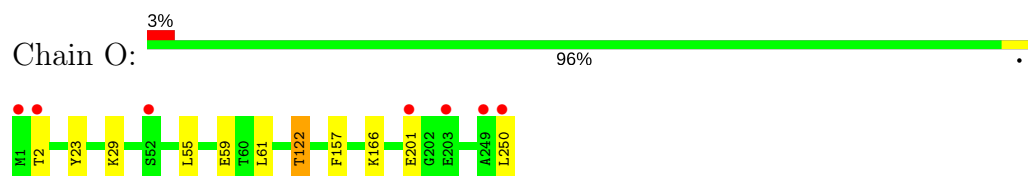
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

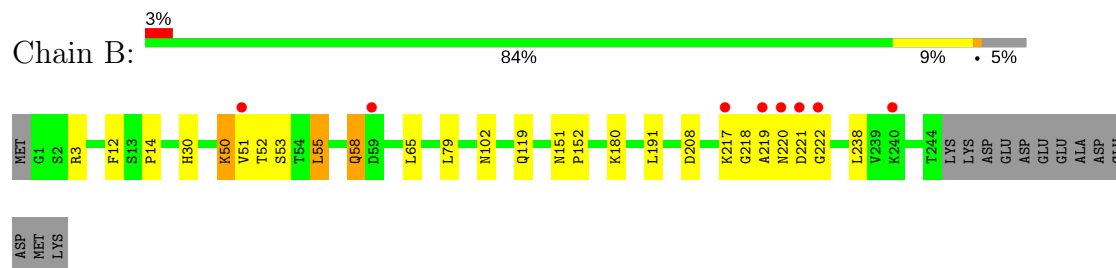
- Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-2



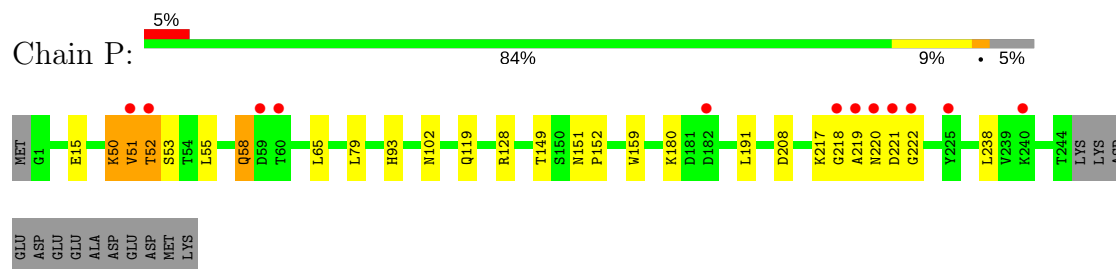
- Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-2



- Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE-3

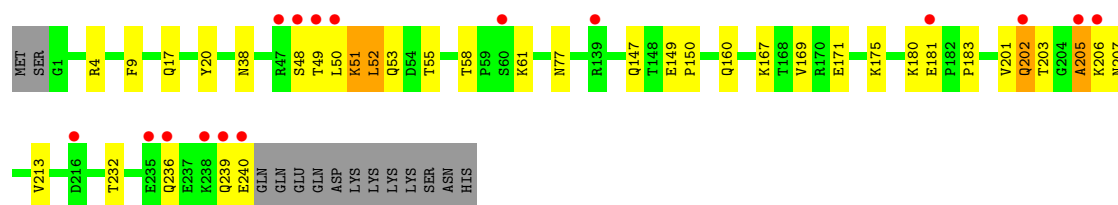


- Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE-3

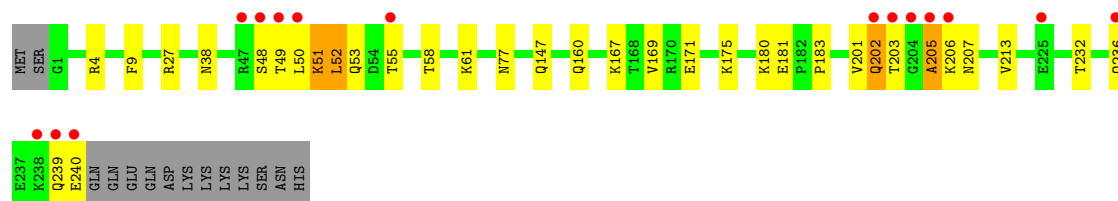
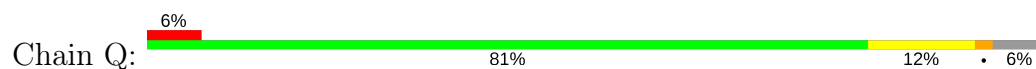


- Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4

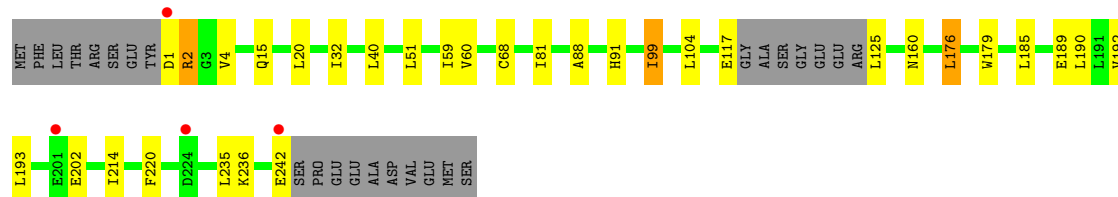
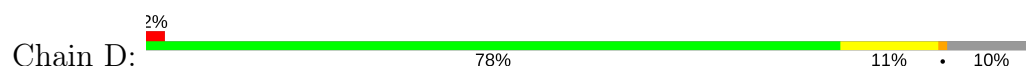




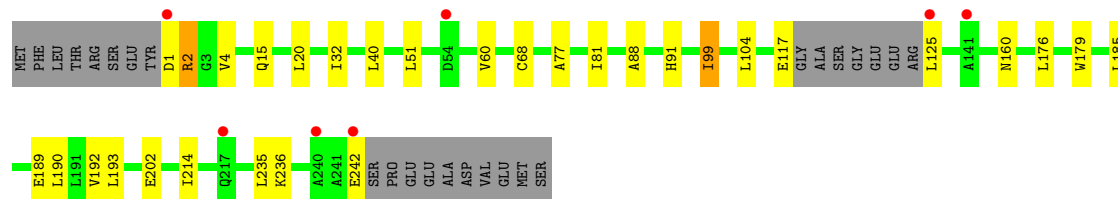
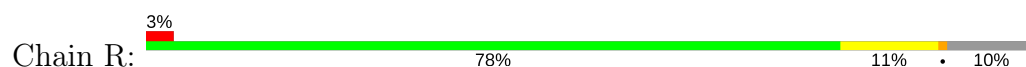
• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4



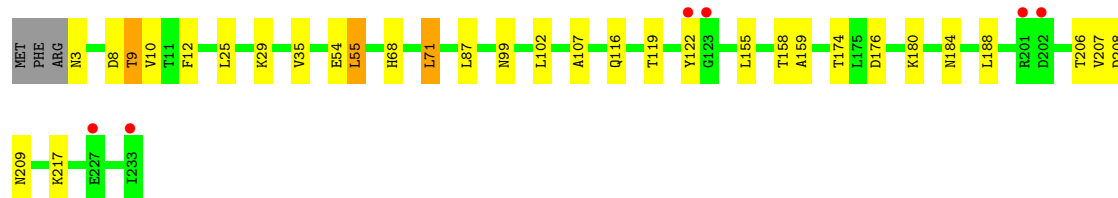
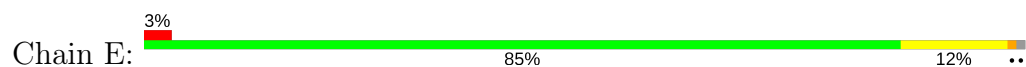
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-5



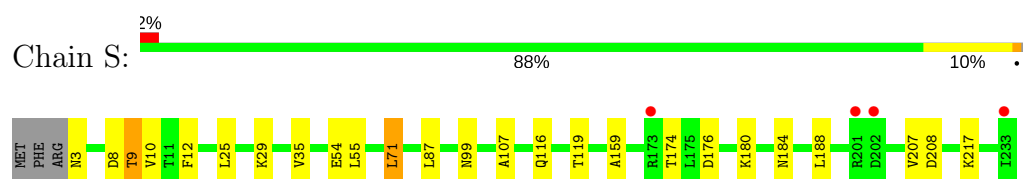
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-5



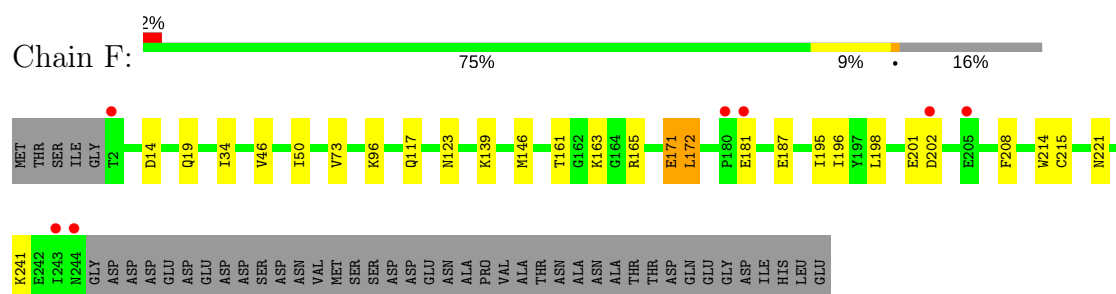
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-6



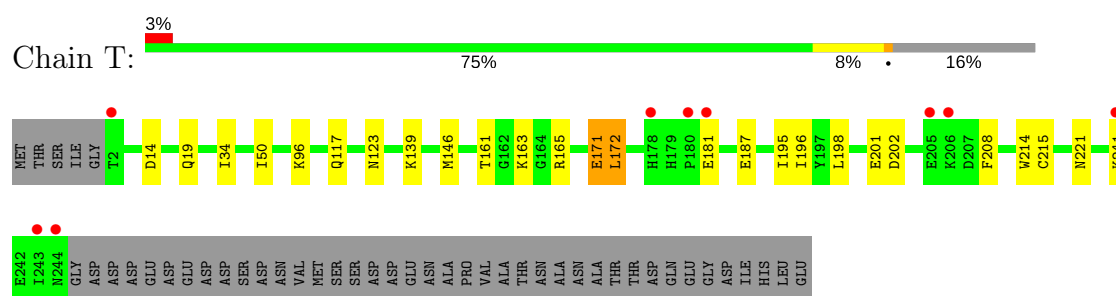
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-6



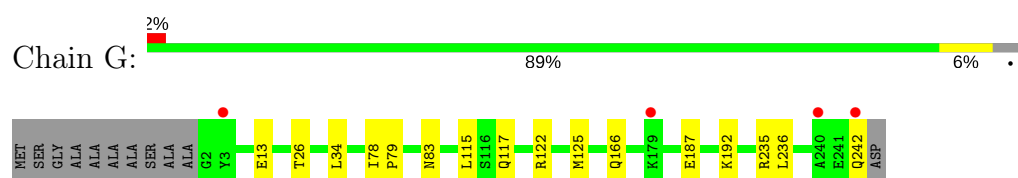
• Molecule 6: PROTEASOME SUBUNIT ALPHA TYPE-7



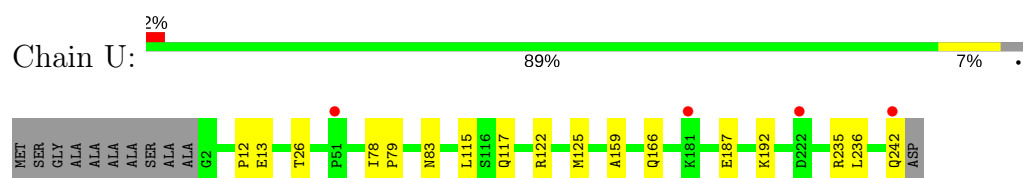
• Molecule 6: PROTEASOME SUBUNIT ALPHA TYPE-7



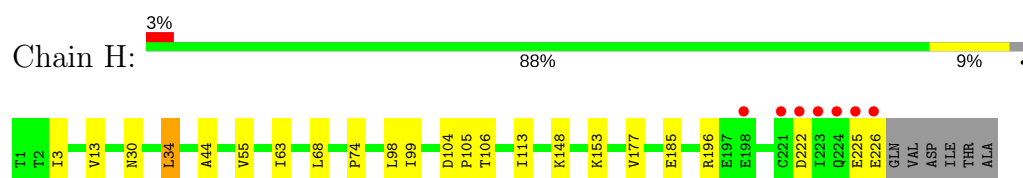
• Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-1



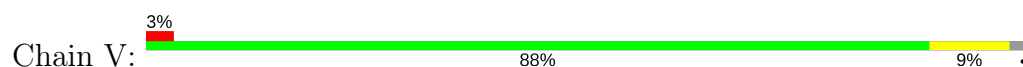
• Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-1

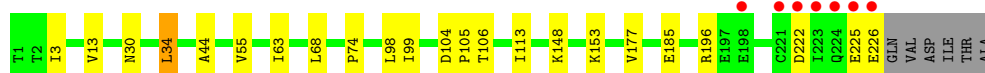


• Molecule 8: PROTEASOME SUBUNIT BETA TYPE-2



• Molecule 8: PROTEASOME SUBUNIT BETA TYPE-2





• Molecule 9: PROTEASOME SUBUNIT BETA TYPE-3

Chain I: 93% 6%



• Molecule 9: PROTEASOME SUBUNIT BETA TYPE-3

Chain W: 93% 6%



• Molecule 10: PROTEASOME SUBUNIT BETA TYPE-4

Chain J: 88% 10% 2%



• Molecule 10: PROTEASOME SUBUNIT BETA TYPE-4

Chain X: 88% 10% 2%



• Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5

Chain K: 91% 7%



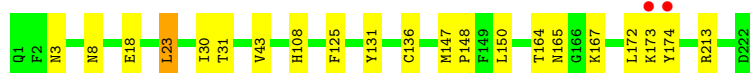
• Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5

Chain Y: 90% 8%

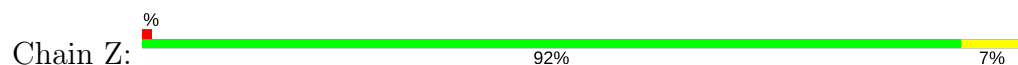


• Molecule 12: PROTEASOME SUBUNIT BETA TYPE-6

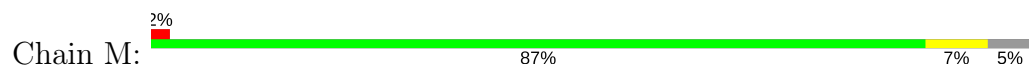
Chain L: 91% 9%



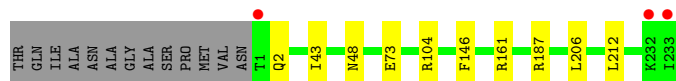
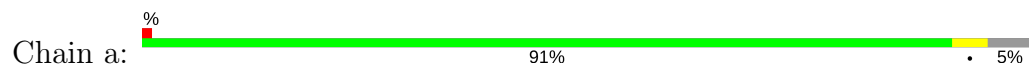
- Molecule 12: PROTEASOME SUBUNIT BETA TYPE-6



- Molecule 13: PROTEASOME SUBUNIT BETA TYPE-7



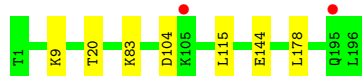
- Molecule 13: PROTEASOME SUBUNIT BETA TYPE-7



- Molecule 14: PROTEASOME SUBUNIT BETA TYPE-1



- Molecule 14: PROTEASOME SUBUNIT BETA TYPE-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.58Å 300.82Å 146.29Å 90.00° 113.20° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-2.40) 97.0 (15.00-2.40)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.00 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.177 , 0.195 0.181 , 0.197	Depositor DCC
$R_{free}$ test set	20336 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.6	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	51115	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/1952	0.50	0/2642
1	O	0.27	0/1952	0.50	0/2642
2	B	0.29	0/1934	0.54	0/2618
2	P	0.29	0/1934	0.54	0/2618
3	C	0.28	0/1910	0.55	0/2586
3	Q	0.28	0/1910	0.55	0/2586
4	D	0.27	0/1837	0.52	0/2475
4	R	0.27	0/1837	0.52	0/2475
5	E	0.28	0/1800	0.52	1/2433 (0.0%)
5	S	0.28	0/1800	0.52	1/2433 (0.0%)
6	F	0.28	0/1932	0.49	0/2609
6	T	0.28	0/1932	0.49	0/2609
7	G	0.28	0/1945	0.52	0/2634
7	U	0.28	0/1945	0.52	0/2634
8	H	0.32	0/1750	0.52	0/2373
8	V	0.26	0/1750	0.51	0/2373
9	I	0.28	0/1611	0.51	0/2174
9	W	0.28	0/1611	0.51	0/2174
10	J	0.27	0/1589	0.52	0/2142
10	X	0.27	0/1589	0.52	0/2142
11	K	0.26	0/1674	0.53	1/2264 (0.0%)
11	Y	0.26	0/1674	0.53	1/2264 (0.0%)
12	L	0.30	0/1795	0.51	0/2420
12	Z	0.27	0/1795	0.51	0/2420
13	M	0.34	0/1855	0.59	0/2514
13	a	0.34	0/1855	0.58	0/2514
14	N	0.26	0/1541	0.49	0/2087
14	b	0.26	0/1541	0.49	0/2087
All	All	0.28	0/50250	0.52	4/67942 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	4	LEU	CA-CB-CG	5.70	128.40	115.30
11	Y	4	LEU	CA-CB-CG	5.68	128.37	115.30
5	E	71	LEU	CA-CB-CG	5.04	126.90	115.30
5	S	71	LEU	CA-CB-CG	5.01	126.83	115.30

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	3	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	16	0
2	P	1904	0	1904	19	0
3	C	1881	0	1895	9	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	12	0
4	R	1813	0	1797	11	0
5	E	1773	0	1775	10	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	9	0
6	T	1892	0	1883	8	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	8	0
8	V	1719	0	1719	8	0
9	I	1581	0	1574	4	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	7	0
11	K	1637	0	1583	6	0
11	Y	1637	0	1583	7	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1824	0	1832	5	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	9	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	K	6	0	7	0	0
16	Y	6	0	7	0	0
17	A	79	0	0	0	0
17	B	62	0	0	0	0
17	C	48	0	0	0	0
17	D	56	0	0	0	0
17	E	18	0	0	0	0
17	F	67	0	0	0	0
17	G	83	0	0	0	0
17	H	66	0	0	0	0
17	I	73	0	0	0	0
17	J	85	0	0	0	0
17	K	77	0	0	0	0
17	L	69	0	0	1	0
17	M	81	0	0	1	0
17	N	61	0	0	0	0
17	O	42	0	0	0	0
17	P	52	0	0	1	0
17	Q	31	0	0	0	0
17	R	50	0	0	0	0
17	S	24	0	0	0	0
17	T	62	0	0	0	0
17	U	62	0	0	0	0
17	V	58	0	0	0	0
17	W	68	0	0	0	0
17	X	66	0	0	0	0
17	Y	69	0	0	0	0
17	Z	81	0	0	0	0
17	a	84	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	b	66	0	0	0	0
All	All	51115	0	49120	180	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 (180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:50:LYS:HA	2:P:50:LYS:HE3	1.28	1.13
2:P:52:THR:HG22	2:P:53:SER:N	1.82	0.95
2:B:52:THR:HG22	2:B:53:SER:N	1.89	0.88
2:P:52:THR:CG2	2:P:53:SER:N	2.38	0.86
2:P:50:LYS:HA	2:P:50:LYS:CE	2.01	0.85
2:B:30:HIS:O	2:B:50:LYS:HE3	1.86	0.74
2:B:52:THR:CG2	2:B:53:SER:N	2.53	0.72
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.75	0.68
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.76	0.67
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.77	0.67
2:P:52:THR:CG2	2:P:53:SER:H	2.05	0.67
11:K:53:GLN:O	11:K:57:THR:HG23	1.95	0.66
3:C:51:LYS:O	3:C:52:LEU:HB2	1.95	0.66
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.77	0.66
2:B:12:PHE:H	3:C:17:GLN:HE22	1.44	0.65
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.96	0.65
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.96	0.65
2:B:52:THR:HG22	2:B:53:SER:O	1.97	0.63
2:P:217:LYS:O	2:P:219:ALA:N	2.33	0.62
7:U:187:GLU:HG2	7:U:192:LYS:HB3	1.82	0.61
2:B:217:LYS:O	2:B:219:ALA:N	2.33	0.61
7:G:187:GLU:HG2	7:G:192:LYS:HB3	1.82	0.60
5:E:12:PHE:H	6:F:19:GLN:HE22	1.50	0.59
1:A:176:GLU:HG2	2:B:55:LEU:HD22	1.83	0.59
5:S:12:PHE:H	6:T:19:GLN:HE22	1.52	0.58
14:N:20:THR:HG22	14:N:31:THR:OG1	2.04	0.58
2:P:52:THR:HG22	2:P:53:SER:C	2.25	0.58
3:C:201:VAL:O	3:C:202:GLN:CB	2.53	0.57
6:T:146:MET:CE	6:T:161:THR:HB	2.35	0.56
6:F:146:MET:CE	6:F:161:THR:HB	2.35	0.56
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.53	0.56
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.88	0.56
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.88	0.55
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.87	0.54
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.37	0.54
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.54
14:N:35:THR:HG21	14:N:45:ARG:HE	1.71	0.54
2:P:52:THR:HG22	2:P:53:SER:CA	2.38	0.54
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.53
2:B:52:THR:CG2	2:B:53:SER:H	2.20	0.53
5:S:9:THR:HG21	5:S:119:THR:HA	1.91	0.53
14:N:20:THR:CG2	14:N:31:THR:OG1	2.57	0.53
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.92	0.52
5:E:9:THR:HG21	5:E:119:THR:HA	1.90	0.52
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.92	0.52
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.92	0.49
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.94	0.49
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.95	0.49
14:N:35:THR:CG2	14:N:45:ARG:HE	2.26	0.49
2:P:93:HIS:HB3	17:P:302:HOH:O	2.13	0.49
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.95	0.49
6:T:34:ILE:HG12	6:T:196:ILE:HD11	1.95	0.49
10:J:149:ARG:O	10:J:152:MET:HG3	2.13	0.49
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.47	0.49
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.48	0.49
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.95	0.49
6:F:146:MET:HE1	6:F:161:THR:HB	1.93	0.48
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.62	0.48
10:X:149:ARG:O	10:X:152:MET:HG3	2.12	0.48
6:F:34:ILE:HG12	6:F:196:ILE:HD11	1.95	0.48
14:N:13:ILE:HG21	14:N:175:MET:CE	2.43	0.48
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.48	0.48
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.14	0.48
13:M:159:VAL:HG23	13:M:159:VAL:O	2.14	0.47
6:T:146:MET:HE3	6:T:161:THR:HB	1.95	0.47
5:E:176:ASP:O	5:E:180:LYS:HD3	2.15	0.47
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.49	0.47
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.97	0.47
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.50	0.47
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.96	0.47
5:S:176:ASP:O	5:S:180:LYS:HD3	2.15	0.47
9:W:98:ARG:HD2	9:W:126:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:52:THR:HG22	2:P:53:SER:O	2.15	0.46
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.97	0.46
9:I:98:ARG:HD2	9:I:126:ILE:HG12	1.97	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.98	0.46
13:M:96:LEU:O	13:M:100:MET:HG2	2.15	0.46
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.46	0.46
6:T:146:MET:HE1	6:T:161:THR:HB	1.97	0.46
2:B:52:THR:HG22	2:B:53:SER:H	1.72	0.46
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.97	0.46
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.46	0.45
4:D:176:LEU:HD22	5:E:55:LEU:HD22	1.98	0.45
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.46	0.45
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.97	0.45
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.46	0.45
2:P:52:THR:CG2	2:P:53:SER:O	2.64	0.45
2:B:52:THR:HG22	2:B:53:SER:C	2.37	0.45
8:V:225:GLU:O	8:V:226:GLU:HB2	2.16	0.45
2:P:15:GLU:O	3:Q:27:ARG:NH1	2.47	0.45
8:H:225:GLU:O	8:H:226:GLU:HB2	2.16	0.44
3:Q:232:THR:O	3:Q:236:GLN:HG3	2.18	0.44
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.00	0.44
10:J:1:MET:CB	10:J:34:LYS:HE3	2.48	0.44
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.00	0.44
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.00	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.48	0.44
12:L:213:ARG:NH1	17:L:331:HOH:O	2.51	0.44
3:C:232:THR:O	3:C:236:GLN:HG3	2.17	0.44
6:F:146:MET:HE3	6:F:161:THR:HB	1.99	0.44
10:X:1:MET:CB	10:X:34:LYS:HE3	2.48	0.44
11:K:12:ILE:HB	11:K:180:VAL:HB	2.00	0.44
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	2.00	0.44
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.00	0.43
2:P:58:GLN:NE2	2:P:208:ASP:HA	2.33	0.43
2:P:52:THR:HG23	2:P:53:SER:H	1.79	0.43
6:T:171:GLU:HB3	6:T:195:ILE:HG12	2.00	0.43
8:V:3:ILE:HG22	8:V:99:ILE:HD12	2.00	0.43
3:C:201:VAL:O	3:C:202:GLN:HB2	2.18	0.43
3:C:205:ALA:C	3:C:207:ASN:H	2.21	0.43
8:H:3:ILE:HG22	8:H:99:ILE:HD12	2.00	0.43
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.48	0.43
3:Q:205:ALA:C	3:Q:207:ASN:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:148:LYS:HE3	8:V:177:VAL:HG11	2.00	0.43
2:B:30:HIS:O	2:B:50:LYS:CE	2.60	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.43
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.01	0.43
8:H:148:LYS:HE3	8:H:177:VAL:HG11	2.00	0.43
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.18	0.43
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.43
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.00	0.43
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.49	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.01	0.42
10:X:168:LEU:O	10:X:172:MET:HB2	2.19	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
4:D:1:ASP:O	4:D:2:ARG:HB2	2.19	0.42
6:F:171:GLU:HB3	6:F:195:ILE:HG12	2.00	0.42
10:J:168:LEU:O	10:J:172:MET:HB2	2.19	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.42
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.01	0.42
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.54	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.02	0.42
2:P:50:LYS:CA	2:P:50:LYS:CE	2.85	0.42
4:R:1:ASP:O	4:R:2:ARG:HB2	2.19	0.42
10:X:162:LYS:HG3	10:X:195:PHE:CZ	2.55	0.42
4:D:185:LEU:O	4:D:189:GLU:HG3	2.20	0.42
2:B:58:GLN:NE2	2:B:208:ASP:HA	2.34	0.42
12:L:23:LEU:HD13	12:L:43:VAL:HG13	2.00	0.42
6:F:50:ILE:HG13	6:F:208:PHE:HA	2.01	0.42
4:R:185:LEU:O	4:R:189:GLU:HG3	2.20	0.42
12:L:147:MET:N	12:L:148:PRO:CD	2.82	0.42
13:M:2:GLN:NE2	17:M:377:HOH:O	2.53	0.42
4:D:60:VAL:HG11	4:D:81:ILE:HG21	2.03	0.41
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.60	0.41
6:T:50:ILE:HG13	6:T:208:PHE:HA	2.01	0.41
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.01	0.41
8:H:98:LEU:HB2	8:H:113:ILE:CG2	2.50	0.41
14:N:20:THR:HG23	14:N:28:ASN:HB3	2.02	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
8:V:34:LEU:HD12	8:V:44:ALA:HB2	2.02	0.41
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.86	0.41
8:H:34:LEU:HD12	8:H:44:ALA:HB2	2.02	0.41
10:J:162:LYS:HG3	10:J:195:PHE:CZ	2.55	0.41
2:P:149:THR:HG1	2:P:159:TRP:HE1	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:60:VAL:HG11	4:R:81:ILE:HG21	2.02	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.03	0.41
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.34	0.41
12:L:164:THR:O	12:L:167:LYS:HE3	2.21	0.41
4:R:4:VAL:HG13	4:R:15:GLN:HG3	2.03	0.41
4:R:77:ALA:O	4:R:81:ILE:HG12	2.21	0.41
4:D:4:VAL:HG13	4:D:15:GLN:HG3	2.03	0.41
5:E:35:VAL:HG22	5:E:159:ALA:HB2	2.03	0.41
7:G:34:LEU:HD23	7:G:34:LEU:C	2.40	0.41
11:Y:13:ILE:HG13	11:Y:153:ALA:HB1	2.03	0.41
5:E:68:HIS:HE1	5:E:102:LEU:O	2.04	0.41
8:V:98:LEU:HB2	8:V:113:ILE:CG2	2.50	0.41
5:E:155:LEU:HD13	5:E:158:THR:HB	2.03	0.40
5:E:206:THR:OG1	5:E:209:ASN:HB2	2.21	0.40
6:F:46:VAL:HB	6:F:73:VAL:HG21	2.03	0.40
5:S:35:VAL:HG22	5:S:159:ALA:HB2	2.03	0.40
1:A:1:MET:CG	1:A:2:THR:N	2.85	0.40
3:C:9:PHE:H	4:D:15:GLN:HE22	1.69	0.40
1:O:55:LEU:HB3	7:U:159:ALA:O	2.21	0.40
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.57	0.40
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.57	0.40
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.40
1:A:115:ALA:HB1	1:A:154:GLY:O	2.21	0.40
13:M:128:ARG:HH11	13:M:138:SER:HB2	1.87	0.40
12:Z:164:THR:O	12:Z:167:LYS:HE3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	6 (2%)	2 (1%)	22 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	22	33
2	B	242/258 (94%)	233 (96%)	4 (2%)	5 (2%)	8	9
2	P	242/258 (94%)	232 (96%)	4 (2%)	6 (2%)	6	6
3	C	238/254 (94%)	231 (97%)	3 (1%)	4 (2%)	11	13
3	Q	238/254 (94%)	230 (97%)	4 (2%)	4 (2%)	11	13
4	D	231/260 (89%)	227 (98%)	3 (1%)	1 (0%)	38	54
4	R	231/260 (89%)	227 (98%)	3 (1%)	1 (0%)	38	54
5	E	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
5	S	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
6	F	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
9	W	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	J	193/198 (98%)	187 (97%)	6 (3%)	0	100	100
10	X	193/198 (98%)	187 (97%)	6 (3%)	0	100	100
11	K	209/212 (99%)	201 (96%)	8 (4%)	0	100	100
11	Y	209/212 (99%)	201 (96%)	8 (4%)	0	100	100
12	L	220/222 (99%)	216 (98%)	3 (1%)	1 (0%)	32	46
12	Z	220/222 (99%)	216 (98%)	3 (1%)	1 (0%)	32	46
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6282/6614 (95%)	6102 (97%)	153 (2%)	27 (0%)	38	54

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR

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Mol	Chain	Res	Type
2	B	218	GLY
2	B	222	GLY
3	C	202	GLN
3	C	205	ALA
1	O	2	THR
2	P	51	VAL
2	P	218	GLY
2	P	222	GLY
3	Q	202	GLN
3	Q	205	ALA
1	A	166	LYS
2	B	51	VAL
1	O	166	LYS
2	B	220	ASN
12	L	165	ASN
2	P	220	ASN
12	Z	165	ASN
4	D	2	ARG
4	R	2	ARG
2	B	221	ASP
3	C	183	PRO
3	C	239	GLN
2	P	52	THR
2	P	221	ASP
3	Q	183	PRO
3	Q	239	GLN

### 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%)	202 (97%)	7 (3%)	43	64
1	O	209/209 (100%)	202 (97%)	7 (3%)	43	64
2	B	203/216 (94%)	193 (95%)	10 (5%)	29	46
2	P	203/216 (94%)	192 (95%)	11 (5%)	26	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	212/226 (94%)	188 (89%)	24 (11%)	7	9
3	Q	212/226 (94%)	188 (89%)	24 (11%)	7	9
4	D	194/215 (90%)	179 (92%)	15 (8%)	15	23
4	R	194/215 (90%)	179 (92%)	15 (8%)	15	23
5	E	190/193 (98%)	173 (91%)	17 (9%)	11	17
5	S	190/193 (98%)	173 (91%)	17 (9%)	11	17
6	F	201/239 (84%)	183 (91%)	18 (9%)	11	16
6	T	201/239 (84%)	183 (91%)	18 (9%)	11	16
7	G	206/210 (98%)	195 (95%)	11 (5%)	26	42
7	U	206/210 (98%)	195 (95%)	11 (5%)	26	42
8	H	185/190 (97%)	175 (95%)	10 (5%)	26	41
8	V	185/190 (97%)	175 (95%)	10 (5%)	26	41
9	I	172/173 (99%)	165 (96%)	7 (4%)	35	54
9	W	172/173 (99%)	165 (96%)	7 (4%)	35	54
10	J	173/175 (99%)	166 (96%)	7 (4%)	36	55
10	X	173/175 (99%)	166 (96%)	7 (4%)	36	55
11	K	168/169 (99%)	158 (94%)	10 (6%)	22	35
11	Y	168/169 (99%)	158 (94%)	10 (6%)	22	35
12	L	185/185 (100%)	175 (95%)	10 (5%)	26	41
12	Z	185/185 (100%)	174 (94%)	11 (6%)	23	36
13	M	199/208 (96%)	188 (94%)	11 (6%)	25	40
13	a	199/208 (96%)	189 (95%)	10 (5%)	28	45
14	N	162/162 (100%)	155 (96%)	7 (4%)	33	52
14	b	162/162 (100%)	155 (96%)	7 (4%)	33	52
All	All	5318/5540 (96%)	4989 (94%)	329 (6%)	21	34

All (329) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	59	GLU
1	A	61	LEU
1	A	122	THR
1	A	157	PHE

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Mol	Chain	Res	Type
1	A	201	GLU
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	58	GLN
2	B	65	LEU
2	B	79	LEU
2	B	102	ASN
2	B	119	GLN
2	B	180	LYS
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	48	SER
3	C	49	THR
3	C	50	LEU
3	C	51	LYS
3	C	52	LEU
3	C	53	GLN
3	C	55	THR
3	C	58	THR
3	C	61	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	167	LYS
3	C	169	VAL
3	C	171	GLU
3	C	175	LYS
3	C	180	LYS
3	C	181	GLU
3	C	203	THR
3	C	206	LYS
3	C	213	VAL
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	68	CYS
4	D	99	ILE
4	D	117	GLU

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Mol	Chain	Res	Type
4	D	125	LEU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	3	ASN
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	174	THR
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL
5	E	208	ASP
5	E	217	LYS
6	F	14	ASP
6	F	96	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	163	LYS
6	F	165	ARG
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	187	GLU
6	F	198	LEU
6	F	201	GLU
6	F	202	ASP
6	F	214	TRP
6	F	215	CYS

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Mol	Chain	Res	Type
6	F	221	ASN
6	F	241	LYS
7	G	13	GLU
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	166	GLN
7	G	235	ARG
7	G	236	LEU
7	G	242	GLN
8	H	13	VAL
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	106	THR
8	H	153	LYS
8	H	185	GLU
8	H	196	ARG
8	H	222	ASP
9	I	37	ASN
9	I	96	GLU
9	I	117	LYS
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	2	ASP
10	J	3	ILE
10	J	23	ARG
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	57	THR
11	K	67	GLU

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Mol	Chain	Res	Type
11	K	97	MET
11	K	104	TYR
11	K	107	LYS
11	K	128	CYS
11	K	148	LEU
12	L	3	ASN
12	L	18	GLU
12	L	23	LEU
12	L	31	THR
12	L	108	HIS
12	L	136	CYS
12	L	150	LEU
12	L	172	LEU
12	L	173	LYS
12	L	174	TYR
13	M	2	GLN
13	M	43	ILE
13	M	48	ASN
13	M	73	GLU
13	M	104	ARG
13	M	106	LYS
13	M	146	PHE
13	M	161	ARG
13	M	187	ARG
13	M	206	LEU
13	M	212	LEU
14	N	9	LYS
14	N	20	THR
14	N	83	LYS
14	N	104	ASP
14	N	115	LEU
14	N	144	GLU
14	N	178	LEU
1	O	29	LYS
1	O	59	GLU
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	201	GLU
1	O	250	LEU
2	P	50	LYS
2	P	51	VAL

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Mol	Chain	Res	Type
2	P	55	LEU
2	P	58	GLN
2	P	65	LEU
2	P	79	LEU
2	P	102	ASN
2	P	119	GLN
2	P	180	LYS
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	48	SER
3	Q	49	THR
3	Q	50	LEU
3	Q	51	LYS
3	Q	52	LEU
3	Q	53	GLN
3	Q	55	THR
3	Q	58	THR
3	Q	61	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	167	LYS
3	Q	169	VAL
3	Q	171	GLU
3	Q	175	LYS
3	Q	180	LYS
3	Q	181	GLU
3	Q	203	THR
3	Q	206	LYS
3	Q	213	VAL
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	68	CYS
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	190	LEU

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Mol	Chain	Res	Type
4	R	193	LEU
4	R	202	GLU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	3	ASN
5	S	8	ASP
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	174	THR
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
5	S	208	ASP
5	S	217	LYS
6	T	14	ASP
6	T	96	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	163	LYS
6	T	165	ARG
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	187	GLU
6	T	198	LEU
6	T	201	GLU
6	T	202	ASP
6	T	214	TRP
6	T	215	CYS
6	T	221	ASN
6	T	241	LYS
7	U	13	GLU

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Mol	Chain	Res	Type
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	166	GLN
7	U	235	ARG
7	U	236	LEU
7	U	242	GLN
8	V	13	VAL
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	106	THR
8	V	153	LYS
8	V	185	GLU
8	V	196	ARG
8	V	222	ASP
9	W	37	ASN
9	W	96	GLU
9	W	117	LYS
9	W	126	ILE
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	2	ASP
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
10	X	110	LYS
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	57	THR
11	Y	67	GLU
11	Y	97	MET
11	Y	104	TYR
11	Y	107	LYS

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Mol	Chain	Res	Type
11	Y	128	CYS
11	Y	148	LEU
12	Z	3	ASN
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	108	HIS
12	Z	136	CYS
12	Z	150	LEU
12	Z	172	LEU
12	Z	173	LYS
12	Z	174	TYR
13	a	2	GLN
13	a	43	ILE
13	a	48	ASN
13	a	73	GLU
13	a	104	ARG
13	a	146	PHE
13	a	161	ARG
13	a	187	ARG
13	a	206	LEU
13	a	212	LEU
14	b	9	LYS
14	b	20	THR
14	b	83	LYS
14	b	104	ASP
14	b	115	LEU
14	b	144	GLU
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN

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Mol	Chain	Res	Type
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	100	ASN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	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	186	ASN
8	H	66	HIS
8	H	114	HIS
8	H	116	HIS
8	H	165	ASN
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN

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Mol	Chain	Res	Type
12	L	49	ASN
12	L	158	ASN
13	M	48	ASN
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	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
4	R	15	GLN
4	R	100	ASN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	120	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	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN

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Mol	Chain	Res	Type
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
8	V	30	ASN
8	V	66	HIS
8	V	114	HIS
8	V	116	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	190	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
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 ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 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	$\# Z  > 2$
16	ABA	K	301	11	5,5,6	1.39	1 (20%)	3,5,7	0.89	0
16	ABA	Y	301	11	5,5,6	1.41	1 (20%)	3,5,7	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	ABA	K	301	11	-	0/2/4/6	0/0/0/0
16	ABA	Y	301	11	-	0/2/4/6	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	301	ABA	CA-C	2.52	1.53	1.50
16	Y	301	ABA	CA-C	2.58	1.53	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.41	11 (4%) 35 33	33, 46, 82, 120	0
1	O	250/250 (100%)	-0.31	7 (2%) 53 51	39, 55, 102, 134	0
2	B	244/258 (94%)	-0.30	8 (3%) 47 45	33, 51, 95, 158	0
2	P	244/258 (94%)	-0.17	12 (4%) 30 29	37, 54, 105, 160	0
3	C	240/254 (94%)	-0.15	16 (6%) 19 17	33, 56, 123, 146	0
3	Q	240/254 (94%)	0.06	15 (6%) 21 19	36, 65, 146, 163	0
4	D	235/260 (90%)	-0.38	4 (1%) 70 68	37, 57, 94, 141	0
4	R	235/260 (90%)	-0.32	7 (2%) 51 49	39, 60, 97, 131	0
5	E	231/234 (98%)	-0.33	6 (2%) 56 54	41, 60, 96, 135	0
5	S	231/234 (98%)	-0.24	4 (1%) 70 68	42, 66, 107, 152	0
6	F	243/288 (84%)	-0.40	7 (2%) 52 50	33, 53, 98, 141	0
6	T	243/288 (84%)	-0.29	9 (3%) 42 41	36, 60, 116, 150	0
7	G	241/252 (95%)	-0.46	4 (1%) 70 68	32, 48, 84, 129	0
7	U	241/252 (95%)	-0.40	4 (1%) 70 68	37, 53, 89, 126	0
8	H	226/232 (97%)	-0.37	7 (3%) 49 47	34, 45, 81, 154	0
8	V	226/232 (97%)	-0.29	7 (3%) 49 47	36, 51, 88, 161	0
9	I	204/205 (99%)	-0.69	1 (0%) 90 89	31, 43, 70, 105	0
9	W	204/205 (99%)	-0.59	2 (0%) 82 80	31, 45, 77, 102	0
10	J	195/198 (98%)	-0.51	3 (1%) 74 72	31, 46, 74, 138	0
10	X	195/198 (98%)	-0.45	4 (2%) 64 61	35, 48, 77, 143	0
11	K	211/212 (99%)	-0.53	0 100 100	33, 46, 72, 86	0
11	Y	211/212 (99%)	-0.54	1 (0%) 90 89	34, 46, 72, 93	0
12	L	222/222 (100%)	-0.57	2 (0%) 84 82	33, 49, 78, 133	0
12	Z	222/222 (100%)	-0.58	2 (0%) 84 82	28, 47, 76, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.56	4 (1%)	70 68	31, 48, 76, 144	0
13	a	233/246 (94%)	-0.51	3 (1%)	77 75	31, 46, 75, 142	0
14	N	196/196 (100%)	-0.58	2 (1%)	82 80	31, 44, 73, 114	0
14	b	196/196 (100%)	-0.57	2 (1%)	82 80	33, 45, 73, 109	0
All	All	6342/6614 (95%)	-0.40	154 (2%)	59 56	28, 51, 95, 163	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	10.8
3	Q	49	THR	9.5
2	P	219	ALA	9.0
8	V	224	GLN	8.3
8	V	223	ILE	8.3
10	J	1	MET	7.7
13	a	233	ILE	7.6
8	V	222	ASP	7.5
2	B	221	ASP	7.1
3	Q	50	LEU	6.8
8	V	221	CYS	6.6
2	P	220	ASN	6.5
3	C	236	GLN	6.3
8	H	224	GLN	6.2
3	Q	206	LYS	6.0
8	V	226	GLU	5.9
8	H	223	ILE	5.7
3	C	49	THR	5.3
3	C	206	LYS	5.3
12	L	174	TYR	5.3
5	S	202	ASP	5.2
13	M	233	ILE	5.2
2	P	51	VAL	5.0
13	a	232	LYS	5.0
8	H	222	ASP	4.8
3	Q	236	GLN	4.6
6	T	243	ILE	4.6
2	B	219	ALA	4.5
2	P	59	ASP	4.5
9	W	1	SER	4.5
5	E	202	ASP	4.5
2	P	221	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	O	249	ALA	4.3
10	J	194	ASP	4.3
8	H	226	GLU	4.3
10	X	194	ASP	4.2
2	B	51	VAL	4.1
2	P	222	GLY	4.1
13	M	232	LYS	4.0
3	Q	48	SER	3.9
8	H	221	CYS	3.8
4	R	1	ASP	3.7
3	C	205	ALA	3.6
8	H	225	GLU	3.6
1	O	2	THR	3.6
3	Q	239	GLN	3.6
10	X	193	ASP	3.6
6	T	244	ASN	3.5
3	C	238	LYS	3.5
3	Q	238	LYS	3.5
1	A	249	ALA	3.5
3	Q	204	GLY	3.5
2	P	218	GLY	3.4
1	O	1	MET	3.4
5	E	122	TYR	3.4
6	T	181	GLU	3.3
8	V	225	GLU	3.3
3	C	50	LEU	3.3
6	T	180	PRO	3.3
1	A	1	MET	3.3
4	D	242	GLU	3.3
3	Q	202	GLN	3.3
7	U	242	GLN	3.3
5	E	123	GLY	3.2
9	I	1	SER	3.1
3	Q	225	GLU	3.1
1	O	201	GLU	3.1
3	C	239	GLN	3.0
6	F	244	ASN	3.0
6	F	205	GLU	3.0
1	A	2	THR	3.0
10	J	193	ASP	3.0
1	A	248	GLU	3.0
3	Q	205	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
3	Q	240	GLU	2.9
3	C	216	ASP	2.9
2	B	220	ASN	2.9
1	O	250	LEU	2.9
12	Z	174	TYR	2.9
3	Q	203	THR	2.8
1	A	201	GLU	2.8
5	E	201	ARG	2.8
8	H	198	GLU	2.8
5	S	233	ILE	2.8
6	F	180	PRO	2.8
6	F	202	ASP	2.7
14	b	105	LYS	2.7
9	W	192	ASP	2.7
14	b	195	GLN	2.7
6	F	181	GLU	2.7
7	G	240	ALA	2.6
1	A	250	LEU	2.6
4	D	1	ASP	2.6
2	P	240	LYS	2.6
3	C	181	GLU	2.6
7	G	242	GLN	2.6
8	V	198	GLU	2.6
3	C	47	ARG	2.6
3	Q	55	THR	2.6
5	S	201	ARG	2.6
3	C	202	GLN	2.6
2	B	59	ASP	2.6
6	T	2	THR	2.5
2	B	217	LYS	2.5
7	G	179	LYS	2.5
4	R	240	ALA	2.5
1	A	54	PRO	2.5
12	Z	167	LYS	2.5
2	P	225	TYR	2.5
3	C	240	GLU	2.5
4	R	242	GLU	2.5
6	F	243	ILE	2.4
2	P	60	THR	2.4
4	R	217	GLN	2.4
3	C	235	GLU	2.4
1	A	203	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	227	GLU	2.4
11	Y	212	GLY	2.3
5	E	233	ILE	2.3
1	O	203	GLU	2.3
13	a	1	THR	2.3
4	R	125	LEU	2.3
2	P	52	THR	2.3
5	S	173	ARG	2.3
7	U	181	LYS	2.3
14	N	195	GLN	2.3
6	T	241	LYS	2.3
7	U	51	PRO	2.3
1	A	231	LYS	2.3
1	O	52	SER	2.3
4	R	54	ASP	2.3
13	M	1	THR	2.3
4	D	201	GLU	2.3
3	C	139	ARG	2.2
12	L	173	LYS	2.2
7	G	3	TYR	2.2
14	N	105	LYS	2.2
2	P	182	ASP	2.2
6	T	178	HIS	2.2
1	A	229	THR	2.2
7	U	222	ASP	2.2
6	T	205	GLU	2.2
1	A	62	SER	2.2
13	M	47	ASP	2.1
2	B	222	GLY	2.1
4	R	141	ALA	2.1
3	C	48	SER	2.1
3	C	60	SER	2.1
4	D	224	ASP	2.1
2	B	240	LYS	2.1
10	X	72	ASP	2.0
6	F	2	THR	2.0
6	T	206	LYS	2.0
3	Q	47	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	MG	K	303	1/1	0.98	0.39	13.29	48,48,48,48	0
15	MG	J	201	1/1	0.93	0.31	11.17	56,56,56,56	0
15	MG	I	302	1/1	0.89	0.27	4.59	79,79,79,79	0
16	ABA	K	301	6/7	0.92	0.17	3.03	43,45,46,48	0
16	ABA	Y	301	6/7	0.95	0.15	1.13	44,45,47,49	0
15	MG	G	301	1/1	0.99	0.05	-1.37	43,43,43,43	0
15	MG	Y	302	1/1	0.99	0.06	-1.44	37,37,37,37	0
15	MG	N	201	1/1	0.98	0.07	-1.51	43,43,43,43	0
15	MG	K	302	1/1	0.97	0.06	-1.65	42,42,42,42	0
15	MG	Z	301	1/1	0.98	0.08	-1.77	57,57,57,57	0
15	MG	I	301	1/1	0.99	0.04	-2.14	45,45,45,45	0
15	MG	V	301	1/1	0.98	0.05	-2.17	52,52,52,52	0
15	MG	H	301	1/1	0.87	0.23	-	83,83,83,83	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.