



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:10 PM GMT

PDB ID : 4QWJ  
Title : yCP beta5-A49T-mutant in complex with carfilzomib  
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.  
Deposited on : 2014-07-16  
Resolution : 2.90 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

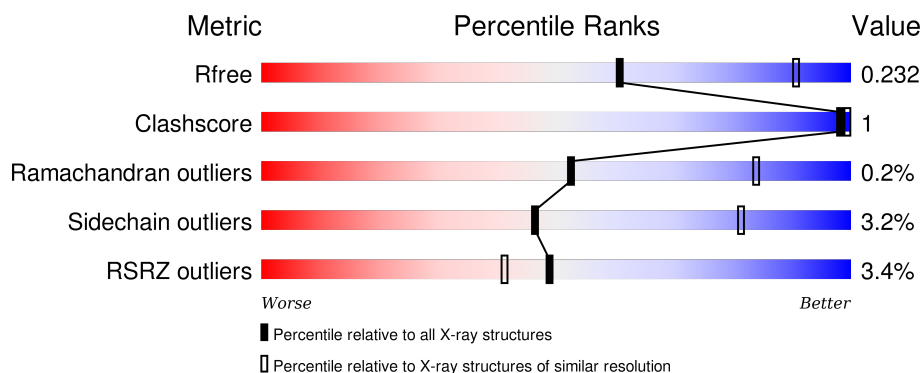
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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>5%</div> <div>98%</div> <div>.</div> </div>
1	O	250	<div> <div>4%</div> <div>98%</div> <div>.</div> </div>
2	B	258	<div> <div>6%</div> <div>90%</div> <div>5% 5%</div> </div>
2	P	258	<div> <div>4%</div> <div>90%</div> <div>. . 5%</div> </div>
3	C	254	<div> <div>7%</div> <div>89%</div> <div>. . 6%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	
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	K	302	-	-	-	X
16	CL	N	203	-	-	-	X
17	3BV	H	301	-	-	-	X
17	3BV	K	301	-	-	-	X
17	3BV	N	201	-	-	-	X
17	3BV	V	301	-	-	-	X
17	3BV	b	201	-	-	-	X
18	MES	K	303	-	-	-	X
18	MES	Y	303	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49730 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	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	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			

*Continued on next page...*

*Continued from previous page...*

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	212	Total	C	N	O	S	0	0	0
			1646	1046	280	313	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1646	1046	280	313	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	49	THR	ALA	ENGINEERED MUTATION	UNP P30656
Y	49	THR	ALA	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	230	Total	C	N	O	S	0	0	0
			1797	1137	307	346	7			
13	a	228	Total	C	N	O	S	0	0	0
			1786	1131	305	343	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			

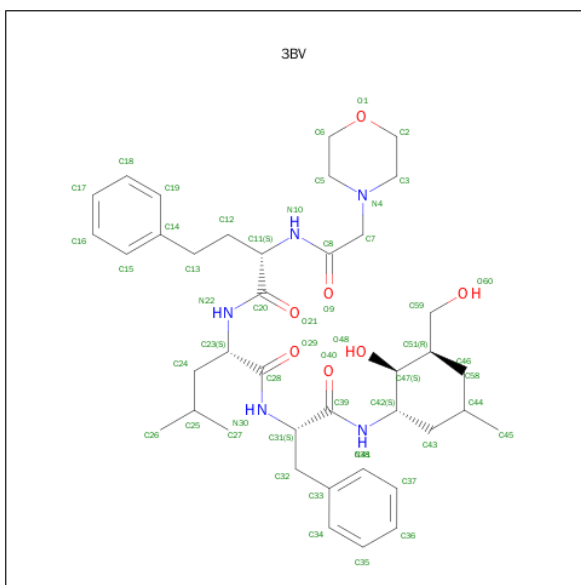
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

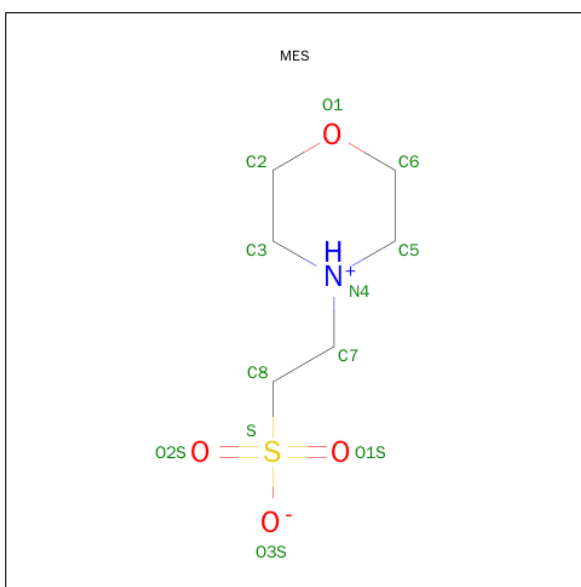
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	b	1	Total Cl 1 1	0	0
16	N	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is N-{(2S)-2-[(MORPHOLIN-4-YLACETYL)AMINO]-4-PHENYLBUTANOYL}-L-LEUCYL-N-[(2R,3S,4S)-1,3-DIHYDROXY-2,6-DIMETHYLHEPTAN-4-YL]-L-PHENYLALANINAMIDE (three-letter code: 3BV) (formula: C<sub>40</sub>H<sub>61</sub>N<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			52	40	5	7		
17	K	1	Total	C	N	O	0	0
			52	40	5	7		
17	N	1	Total	C	N	O	0	0
			52	40	5	7		
17	V	1	Total	C	N	O	0	0
			52	40	5	7		
17	Y	1	Total	C	N	O	0	0
			52	40	5	7		
17	b	1	Total	C	N	O	0	0
			52	40	5	7		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	9	Total	O	0	0
			9	9		
19	B	6	Total	O	0	0
			6	6		
19	C	3	Total	O	0	0
			3	3		
19	D	3	Total	O	0	0
			3	3		
19	E	4	Total	O	0	0
			4	4		
19	F	11	Total	O	0	0
			11	11		
19	G	6	Total	O	0	0
			6	6		
19	H	4	Total	O	0	0
			4	4		
19	I	3	Total	O	0	0
			3	3		
19	J	9	Total	O	0	0
			9	9		

*Continued on next page...*

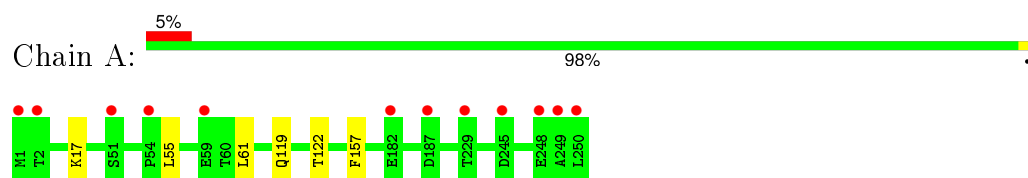
*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	3	Total O 3 3	0	0
19	L	6	Total O 6 6	0	0
19	M	9	Total O 9 9	0	0
19	N	2	Total O 2 2	0	0
19	O	2	Total O 2 2	0	0
19	P	3	Total O 3 3	0	0
19	Q	3	Total O 3 3	0	0
19	R	3	Total O 3 3	0	0
19	S	4	Total O 4 4	0	0
19	T	7	Total O 7 7	0	0
19	U	4	Total O 4 4	0	0
19	V	4	Total O 4 4	0	0
19	W	3	Total O 3 3	0	0
19	X	8	Total O 8 8	0	0
19	Y	7	Total O 7 7	0	0
19	Z	6	Total O 6 6	0	0
19	a	8	Total O 8 8	0	0
19	b	8	Total O 8 8	0	0

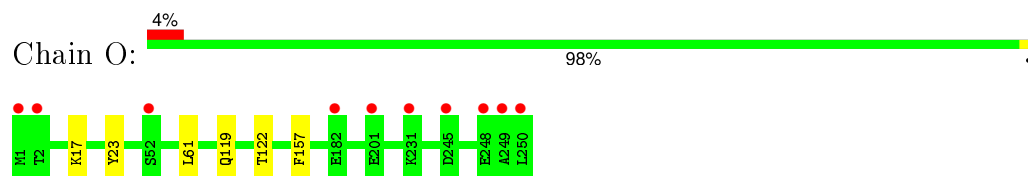
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

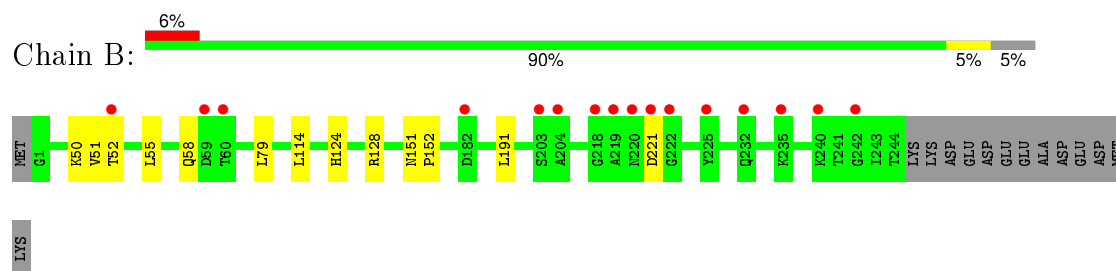
- Molecule 1: Proteasome subunit alpha type-2



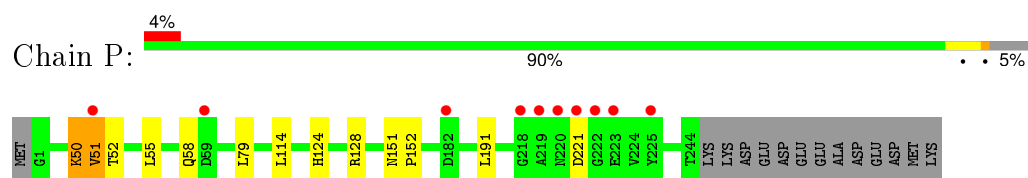
- Molecule 1: Proteasome subunit alpha type-2



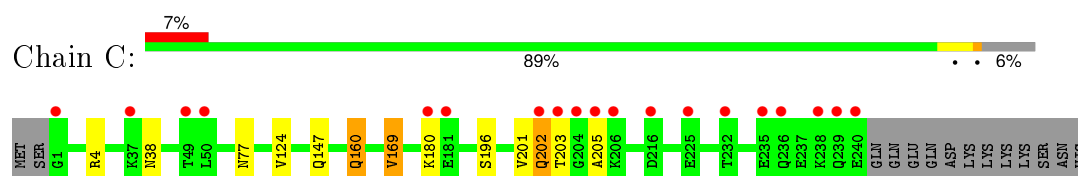
- Molecule 2: Proteasome subunit alpha type-3



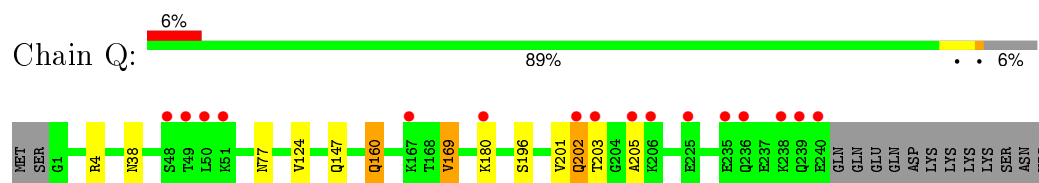
- Molecule 2: Proteasome subunit alpha type-3



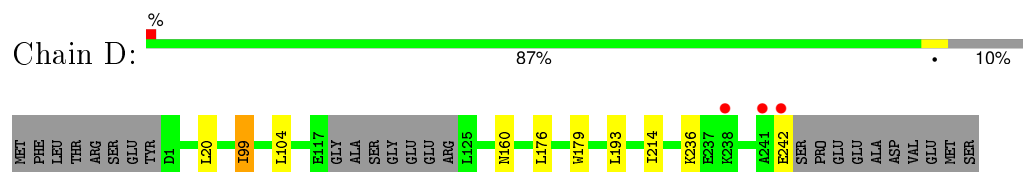
- Molecule 3: Proteasome subunit alpha type-4



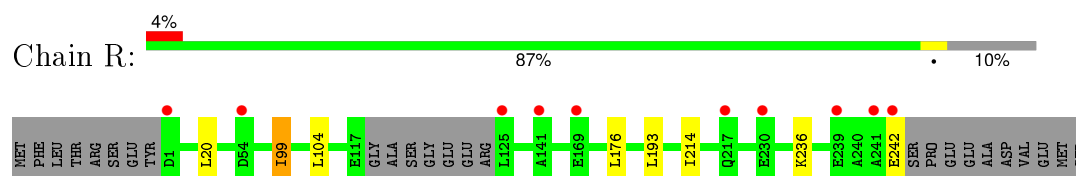
- Molecule 3: Proteasome subunit alpha type-4



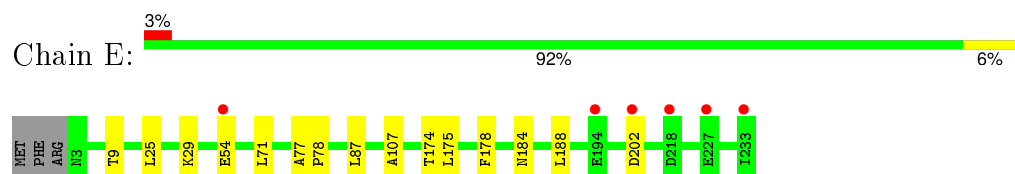
- Molecule 4: Proteasome subunit alpha type-5



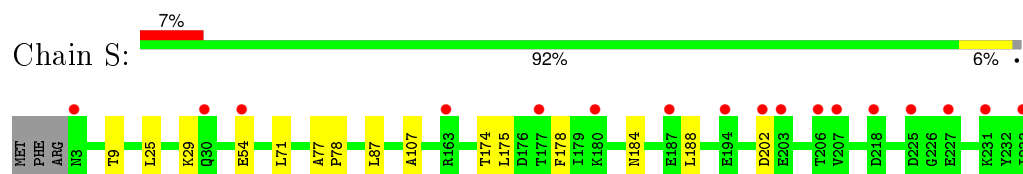
- Molecule 4: Proteasome subunit alpha type-5



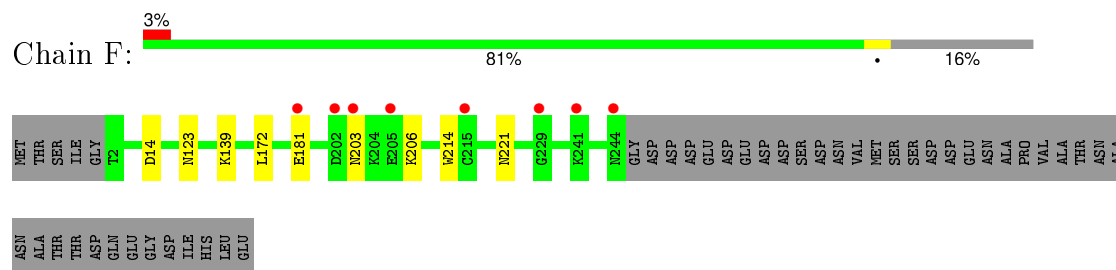
- Molecule 5: Proteasome subunit alpha type-6



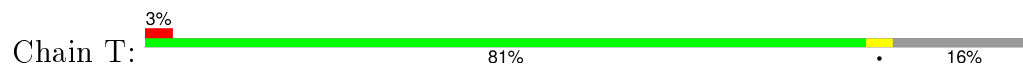
- Molecule 5: Proteasome subunit alpha type-6

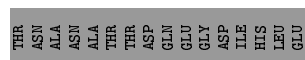


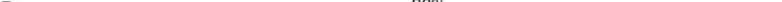
- Molecule 6: Probable proteasome subunit alpha type-7



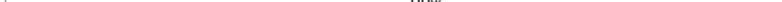
- Molecule 6: Probable proteasome subunit alpha type-7



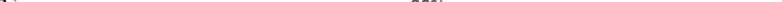


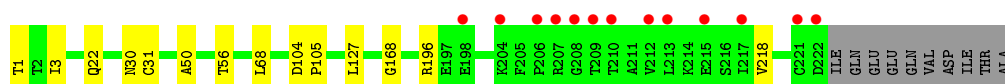
Chain G:  3% 90% 5%

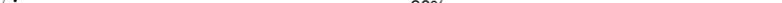


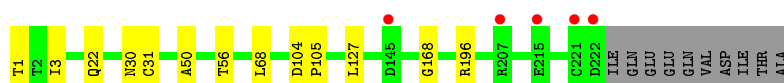
Chain U:  3% 90% 5%

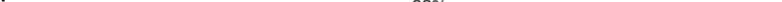


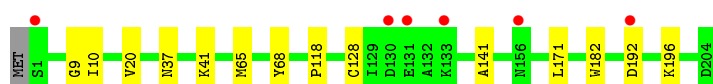
Chain H:  6% 90% 6%

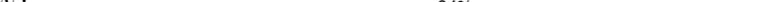


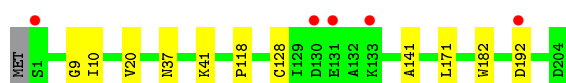
Chain V:  2% 90% 6%



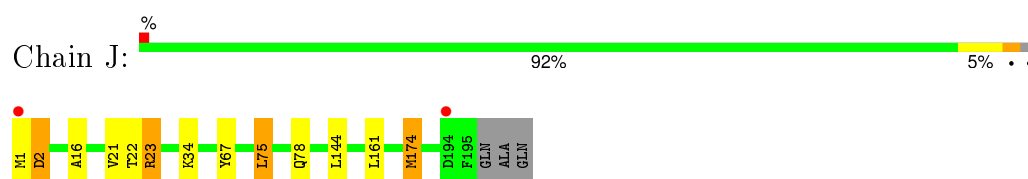
Chain I: 



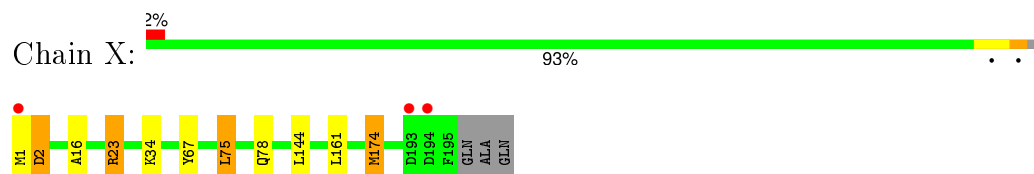
Chain W:  2% 94% 5%



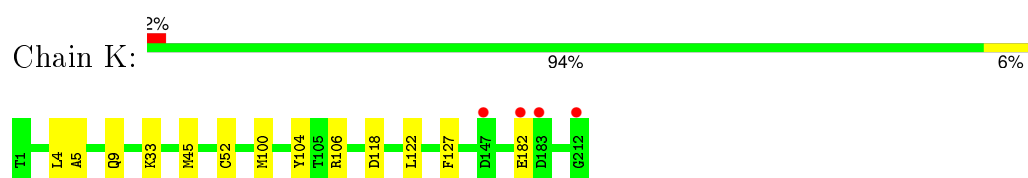
WORLDWIDE  
**PDB**  
PROTEIN DATA BANK



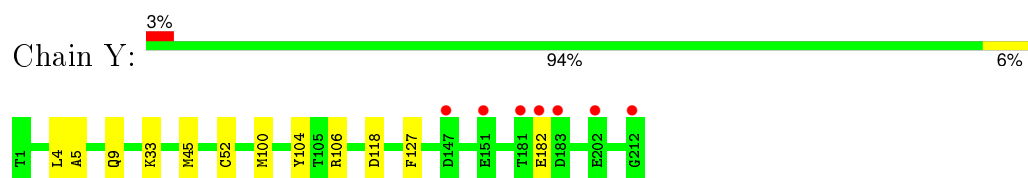
- Molecule 10: Proteasome subunit beta type-4



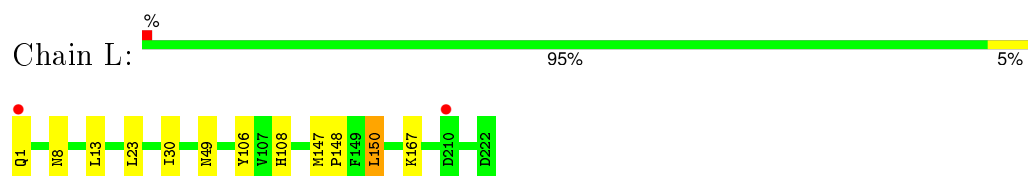
- Molecule 11: Proteasome subunit beta type-5



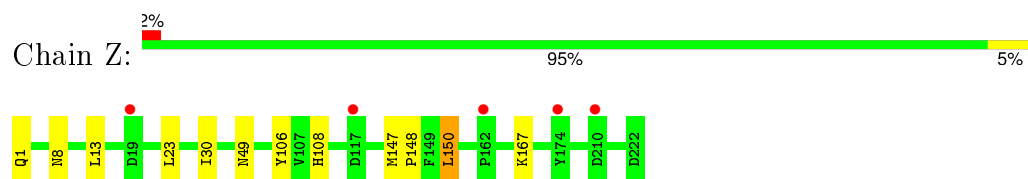
- Molecule 11: Proteasome subunit beta type-5



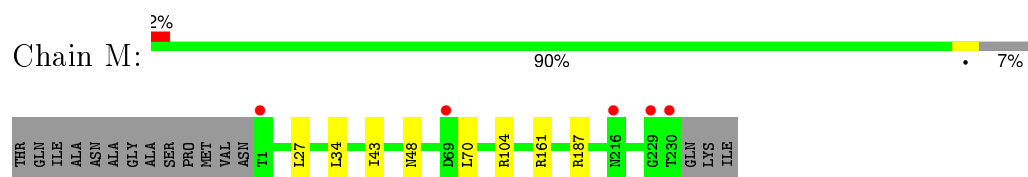
- Molecule 12: Proteasome subunit beta type-6



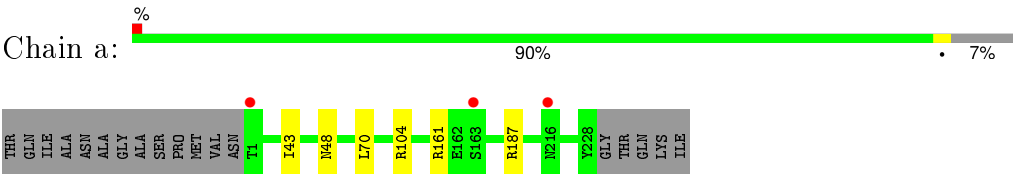
- Molecule 12: Proteasome subunit beta type-6



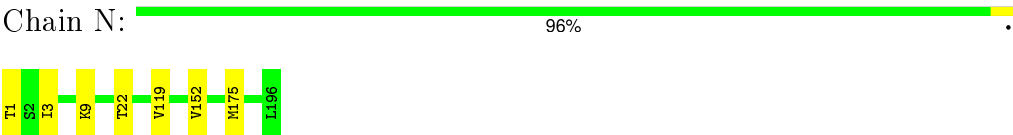
- Molecule 13: Proteasome subunit beta type-7



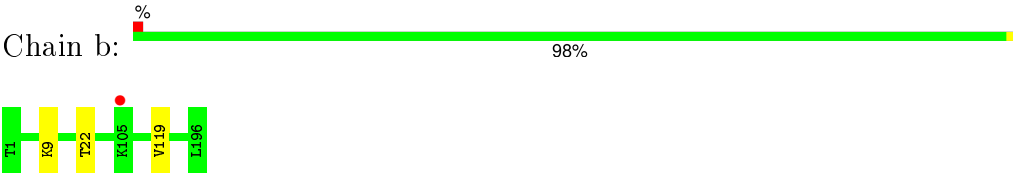
- Molecule 13: Proteasome subunit beta type-7



• 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, $\alpha$ , $\beta$ , $\gamma$	136.71Å 300.14Å 145.28Å 90.00° 113.16° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.90) 98.7 (15.00-2.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.191 , 0.228 0.197 , 0.232	Depositor DCC
$R_{free}$ test set	11608 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 232156 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	49730	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, 3BV, MES, 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	0.27	0/1952	0.48	0/2642
1	O	0.27	0/1952	0.48	0/2642
2	B	0.27	0/1934	0.50	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.27	0/1910	0.51	0/2586
3	Q	0.27	0/1910	0.51	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.27	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.48	0/2433
6	F	0.27	0/1932	0.46	0/2609
6	T	0.27	0/1932	0.46	0/2609
7	G	0.28	0/1945	0.48	0/2634
7	U	0.28	0/1945	0.48	0/2634
8	H	0.27	0/1715	0.48	0/2326
8	V	0.26	0/1715	0.47	0/2326
9	I	0.28	0/1611	0.49	0/2174
9	W	0.27	0/1611	0.48	0/2174
10	J	0.27	0/1589	0.48	0/2142
10	X	0.28	0/1589	0.49	0/2142
11	K	0.27	0/1683	0.50	0/2277
11	Y	0.27	0/1683	0.50	0/2277
12	L	0.28	0/1795	0.48	0/2420
12	Z	0.28	0/1795	0.48	0/2420
13	M	0.28	0/1828	0.51	0/2480
13	a	0.28	0/1817	0.51	0/2465
14	N	0.26	0/1541	0.47	0/2087
14	b	0.26	0/1541	0.47	0/2087
All	All	0.27	0/50133	0.48	0/67791

There are no bond length outliers.

There are no bond angle outliers.

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	4	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	2	0
4	R	1813	0	1797	1	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	0	0
6	T	1892	0	1883	0	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0
8	H	1684	0	1686	5	0
8	V	1684	0	1686	4	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	10	0
10	X	1561	0	1569	6	0
11	K	1646	0	1595	8	0
11	Y	1646	0	1595	7	0
12	L	1757	0	1711	4	0
12	Z	1757	0	1711	4	0
13	M	1797	0	1800	1	0
13	a	1786	0	1790	0	0
14	N	1512	0	1478	2	0
14	b	1512	0	1478	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	52	0	59	1	0
17	K	52	0	59	4	0
17	N	52	0	59	1	0
17	V	52	0	59	1	0
17	Y	52	0	59	3	0
17	b	52	0	59	0	0
18	K	12	0	13	0	0
18	Y	12	0	13	0	0
19	A	9	0	0	0	0
19	B	6	0	0	0	0
19	C	3	0	0	0	0
19	D	3	0	0	0	0
19	E	4	0	0	0	0
19	F	11	0	0	0	0
19	G	6	0	0	0	0
19	H	4	0	0	0	0
19	I	3	0	0	0	0
19	J	9	0	0	0	0
19	K	3	0	0	0	0
19	L	6	0	0	0	0
19	M	9	0	0	0	0
19	N	2	0	0	0	0
19	O	2	0	0	0	0
19	P	3	0	0	0	0
19	Q	3	0	0	0	0
19	R	3	0	0	0	0
19	S	4	0	0	0	0
19	T	7	0	0	0	0
19	U	4	0	0	0	0
19	V	4	0	0	0	0
19	W	3	0	0	0	0
19	X	8	0	0	0	0
19	Y	7	0	0	1	0
19	Z	6	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	a	8	0	0	0	0
19	b	8	0	0	0	0
All	All	49730	0	49364	97	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 1.

All (97) 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)
10:J:23:ARG:HH11	10:J:23:ARG:HG2	1.39	0.87
10:J:1:MET:O	10:J:2:ASP:HB2	1.88	0.73
10:X:1:MET:O	10:X:2:ASP:HB2	1.89	0.70
10:J:23:ARG:NH1	10:J:23:ARG:HG2	2.07	0.69
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.82	0.62
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.82	0.60
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.84	0.59
17:N:201:3BV:O48	17:N:201:3BV:O60	2.21	0.58
8:H:168:GLY:O	17:H:301:3BV:H57	2.04	0.57
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.86	0.56
7:G:23:PHE:O	7:G:26:THR:HB	2.06	0.55
10:J:22:THR:O	10:J:23:ARG:HG2	2.06	0.55
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.89	0.55
8:V:168:GLY:O	17:V:301:3BV:H57	2.06	0.55
7:U:23:PHE:O	7:U:26:THR:HB	2.07	0.55
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.75	0.52
10:J:174:MET:HA	10:X:174:MET:HA	1.92	0.51
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.94	0.50
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.94	0.50
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.92	0.50
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.76	0.49
3:C:201:VAL:O	3:C:202:GLN:CB	2.61	0.49
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.47	0.49
11:K:33:LYS:NZ	17:K:301:3BV:H58	2.28	0.49
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.94	0.49
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.95	0.48
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.60	0.48
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.48	0.48
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.95	0.48
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.95	0.48
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.95	0.48
11:Y:33:LYS:NZ	17:Y:301:3BV:H58	2.28	0.47
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.96	0.47
17:K:301:3BV:H2	12:L:108:HIS:NE2	2.29	0.47
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.30	0.46
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.97	0.46
3:C:201:VAL:HG13	3:C:202:GLN:N	2.30	0.46
10:J:23:ARG:NH1	10:J:23:ARG:CG	2.73	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.99	0.45
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.33	0.44
14:N:1:THR:CG2	14:N:3:ILE:HG23	2.48	0.44
7:G:26:THR:HG21	7:G:131:ILE:HD12	2.00	0.44
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.18	0.44
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.82	0.44
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.00	0.44
8:H:50:ALA:HB2	9:I:128:CYS:HB2	2.00	0.44
17:Y:301:3BV:H59	17:Y:301:3BV:H44	1.93	0.43
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.00	0.43
1:O:119:GLN:O	1:O:122:THR:HB	2.18	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.43
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.43
12:Z:108:HIS:HB3	19:Z:401:HOH:O	2.18	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.43
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.01	0.43
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.53	0.43
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.43
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.18	0.43
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.99	0.43
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.99	0.43
12:L:147:MET:N	12:L:148:PRO:HD2	2.33	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.43
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.00	0.43
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.01	0.43
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.53	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.01	0.43
3:C:201:VAL:O	3:C:202:GLN:HB2	2.17	0.42
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.00	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
8:H:1:THR:CG2	8:H:3:ILE:HG23	2.50	0.42
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.50	0.42
1:A:119:GLN:O	1:A:122:THR:HB	2.19	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:23:ARG:HG2	19:Y:403:HOH:O	2.19	0.42
11:Y:33:LYS:HZ1	17:Y:301:3BV:H58	1.84	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
8:V:1:THR:CG2	8:V:3:ILE:HG23	2.50	0.41
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.50	0.41
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.03	0.41
11:K:100:MET:CE	11:K:127:PHE:HB2	2.51	0.41
11:K:33:LYS:HZ1	17:K:301:3BV:H58	1.86	0.41
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.03	0.41
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.03	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.84	0.41
10:J:1:MET:HA	10:J:34:LYS:CE	2.50	0.41
9:I:65:MET:O	9:I:68:TYR:HB3	2.21	0.41
11:Y:104:TYR:CD1	11:Y:182:GLU:HA	2.56	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.56	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.85	0.40
10:X:1:MET:HA	10:X:34:LYS:CE	2.51	0.40
2:P:50:LYS:O	2:P:51:VAL:C	2.60	0.40
14:N:152:VAL:HA	14:N:175:MET:HE1	2.03	0.40
17:K:301:3BV:O48	17:K:301:3BV:O60	2.39	0.40
11:K:104:TYR:CD1	11:K:182:GLU:HA	2.56	0.40
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.57	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%)	241 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	24	60
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	24	60
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	24	60
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	24	60
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	232 (96%)	9 (4%)	0	100	100
6	T	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	34	71
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	34	71
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
11	Y	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	228/246 (93%)	221 (97%)	7 (3%)	0	100	100
13	a	226/246 (92%)	220 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6268/6614 (95%)	6097 (97%)	161 (3%)	10 (0%)	52	84

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
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
2	B	221	ASP
2	P	221	ASP

### 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%)	206 (99%)	3 (1%)	74	93
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	93
2	B	203/216 (94%)	196 (97%)	7 (3%)	44	79
2	P	203/216 (94%)	196 (97%)	7 (3%)	44	79
3	C	212/226 (94%)	204 (96%)	8 (4%)	40	76
3	Q	212/226 (94%)	204 (96%)	8 (4%)	40	76
4	D	194/215 (90%)	187 (96%)	7 (4%)	42	78
4	R	194/215 (90%)	187 (96%)	7 (4%)	42	78
5	E	190/193 (98%)	181 (95%)	9 (5%)	32	68
5	S	190/193 (98%)	181 (95%)	9 (5%)	32	68
6	F	201/239 (84%)	192 (96%)	9 (4%)	34	70
6	T	201/239 (84%)	192 (96%)	9 (4%)	34	70
7	G	206/210 (98%)	199 (97%)	7 (3%)	44	79
7	U	206/210 (98%)	199 (97%)	7 (3%)	44	79
8	H	181/190 (95%)	174 (96%)	7 (4%)	39	75
8	V	181/190 (95%)	174 (96%)	7 (4%)	39	75
9	I	172/173 (99%)	168 (98%)	4 (2%)	58	87

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	172/173 (99%)	168 (98%)	4 (2%)	58	87
10	J	173/175 (99%)	168 (97%)	5 (3%)	50	83
10	X	173/175 (99%)	168 (97%)	5 (3%)	50	83
11	K	170/170 (100%)	166 (98%)	4 (2%)	57	86
11	Y	170/170 (100%)	166 (98%)	4 (2%)	57	86
12	L	185/185 (100%)	179 (97%)	6 (3%)	46	81
12	Z	185/185 (100%)	179 (97%)	6 (3%)	46	81
13	M	196/208 (94%)	190 (97%)	6 (3%)	47	82
13	a	195/208 (94%)	189 (97%)	6 (3%)	47	82
14	N	162/162 (100%)	159 (98%)	3 (2%)	65	89
14	b	162/162 (100%)	159 (98%)	3 (2%)	65	89
All	All	5307/5542 (96%)	5137 (97%)	170 (3%)	46	81

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	114	LEU
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	20	LEU
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	174	THR
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	115	LEU
7	G	125	MET
7	G	154	TYR
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN
8	H	31	CYS
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	23	ARG
10	J	75	LEU
10	J	78	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
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	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	22	THR
14	N	119	VAL
1	O	17	LYS
1	O	61	LEU
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	114	LEU
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	20	LEU
4	R	99	ILE
4	R	176	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	R	193	LEU
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	174	THR
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	115	LEU
7	U	125	MET
7	U	154	TYR
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	22	GLN
8	V	30	ASN
8	V	31	CYS
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	23	ARG
10	X	75	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	106	ARG
11	Y	118	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
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	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	22	THR
14	b	119	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
4	D	160	ASN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	99	ASN
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	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	117	GLN
7	G	121	GLN
8	H	66	HIS
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
11	K	179	HIS
12	L	3	ASN
12	L	70	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
1	O	94	HIS
2	P	20	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN
5	S	151	ASN
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	117	GLN
7	U	121	GLN
9	W	37	ASN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	179	HIS
12	Z	3	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	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 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 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$
17	3BV	H	301	8	53,54,54	1.15	3 (5%)	67,71,71	1.38	9 (13%)
17	3BV	K	301	11	53,54,54	1.12	3 (5%)	67,71,71	1.72	10 (14%)
18	MES	K	303	-	11,12,12	0.66	0	14,16,16	1.50	2 (14%)
17	3BV	N	201	14	53,54,54	1.28	4 (7%)	67,71,71	1.32	8 (11%)
17	3BV	V	301	8	53,54,54	1.13	3 (5%)	67,71,71	1.38	10 (14%)
17	3BV	Y	301	11	53,54,54	1.13	3 (5%)	67,71,71	1.74	10 (14%)
18	MES	Y	303	-	11,12,12	0.67	0	14,16,16	1.55	2 (14%)
17	3BV	b	201	14	53,54,54	1.26	3 (5%)	67,71,71	1.32	8 (11%)

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
17	3BV	H	301	8	-	0/59/67/67	0/3/3/3
17	3BV	K	301	11	-	0/59/67/67	0/3/3/3
18	MES	K	303	-	-	0/6/14/14	0/1/1/1
17	3BV	N	201	14	-	0/59/67/67	0/3/3/3
17	3BV	V	301	8	-	0/59/67/67	0/3/3/3
17	3BV	Y	301	11	-	0/59/67/67	0/3/3/3
18	MES	Y	303	-	-	0/6/14/14	0/1/1/1
17	3BV	b	201	14	-	0/59/67/67	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	301	3BV	C32-C33	-4.33	1.40	1.51
17	b	201	3BV	C32-C33	-4.32	1.40	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	3BV	C32-C33	-4.32	1.40	1.51
17	N	201	3BV	C32-C33	-4.28	1.40	1.51
17	Y	301	3BV	C32-C33	-4.24	1.40	1.51
17	V	301	3BV	C32-C33	-4.13	1.41	1.51
17	K	301	3BV	C13-C14	-3.71	1.41	1.51
17	N	201	3BV	C13-C14	-3.62	1.41	1.51
17	Y	301	3BV	C13-C14	-3.61	1.41	1.51
17	b	201	3BV	C13-C14	-3.60	1.41	1.51
17	H	301	3BV	C13-C14	-3.24	1.42	1.51
17	V	301	3BV	C13-C14	-3.15	1.42	1.51
17	N	201	3BV	C59-C51	2.01	1.55	1.52
17	K	301	3BV	C51-C47	4.15	1.61	1.53
17	Y	301	3BV	C51-C47	4.33	1.61	1.53
17	V	301	3BV	C51-C47	4.46	1.61	1.53
17	H	301	3BV	C51-C47	4.51	1.62	1.53
17	b	201	3BV	C51-C47	5.39	1.63	1.53
17	N	201	3BV	C51-C47	5.57	1.64	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	301	3BV	C43-C42-N41	-6.89	100.88	110.15
17	K	301	3BV	C43-C42-N41	-6.80	101.00	110.15
17	H	301	3BV	C43-C42-N41	-5.58	102.65	110.15
17	V	301	3BV	C43-C42-N41	-5.51	102.74	110.15
17	b	201	3BV	C58-C51-C59	-4.65	103.73	109.86
17	N	201	3BV	C58-C51-C59	-4.65	103.73	109.86
17	Y	301	3BV	C58-C51-C59	-4.63	103.75	109.86
17	K	301	3BV	C58-C51-C59	-4.24	104.28	109.86
17	V	301	3BV	O1-C6-C5	-4.01	102.66	111.84
17	H	301	3BV	O1-C6-C5	-4.00	102.67	111.84
17	b	201	3BV	C43-C42-N41	-3.87	104.94	110.15
17	K	301	3BV	C7-N4-C3	-3.82	105.43	111.07
17	Y	301	3BV	C7-N4-C3	-3.80	105.45	111.07
17	K	301	3BV	C33-C32-C31	-3.73	102.57	113.41
17	N	201	3BV	C43-C42-N41	-3.69	105.19	110.15
17	Y	301	3BV	C33-C32-C31	-3.69	102.68	113.41
17	K	301	3BV	O1-C2-C3	-3.54	103.73	111.84
17	Y	301	3BV	O1-C2-C3	-3.46	103.92	111.84
17	H	301	3BV	C58-C51-C59	-3.41	105.36	109.86
17	V	301	3BV	C58-C51-C59	-3.32	105.48	109.86
17	N	201	3BV	O1-C6-C5	-3.13	104.67	111.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	301	3BV	C6-C5-N4	-3.07	105.48	110.12
17	b	201	3BV	O1-C6-C5	-3.03	104.89	111.84
17	b	201	3BV	C33-C32-C31	-3.02	104.63	113.41
17	N	201	3BV	C33-C32-C31	-2.97	104.76	113.41
17	K	301	3BV	C6-C5-N4	-2.88	105.75	110.12
17	N	201	3BV	C12-C11-C20	-2.87	103.34	110.32
17	b	201	3BV	C12-C11-C20	-2.85	103.38	110.32
17	N	201	3BV	O1-C2-C3	-2.84	105.32	111.84
17	V	301	3BV	C25-C24-C23	-2.83	107.14	115.50
17	H	301	3BV	C25-C24-C23	-2.80	107.20	115.50
17	b	201	3BV	O1-C2-C3	-2.79	105.44	111.84
17	H	301	3BV	C33-C32-C31	-2.71	105.52	113.41
17	V	301	3BV	C33-C32-C31	-2.69	105.59	113.41
17	N	201	3BV	C12-C13-C14	-2.62	103.04	113.14
17	b	201	3BV	C12-C13-C14	-2.60	103.11	113.14
17	Y	301	3BV	O60-C59-C51	-2.57	105.89	111.34
17	K	301	3BV	O60-C59-C51	-2.56	105.92	111.34
17	V	301	3BV	C6-C5-N4	-2.55	106.26	110.12
17	H	301	3BV	C6-C5-N4	-2.55	106.26	110.12
17	K	301	3BV	O1-C6-C5	-2.48	106.16	111.84
17	Y	301	3BV	O1-C6-C5	-2.45	106.21	111.84
17	V	301	3BV	O60-C59-C51	-2.30	106.47	111.34
17	H	301	3BV	O60-C59-C51	-2.24	106.59	111.34
17	H	301	3BV	C13-C12-C11	-2.23	106.31	113.12
17	H	301	3BV	C28-C23-N22	-2.18	105.11	111.26
17	K	301	3BV	C39-C31-N30	-2.18	105.11	111.26
17	V	301	3BV	C13-C12-C11	-2.17	106.47	113.12
17	Y	301	3BV	C39-C31-N30	-2.16	105.18	111.26
17	V	301	3BV	C28-C23-N22	-2.13	105.27	111.26
17	b	201	3BV	C7-N4-C3	-2.03	108.06	111.07
17	N	201	3BV	C7-N4-C3	-2.02	108.08	111.07
17	V	301	3BV	C47-C42-N41	2.03	114.33	110.31
18	Y	303	MES	O2S-S-C8	2.99	109.45	106.91
18	K	303	MES	O2S-S-C8	3.21	109.64	106.91
18	K	303	MES	O1S-S-C8	3.38	109.79	106.91
18	Y	303	MES	O1S-S-C8	3.84	110.18	106.91
17	Y	301	3BV	C7-N4-C5	5.00	118.46	111.07
17	K	301	3BV	C7-N4-C5	5.02	118.50	111.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	3BV	1	0
17	K	301	3BV	4	0
17	N	201	3BV	1	0
17	V	301	3BV	1	0
17	Y	301	3BV	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, 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%)	-0.00	12 (4%) 34 28	44, 62, 101, 154	0
1	O	250/250 (100%)	-0.23	10 (4%) 42 35	43, 63, 106, 150	0
2	B	244/258 (94%)	0.07	16 (6%) 22 16	42, 61, 115, 173	0
2	P	244/258 (94%)	-0.14	10 (4%) 41 34	45, 63, 111, 162	0
3	C	240/254 (94%)	-0.07	19 (7%) 15 10	41, 66, 131, 170	0
3	Q	240/254 (94%)	0.12	16 (6%) 21 15	48, 79, 156, 198	0
4	D	235/260 (90%)	-0.35	3 (1%) 79 78	45, 67, 97, 141	0
4	R	235/260 (90%)	0.02	10 (4%) 39 32	52, 75, 115, 161	0
5	E	231/234 (98%)	-0.16	6 (2%) 59 54	51, 72, 110, 154	0
5	S	231/234 (98%)	0.18	17 (7%) 17 11	51, 74, 116, 141	0
6	F	243/288 (84%)	-0.30	8 (3%) 50 42	43, 65, 122, 152	0
6	T	243/288 (84%)	-0.15	10 (4%) 41 34	40, 69, 120, 156	0
7	G	241/252 (95%)	-0.17	8 (3%) 50 42	43, 62, 106, 159	0
7	U	241/252 (95%)	-0.38	7 (2%) 55 49	41, 59, 95, 142	0
8	H	222/232 (95%)	0.08	13 (5%) 26 19	45, 60, 120, 169	0
8	V	222/232 (95%)	-0.18	5 (2%) 64 59	46, 60, 97, 147	0
9	I	204/205 (99%)	-0.25	6 (2%) 55 49	40, 57, 93, 112	0
9	W	204/205 (99%)	-0.50	5 (2%) 61 55	41, 56, 92, 112	0
10	J	195/198 (98%)	-0.38	2 (1%) 84 82	37, 55, 86, 130	0
10	X	195/198 (98%)	-0.45	3 (1%) 76 74	38, 57, 83, 126	0
11	K	212/212 (100%)	-0.48	4 (1%) 70 66	37, 54, 93, 112	0
11	Y	212/212 (100%)	-0.20	7 (3%) 50 42	38, 57, 94, 116	0
12	L	222/222 (100%)	-0.46	2 (0%) 85 84	37, 57, 89, 117	0
12	Z	222/222 (100%)	-0.16	5 (2%) 64 59	38, 59, 98, 125	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	230/246 (93%)	-0.39	5 (2%) 65 60	37, 58, 86, 102	0
13	a	228/246 (92%)	-0.27	3 (1%) 79 78	38, 57, 84, 108	0
14	N	196/196 (100%)	-0.43	0 100 100	43, 54, 86, 108	0
14	b	196/196 (100%)	-0.46	1 (0%) 91 90	40, 52, 84, 103	0
All	All	6328/6614 (95%)	-0.21	213 (3%) 49 41	37, 62, 108, 198	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	220	ASN	11.1
8	H	221	CYS	10.1
8	V	222	ASP	8.9
2	P	222	GLY	8.0
2	P	220	ASN	7.6
2	B	221	ASP	7.5
8	V	221	CYS	7.3
2	B	242	GLY	7.1
10	X	1	MET	6.3
1	O	249	ALA	6.2
8	H	222	ASP	6.2
1	A	1	MET	6.1
1	O	1	MET	6.1
3	Q	50	LEU	6.1
2	B	219	ALA	5.9
3	C	206	LYS	5.6
10	J	1	MET	5.3
1	A	249	ALA	5.0
2	P	221	ASP	4.9
3	Q	49	THR	4.9
9	W	1	SER	4.8
13	M	230	THR	4.8
5	S	202	ASP	4.8
3	C	239	GLN	4.7
3	Q	238	LYS	4.7
2	B	218	GLY	4.7
6	T	244	ASN	4.7
3	Q	240	GLU	4.6
3	C	238	LYS	4.5
4	R	241	ALA	4.4
11	Y	212	GLY	4.4
2	P	218	GLY	4.1

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	4.1
3	C	49	THR	4.0
3	C	202	GLN	3.9
2	P	51	VAL	3.9
8	H	207	ARG	3.9
11	K	182	GLU	3.8
5	S	54	GLU	3.8
3	Q	239	GLN	3.8
2	B	222	GLY	3.8
1	A	2	THR	3.8
5	E	202	ASP	3.7
11	Y	183	ASP	3.7
8	H	204	LYS	3.7
10	X	193	ASP	3.6
11	Y	147	ASP	3.6
11	Y	182	GLU	3.5
3	C	205	ALA	3.5
3	Q	48	SER	3.5
7	U	222	ASP	3.5
9	I	130	ASP	3.4
8	H	217	ILE	3.3
9	W	131	GLU	3.3
2	B	225	TYR	3.3
2	B	60	THR	3.3
2	B	52	THR	3.3
3	Q	180	LYS	3.2
11	Y	202	GLU	3.2
9	W	130	ASP	3.2
3	C	37	LYS	3.2
2	B	232	GLN	3.2
5	S	177	THR	3.2
8	H	206	PRO	3.2
6	F	202	ASP	3.2
5	S	233	ILE	3.2
8	H	212	VAL	3.1
3	Q	205	ALA	3.1
3	C	236	GLN	3.1
2	B	240	LYS	3.1
7	G	181	LYS	3.1
1	O	231	LYS	3.1
8	H	215	GLU	3.1
13	M	229	GLY	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
9	I	131	GLU	3.1
6	F	244	ASN	3.1
7	G	242	GLN	3.1
1	A	182	GLU	3.1
1	O	201	GLU	3.1
4	R	217	GLN	3.1
12	Z	210	ASP	3.1
4	D	242	GLU	3.0
5	S	218	ASP	3.0
3	Q	236	GLN	3.0
6	T	243	ILE	3.0
9	I	1	SER	3.0
2	P	59	ASP	3.0
1	O	248	GLU	3.0
1	O	2	THR	3.0
5	S	187	GLU	3.0
4	R	242	GLU	3.0
7	G	179	LYS	3.0
10	J	194	ASP	2.9
13	a	1	THR	2.9
6	T	241	LYS	2.9
9	W	133	LYS	2.9
4	R	125	LEU	2.9
7	G	178	LYS	2.9
5	E	54	GLU	2.9
4	R	141	ALA	2.9
6	T	205	GLU	2.9
2	B	182	ASP	2.8
11	K	212	GLY	2.8
4	R	1	ASP	2.8
11	K	147	ASP	2.8
7	G	2	GLY	2.8
1	A	59	GLU	2.8
5	E	233	ILE	2.8
5	S	225	ASP	2.8
10	X	194	ASP	2.8
3	C	225	GLU	2.8
5	S	207	VAL	2.8
7	G	186	ASN	2.8
12	Z	174	TYR	2.8
13	M	1	THR	2.8
12	Z	162	PRO	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	51	SER	2.7
3	C	204	GLY	2.7
6	T	237	ASP	2.7
8	H	208	GLY	2.7
8	H	198	GLU	2.7
1	O	250	LEU	2.7
5	S	231	LYS	2.7
6	F	241	LYS	2.7
5	S	227	GLU	2.7
6	F	215	CYS	2.7
6	T	182	GLY	2.6
5	S	194	GLU	2.6
9	I	133	LYS	2.6
3	C	50	LEU	2.6
11	K	183	ASP	2.6
13	a	163	SER	2.6
3	C	203	THR	2.6
3	Q	225	GLU	2.6
8	H	209	THR	2.6
14	b	105	LYS	2.6
3	C	216	ASP	2.6
5	S	180	LYS	2.5
7	U	242	GLN	2.5
2	B	235	LYS	2.5
8	V	207	ARG	2.5
9	I	192	ASP	2.5
5	E	218	ASP	2.5
3	Q	51	LYS	2.5
9	I	156	ASN	2.5
7	G	222	ASP	2.5
3	C	240	GLU	2.5
5	S	203	GLU	2.5
1	A	187	ASP	2.5
12	Z	19	ASP	2.5
3	C	181	GLU	2.4
1	O	52	SER	2.4
3	Q	206	LYS	2.4
3	C	232	THR	2.4
2	P	225	TYR	2.4
5	E	227	GLU	2.4
1	A	250	LEU	2.4
7	U	3	TYR	2.4

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	Q	235	GLU	2.4
4	R	54	ASP	2.4
1	O	182	GLU	2.4
12	L	210	ASP	2.4
5	S	163	ARG	2.3
1	O	245	ASP	2.3
5	S	206	THR	2.3
7	U	2	GLY	2.3
2	B	59	ASP	2.3
2	P	223	GLU	2.3
4	R	230	GLU	2.3
3	Q	203	THR	2.3
7	U	52	ASP	2.3
6	F	203	ASN	2.3
8	H	210	THR	2.3
7	U	181	LYS	2.3
11	Y	181	THR	2.2
3	Q	167	LYS	2.2
7	U	183	ASP	2.2
6	F	229	GLY	2.2
11	Y	151	GLU	2.2
13	M	216	ASN	2.2
8	H	213	LEU	2.2
13	M	69	ASP	2.2
1	A	54	PRO	2.2
4	R	239	GLU	2.2
6	F	205	GLU	2.2
7	G	188	GLU	2.1
6	T	229	GLY	2.1
6	T	2	THR	2.1
2	P	182	ASP	2.1
8	V	145	ASP	2.1
4	D	241	ALA	2.1
5	E	194	GLU	2.1
1	A	245	ASP	2.1
5	S	3	ASN	2.1
4	D	238	LYS	2.1
6	T	204	LYS	2.1
8	V	215	GLU	2.1
12	L	1	GLN	2.1
2	B	204	ALA	2.1
1	A	229	THR	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
12	Z	117	ASP	2.0
3	C	235	GLU	2.0
4	R	169	GLU	2.0
6	F	181	GLU	2.0
3	Q	202	GLN	2.0
3	C	180	LYS	2.0
13	a	216	ASN	2.0
2	B	203	SER	2.0
6	T	230	ASP	2.0
9	W	192	ASP	2.0
5	S	30	GLN	2.0
3	C	1	GLY	2.0
1	A	248	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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
18	MES	Y	303	12/12	0.85	0.47	24.82	80,90,98,112	0
18	MES	K	303	12/12	0.77	0.55	13.05	94,99,123,130	0
17	3BV	N	201	52/52	0.87	0.26	3.88	44,59,141,142	0
16	CL	N	203	1/1	0.92	0.27	3.66	79,79,79,79	0
17	3BV	b	201	52/52	0.88	0.24	3.51	45,57,131,134	0
17	3BV	V	301	52/52	0.82	0.39	3.21	61,75,120,128	0
17	3BV	K	301	52/52	0.93	0.19	2.96	41,50,108,116	0
17	3BV	H	301	52/52	0.86	0.34	2.40	61,71,123,126	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	MG	K	302	1/1	0.99	0.19	2.34	57,57,57,57	0
15	MG	I	301	1/1	0.95	0.24	1.68	66,66,66,66	0
17	3BV	Y	301	52/52	0.92	0.20	1.41	39,49,105,111	0
16	CL	b	202	1/1	0.96	0.14	-0.19	67,67,67,67	0
15	MG	Z	301	1/1	0.93	0.14	-0.86	64,64,64,64	0
15	MG	G	301	1/1	0.96	0.11	-0.91	58,58,58,58	0
15	MG	N	202	1/1	0.98	0.10	-1.60	51,51,51,51	0
15	MG	Y	302	1/1	0.98	0.09	-2.10	50,50,50,50	0
15	MG	V	302	1/1	0.95	0.06	-3.01	70,70,70,70	0
16	CL	G	302	1/1	0.99	0.18	-	38,38,38,38	0
16	CL	U	301	1/1	0.98	0.15	-	47,47,47,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.