



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:13 PM GMT

PDB ID : 4QV9  
Title : yCP beta5-C63F mutant  
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.  
Deposited on : 2014-07-14  
Resolution : 2.60 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

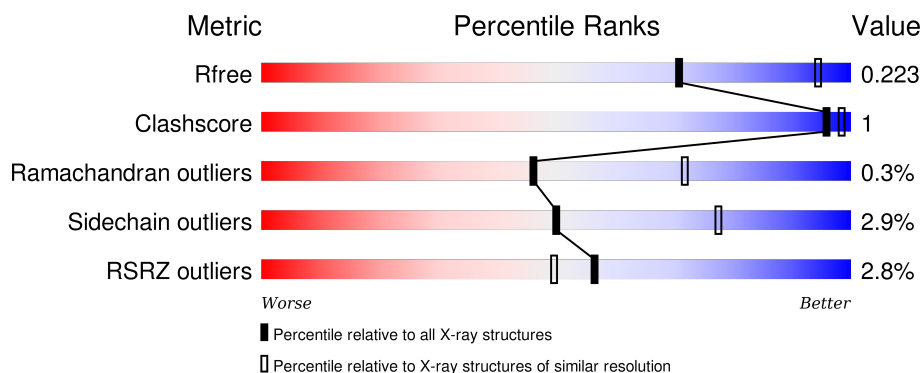
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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>3%</div> <div>98%</div> <div>.</div> </div>
1	O	250	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
2	B	258	<div> <div>4%</div> <div>88%</div> <div>7%</div> <div>5%</div> </div>
2	P	258	<div> <div>5%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
3	C	254	<div> <div>6%</div> <div>87%</div> <div>6%</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	I	301	-	-	-	X
15	MG	K	302	-	-	-	X
15	MG	Z	301	-	-	-	X

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50245 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	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			

*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
			1649	1051	280	312	6			
11	Y	212	Total	C	N	O	S	0	0	0
			1649	1051	280	312	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	63	PHE	CYS	ENGINEERED MUTATION	UNP P30656
Y	63	PHE	CYS	ENGINEERED MUTATION	UNP P30656

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	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	J	1	Total Mg 1 1	0	0
15	K	2	Total Mg 2 2	0	0
15	H	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	U	1	Total Cl 1 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	30	Total O 30 30	0	0
17	B	24	Total O 24 24	0	0
17	C	20	Total O 20 20	0	0
17	D	29	Total O 29 29	0	0
17	E	18	Total O 18 18	0	0
17	F	28	Total O 28 28	0	0
17	G	46	Total O 46 46	0	0

*Continued on next page...*



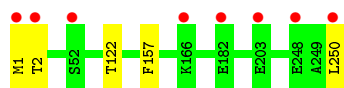
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	32	Total 32	O 32	0	0
17	I	43	Total 43	O 43	0	0
17	J	30	Total 30	O 30	0	0
17	K	44	Total 44	O 44	0	0
17	L	50	Total 50	O 50	0	0
17	M	47	Total 47	O 47	0	0
17	N	37	Total 37	O 37	0	0
17	O	14	Total 14	O 14	0	0
17	P	17	Total 17	O 17	0	0
17	Q	23	Total 23	O 23	0	0
17	R	25	Total 25	O 25	0	0
17	S	9	Total 9	O 9	0	0
17	T	21	Total 21	O 21	0	0
17	U	32	Total 32	O 32	0	0
17	V	28	Total 28	O 28	0	0
17	W	34	Total 34	O 34	0	0
17	X	30	Total 30	O 30	0	0
17	Y	34	Total 34	O 34	0	0
17	Z	31	Total 31	O 31	0	0
17	a	46	Total 46	O 46	0	0
17	b	35	Total 35	O 35	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.

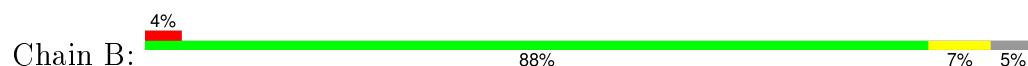
- Molecule 1: Proteasome subunit alpha type-2



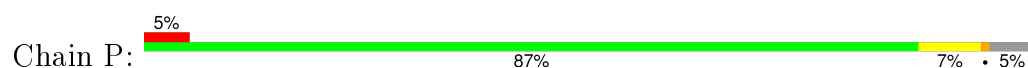
- Molecule 1: Proteasome subunit alpha type-2



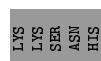
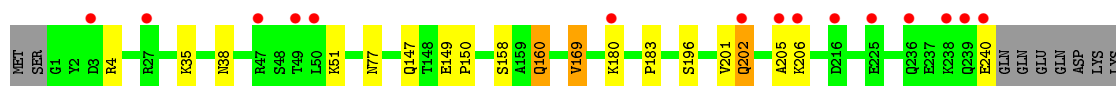
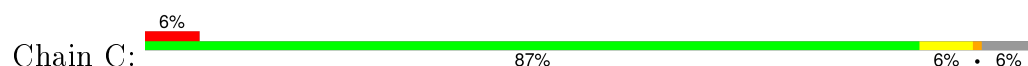
- Molecule 2: Proteasome subunit alpha type-3



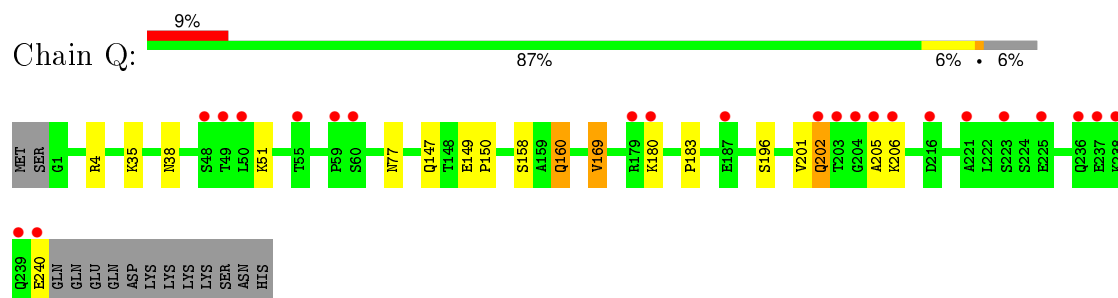
- Molecule 2: Proteasome subunit alpha type-3



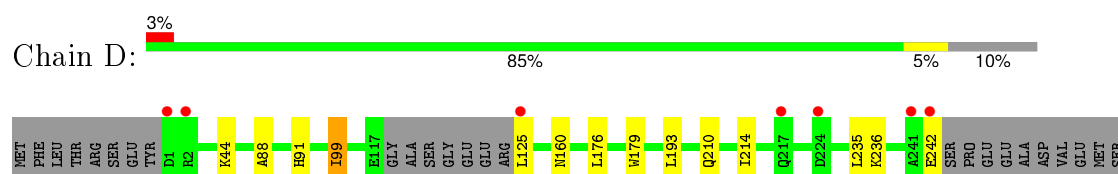
- Molecule 3: Proteasome subunit alpha type-4



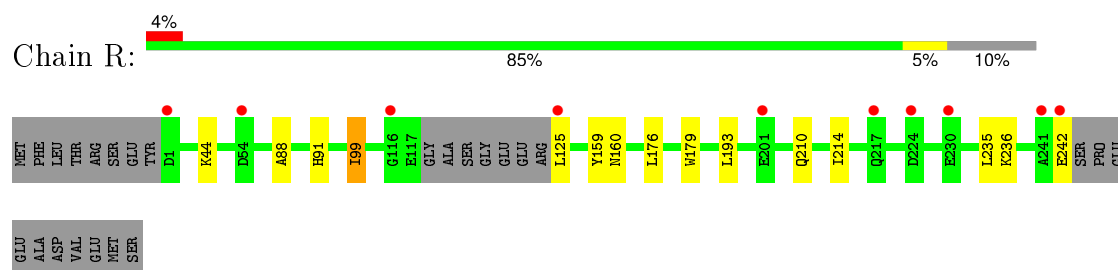
- Molecule 3: Proteasome subunit alpha type-4



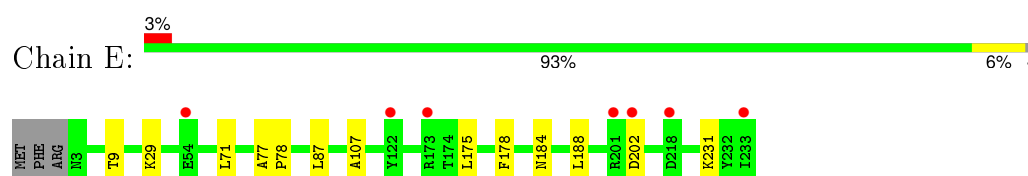
- Molecule 4: Proteasome subunit alpha type-5



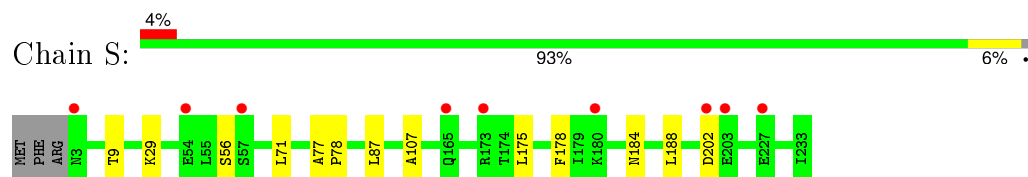
- Molecule 4: Proteasome subunit alpha type-5



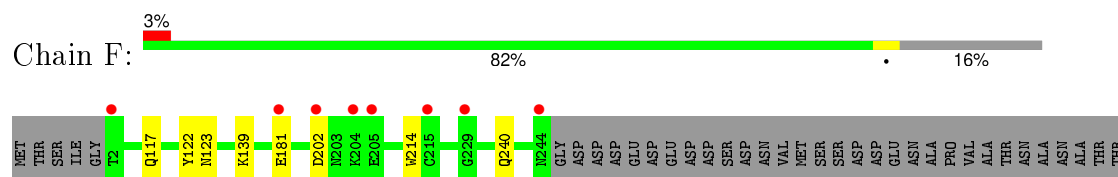
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6




- Molecule 6: Probable proteasome subunit alpha type-7



ASP  
GLN  
GLY  
GLY  
ASP  
ILE  
HIS  
LEU  
GLU

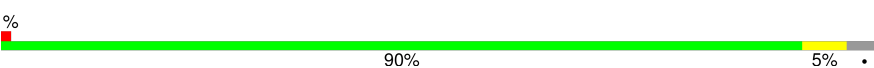
- Molecule 6: Probable proteasome subunit alpha type-7

Chain T: 

MET THR SER ILE GLY T2 Q68 Q117 Y122 M123 K139 E181 E201 D202 E205 E206 I214 C215 D230 Q240 I243 E244 GLY ASP ASP ASP GLU ASP ASP ASP ASP ASP ASP ASP VAL MET SER SER ASP ASP ASP ASN ALA PRO VAL ALA THR ASN ALA

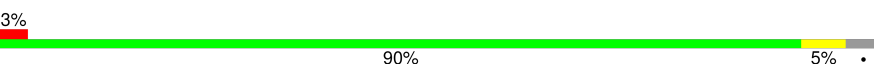
ASN  
ALA  
THR  
THR  
ASP  
GLN  
GLY  
GLY  
ILE  
HIS  
LEU  
GLU

- Molecule 7: Proteasome subunit alpha type-1

Chain G: 

MET SER GLY ALA ALA ALA SER G2 F23 T26 R68 I78 P79 N83 L115 R122 M125 D149 P150 E208 D222 R235 L236 Q242 ASP

- Molecule 7: Proteasome subunit alpha type-1

Chain U: 

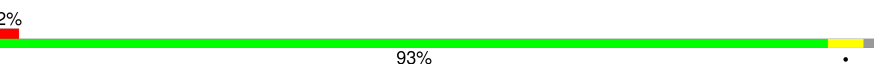
MET SER GLY ALA ALA ALA SER G2 P12 F23 T26 I78 P79 N83 L115 R122 M125 D149 P150 D183 E188 G206 T207 E208 D222 E230 R235 L236 E241 Q242 ASP

- Molecule 8: Proteasome subunit beta type-2

Chain H: 

T4 Q22 N30 A50 E61 T52 E53 T56 Q57 I63 L68 P74 R196 E197 E198 C221 D222 I223 Q224 E225 E226 GLN VAL ASP ILE THR ALA

- Molecule 8: Proteasome subunit beta type-2

Chain V: 

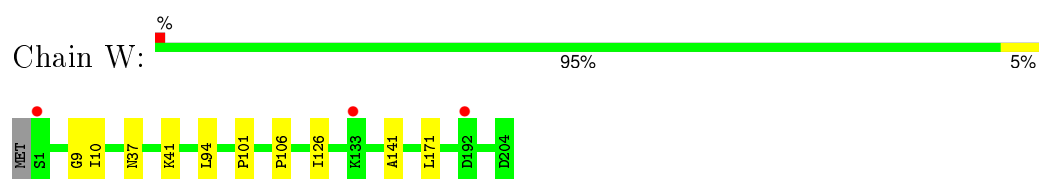
T4 Q22 N30 T52 E53 T56 Q57 L68 D104 P105 D145 R196 D222 I223 Q224 E225 E226 GLN VAL ASP ILE THR ALA

- Molecule 9: Proteasome subunit beta type-3

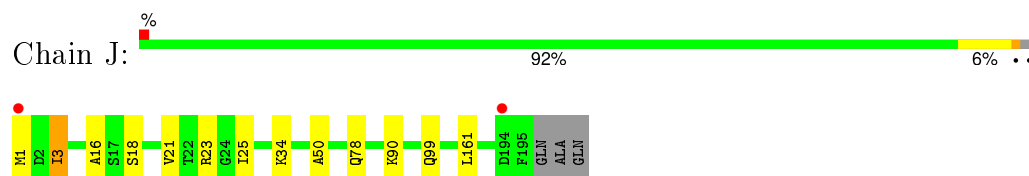
Chain I: 

MET S1 G9 I10 N37 K41 L94 R98 P101 P106 I126 A141 L171 D177 D204

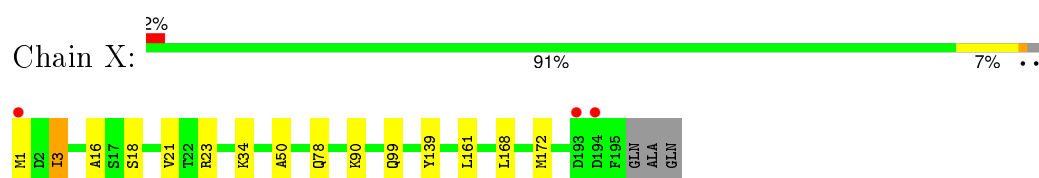
- Molecule 9: Proteasome subunit beta type-3



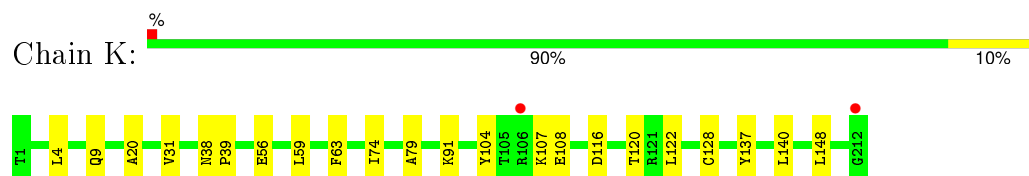
- Molecule 10: Proteasome subunit beta type-4



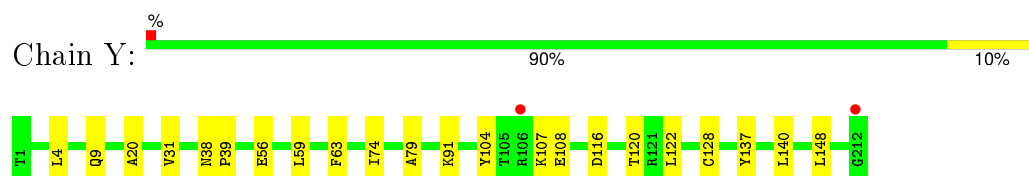
- Molecule 10: Proteasome subunit beta type-4



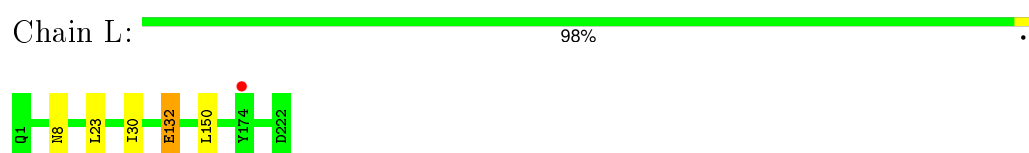
- Molecule 11: Proteasome subunit beta type-5



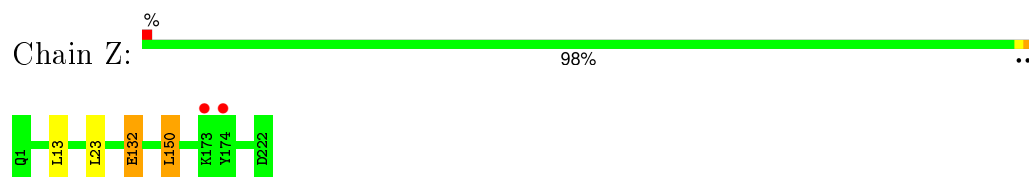
- Molecule 11: Proteasome subunit beta type-5



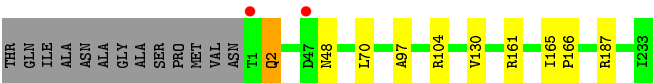
- Molecule 12: Proteasome subunit beta type-6



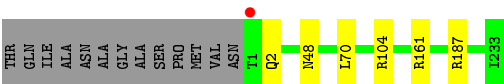
- Molecule 12: Proteasome subunit beta type-6



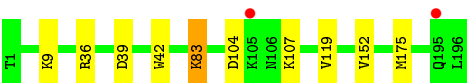
- Molecule 13: Proteasome subunit beta type-7



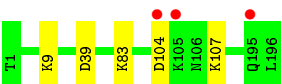
• Molecule 13: Proteasome subunit beta type-7



• 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, $\alpha$ , $\beta$ , $\gamma$	134.20Å 300.45Å 143.41Å 90.00° 113.07° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.60) 98.2 (15.00-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.196 , 0.218 0.202 , 0.223	Depositor DCC
$R_{free}$ test set	15584 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 311693 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	50245	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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, 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	0.26	0/1952	0.46	0/2642
1	O	0.26	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.26	0/1837	0.46	0/2475
4	R	0.26	0/1837	0.46	0/2475
5	E	0.26	0/1800	0.46	0/2433
5	S	0.26	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.26	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.26	0/1945	0.46	0/2634
8	H	0.24	0/1750	0.45	0/2373
8	V	0.25	0/1750	0.45	0/2373
9	I	0.27	0/1611	0.47	0/2174
9	W	0.26	0/1611	0.47	0/2174
10	J	0.26	0/1589	0.48	0/2142
10	X	0.26	0/1589	0.47	0/2142
11	K	0.32	0/1687	0.49	0/2282
11	Y	0.32	0/1687	0.49	0/2282
12	L	0.27	0/1795	0.47	0/2420
12	Z	0.26	0/1795	0.47	0/2420
13	M	0.27	0/1855	0.50	0/2514
13	a	0.27	0/1855	0.50	0/2514
14	N	0.25	0/1541	0.47	0/2087
14	b	0.25	0/1541	0.47	0/2087
All	All	0.27	0/50276	0.47	0/67978

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	1	0
1	O	1915	0	1929	4	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	4	0
8	V	1719	0	1719	3	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	8	0
11	K	1649	0	1599	23	0
11	Y	1649	0	1599	26	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	2	0
13	M	1824	0	1832	3	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	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	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	G	1	0	0	0	0
16	U	1	0	0	0	0
17	A	30	0	0	0	0
17	B	24	0	0	0	0
17	C	20	0	0	0	0
17	D	29	0	0	0	0
17	E	18	0	0	0	0
17	F	28	0	0	0	0
17	G	46	0	0	0	0
17	H	32	0	0	0	0
17	I	43	0	0	0	0
17	J	30	0	0	0	0
17	K	44	0	0	0	0
17	L	50	0	0	0	0
17	M	47	0	0	1	0
17	N	37	0	0	0	0
17	O	14	0	0	0	0
17	P	17	0	0	2	0
17	Q	23	0	0	0	0
17	R	25	0	0	0	0
17	S	9	0	0	0	0
17	T	21	0	0	0	0
17	U	32	0	0	1	0
17	V	28	0	0	0	0
17	W	34	0	0	0	0
17	X	30	0	0	0	0
17	Y	34	0	0	0	0
17	Z	31	0	0	0	0
17	a	46	0	0	0	0
17	b	35	0	0	0	0
All	All	50245	0	49138	139	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 (139) 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)
11:K:63:PHE:HE1	11:K:79:ALA:HB1	1.33	0.91
11:Y:63:PHE:HD1	11:Y:74:ILE:HG21	1.35	0.90
11:Y:59:LEU:HG	11:Y:63:PHE:CE2	2.14	0.82
11:Y:63:PHE:HE1	11:Y:79:ALA:CB	1.92	0.82
11:K:59:LEU:O	11:K:63:PHE:HD2	1.63	0.82
11:K:63:PHE:CE1	11:K:79:ALA:HB1	2.18	0.77
11:K:63:PHE:HE1	11:K:79:ALA:CB	1.99	0.75
11:K:59:LEU:HG	11:K:63:PHE:CE2	2.22	0.74
11:Y:59:LEU:HG	11:Y:63:PHE:HE2	1.50	0.74
11:K:59:LEU:O	11:K:63:PHE:CD2	2.40	0.74
11:Y:63:PHE:HE1	11:Y:79:ALA:HB1	1.58	0.69
11:K:63:PHE:HD1	11:K:74:ILE:HG21	1.59	0.67
11:Y:63:PHE:CE1	11:Y:79:ALA:HB1	2.30	0.67
11:Y:59:LEU:O	11:Y:63:PHE:CD2	2.51	0.64
11:K:63:PHE:CD1	11:K:74:ILE:HG21	2.34	0.63
11:Y:63:PHE:CD1	11:Y:74:ILE:HG21	2.26	0.62
11:K:63:PHE:CE1	11:K:79:ALA:CB	2.82	0.61
11:Y:63:PHE:CE1	11:Y:79:ALA:CB	2.82	0.58
2:P:113:ARG:NE	17:P:301:HOH:O	2.26	0.58
11:Y:59:LEU:HG	11:Y:63:PHE:CZ	2.39	0.58
11:K:56:GLU:HA	11:K:59:LEU:HB2	1.86	0.57
11:K:59:LEU:HG	11:K:63:PHE:HE2	1.68	0.57
2:P:93:HIS:HB3	17:P:301:HOH:O	2.03	0.57
11:Y:56:GLU:HA	11:Y:59:LEU:HB2	1.87	0.56
11:K:59:LEU:HG	11:K:63:PHE:CZ	2.40	0.56
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.89	0.55
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.55
11:Y:63:PHE:HE1	11:Y:79:ALA:CA	2.22	0.53
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.44	0.52
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.45	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
11:Y:59:LEU:O	11:Y:63:PHE:HD2	1.92	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.50
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.50
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.94	0.50
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.46	0.49
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.47	0.49
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.49
3:C:35:LYS:HG2	3:C:158:SER:O	2.13	0.49
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.95	0.49
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.47	0.49
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.48	0.48

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.43	0.48
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.95	0.48
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.94	0.48
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.13	0.48
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.96	0.47
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.96	0.47
14:N:152:VAL:HA	14:N:175:MET:HE1	1.97	0.47
3:C:201:VAL:O	3:C:202:GLN:HB3	2.15	0.47
8:H:52:THR:O	8:H:56:THR:HG23	2.15	0.47
1:O:57:MET:HE1	17:U:421:HOH:O	2.14	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.46
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.51	0.46
8:V:52:THR:O	8:V:56:THR:HG23	2.15	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.15	0.46
11:K:59:LEU:CG	11:K:63:PHE:HE2	2.29	0.45
10:J:50:ALA:O	11:K:91:LYS:NZ	2.50	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.00	0.44
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.51	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.44
2:B:217:LYS:C	2:B:219:ALA:H	2.21	0.44
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.44
2:B:145:TYR:OH	2:B:217:LYS:N	2.51	0.44
11:Y:31:VAL:HA	12:Z:132:GLU:OE2	2.18	0.44
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.00	0.44
2:P:145:TYR:OH	2:P:217:LYS:N	2.50	0.44
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.00	0.43
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.83	0.43
9:I:101:PRO:HB3	9:I:126:ILE:HD12	2.01	0.43
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.00	0.43
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.83	0.43
11:Y:63:PHE:CE1	11:Y:79:ALA:HA	2.53	0.43
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.87	0.43
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.00	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.48	0.43
13:M:2:GLN:NE2	17:M:341:HOH:O	2.50	0.43
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.00	0.43
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.43
11:Y:63:PHE:HE1	11:Y:79:ALA:HA	1.83	0.43
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.00	0.42
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.48	0.42
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.42
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.01	0.42
2:B:221:ASP:O	2:B:223:GLU:N	2.53	0.42
11:K:107:LYS:HG3	11:K:108:GLU:HG3	2.01	0.42
10:J:25:ILE:O	10:X:139:TYR:OH	2.37	0.42
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.52	0.42
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.02	0.42
2:P:217:LYS:C	2:P:219:ALA:H	2.21	0.42
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.01	0.42
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.02	0.42
10:X:1:MET:HB3	10:X:34:LYS:HE3	2.02	0.42
9:I:98:ARG:O	9:I:126:ILE:HD11	2.20	0.42
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.42
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.54	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.42
11:Y:59:LEU:CG	11:Y:63:PHE:HE2	2.25	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.42
2:P:221:ASP:O	2:P:223:GLU:N	2.53	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.50	0.41
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.02	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
8:V:53:GLU:O	8:V:57:GLN:HG2	2.20	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
9:W:94:LEU:HD11	9:W:106:PRO:HG2	2.01	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.83	0.41
11:K:31:VAL:HA	12:L:132:GLU:OE2	2.19	0.41
8:H:53:GLU:O	8:H:57:GLN:HG2	2.21	0.41
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.56	0.41
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	2.01	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.55	0.41
4:D:44:LYS:HE3	4:D:210:GLN:HB2	2.03	0.41
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.03	0.41
4:R:44:LYS:HE3	4:R:210:GLN:HB2	2.03	0.41
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.03	0.41
10:J:1:MET:HB3	10:J:34:LYS:HE3	2.03	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:116:ASP:HB2	11:K:120:THR:HB	2.02	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.52	0.40
10:X:168:LEU:O	10:X:172:MET:HB2	2.21	0.40
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.03	0.40
11:Y:116:ASP:CB	11:Y:120:THR:HB	2.51	0.40
11:K:116:ASP:CB	11:K:120:THR:HB	2.51	0.40
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.56	0.40
11:Y:116:ASP:HB2	11:Y:120:THR:HB	2.02	0.40
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	2.03	0.40
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.56	0.40
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.51	0.40
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.56	0.40
1:O:49:LYS:HG3	1:O:210:GLU:HB2	2.04	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.52	0.40
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	39	65
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	65
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	11	22
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	11	22
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	15	30
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	15	30
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
5	S	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (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	6284/6614 (95%)	6118 (97%)	150 (2%)	16 (0%)	46	72

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	220	ASN
3	C	205	ALA
2	P	220	ASN
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO

### 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	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	90
2	B	203/216 (94%)	199 (98%)	4 (2%)	63	85
2	P	203/216 (94%)	199 (98%)	4 (2%)	63	85
3	C	212/226 (94%)	202 (95%)	10 (5%)	32	59
3	Q	212/226 (94%)	202 (95%)	10 (5%)	32	59
4	D	194/215 (90%)	186 (96%)	8 (4%)	37	66
4	R	194/215 (90%)	186 (96%)	8 (4%)	37	66
5	E	190/193 (98%)	183 (96%)	7 (4%)	41	69
5	S	190/193 (98%)	184 (97%)	6 (3%)	46	74
6	F	201/239 (84%)	194 (96%)	7 (4%)	43	71
6	T	201/239 (84%)	194 (96%)	7 (4%)	43	71
7	G	206/210 (98%)	198 (96%)	8 (4%)	39	68
7	U	206/210 (98%)	198 (96%)	8 (4%)	39	68
8	H	185/190 (97%)	181 (98%)	4 (2%)	60	83
8	V	185/190 (97%)	181 (98%)	4 (2%)	60	83
9	I	172/173 (99%)	170 (99%)	2 (1%)	78	92
9	W	172/173 (99%)	170 (99%)	2 (1%)	78	92
10	J	173/175 (99%)	168 (97%)	5 (3%)	50	77

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	X	173/175 (99%)	168 (97%)	5 (3%)	50	77
11	K	169/169 (100%)	164 (97%)	5 (3%)	48	76
11	Y	169/169 (100%)	164 (97%)	5 (3%)	48	76
12	L	185/185 (100%)	182 (98%)	3 (2%)	70	89
12	Z	185/185 (100%)	182 (98%)	3 (2%)	70	89
13	M	199/208 (96%)	193 (97%)	6 (3%)	48	76
13	a	199/208 (96%)	193 (97%)	6 (3%)	48	76
14	N	162/162 (100%)	157 (97%)	5 (3%)	47	76
14	b	162/162 (100%)	157 (97%)	5 (3%)	47	76
All	All	5320/5540 (96%)	5167 (97%)	153 (3%)	50	77

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	181	GLU
6	F	202	ASP
6	F	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	3	ILE
10	J	23	ARG
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	104	TYR
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	132	GLU
12	L	150	LEU
13	M	2	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	117	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	T	123	ASN
6	T	139	LYS
6	T	181	GLU
6	T	202	ASP
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	22	GLN
8	V	30	ASN
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	3	ILE
10	X	23	ARG
10	X	78	GLN
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	104	TYR
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	132	GLU
12	Z	150	LEU
13	a	2	GLN
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	39	ASP
14	b	83	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	b	104	ASP
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) 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
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
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
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	35	HIS
8	H	66	HIS
9	I	37	ASN
9	I	203	GLN
10	J	55	GLN
11	K	85	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	95	HIS
12	L	158	ASN
13	M	48	ASN
13	M	102	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
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
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
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	35	HIS
9	W	37	ASN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	95	HIS
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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 [i](#)

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%)	-0.30	8 (3%)	51	44	32, 46, 83, 118	0
1	O	250/250 (100%)	-0.19	11 (4%)	38	30	37, 54, 100, 126	0
2	B	244/258 (94%)	-0.12	10 (4%)	41	33	35, 52, 97, 156	0
2	P	244/258 (94%)	-0.09	14 (5%)	27	20	38, 55, 99, 150	0
3	C	240/254 (94%)	-0.08	15 (6%)	23	17	33, 55, 118, 145	0
3	Q	240/254 (94%)	0.24	23 (9%)	10	6	42, 69, 149, 179	0
4	D	235/260 (90%)	-0.27	7 (2%)	54	47	36, 56, 89, 128	0
4	R	235/260 (90%)	-0.11	10 (4%)	39	31	39, 62, 108, 146	0
5	E	231/234 (98%)	-0.22	7 (3%)	54	47	37, 58, 94, 131	0
5	S	231/234 (98%)	-0.01	9 (3%)	43	35	41, 66, 110, 148	0
6	F	243/288 (84%)	-0.35	8 (3%)	50	43	32, 52, 99, 126	0
6	T	243/288 (84%)	-0.20	10 (4%)	41	33	36, 63, 116, 149	0
7	G	241/252 (95%)	-0.43	3 (1%)	81	77	29, 47, 80, 130	0
7	U	241/252 (95%)	-0.29	8 (3%)	50	43	37, 52, 86, 133	0
8	H	226/232 (97%)	-0.30	7 (3%)	52	45	29, 45, 76, 140	0
8	V	226/232 (97%)	-0.31	5 (2%)	65	59	32, 48, 77, 162	0
9	I	204/205 (99%)	-0.61	1 (0%)	91	90	28, 41, 67, 92	0
9	W	204/205 (99%)	-0.55	3 (1%)	76	71	29, 44, 74, 96	0
10	J	195/198 (98%)	-0.44	2 (1%)	84	81	29, 46, 72, 113	0
10	X	195/198 (98%)	-0.41	3 (1%)	76	71	31, 46, 72, 128	0
11	K	212/212 (100%)	-0.44	2 (0%)	85	83	28, 45, 67, 85	0
11	Y	212/212 (100%)	-0.49	2 (0%)	85	83	32, 46, 69, 89	0
12	L	222/222 (100%)	-0.48	1 (0%)	91	90	29, 46, 81, 120	0
12	Z	222/222 (100%)	-0.46	2 (0%)	85	83	27, 47, 84, 121	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	233/246 (94%)	-0.57	2 (0%)	85 83	26, 45, 68, 89	0
13	a	233/246 (94%)	-0.50	1 (0%)	93 91	27, 46, 67, 86	0
14	N	196/196 (100%)	-0.55	2 (1%)	84 81	29, 40, 68, 97	0
14	b	196/196 (100%)	-0.55	3 (1%)	76 71	30, 41, 70, 100	0
All	All	6344/6614 (95%)	-0.31	179 (2%)	56 49	26, 50, 96, 179	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	221	ASP	8.8
2	P	219	ALA	8.6
3	Q	50	LEU	7.9
3	Q	49	THR	7.2
2	P	51	VAL	6.6
10	X	1	MET	6.5
8	V	224	GLN	6.2
2	B	219	ALA	6.1
5	S	202	ASP	5.8
3	Q	206	LYS	5.8
2	B	51	VAL	5.7
2	P	221	ASP	5.6
8	V	226	GLU	5.3
7	U	242	GLN	5.0
5	E	202	ASP	4.8
1	O	2	THR	4.8
12	L	174	TYR	4.8
8	H	226	GLU	4.8
1	A	2	THR	4.7
3	Q	236	GLN	4.6
3	Q	205	ALA	4.6
1	O	1	MET	4.6
3	C	206	LYS	4.5
3	Q	238	LYS	4.5
4	R	241	ALA	4.4
8	H	224	GLN	4.3
3	C	50	LEU	4.3
8	V	222	ASP	4.3
2	B	220	ASN	4.3
3	C	49	THR	4.3
5	S	173	ARG	4.3
10	X	194	ASP	4.2

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	D	242	GLU	4.1
3	C	205	ALA	4.1
8	H	222	ASP	4.1
10	J	1	MET	4.1
2	P	220	ASN	4.0
9	W	1	SER	4.0
6	T	243	ILE	3.9
3	Q	239	GLN	3.9
1	A	1	MET	3.9
6	F	205	GLU	3.8
2	P	59	ASP	3.8
14	b	105	LYS	3.7
3	Q	48	SER	3.7
3	Q	204	GLY	3.7
6	T	244	ASN	3.7
8	H	223	ILE	3.7
4	D	241	ALA	3.7
1	O	52	SER	3.6
14	b	195	GLN	3.5
7	U	222	ASP	3.4
2	P	218	GLY	3.4
12	Z	174	TYR	3.3
2	P	222	GLY	3.3
6	F	181	GLU	3.3
3	Q	240	GLU	3.3
3	C	238	LYS	3.3
3	Q	202	GLN	3.3
1	O	249	ALA	3.2
8	V	223	ILE	3.2
5	S	227	GLU	3.2
7	G	242	GLN	3.1
2	P	203	SER	3.1
6	F	244	ASN	3.1
5	E	233	ILE	3.1
4	R	217	GLN	3.0
10	J	194	ASP	3.0
5	S	180	LYS	3.0
13	a	1	THR	3.0
10	X	193	ASP	3.0
3	Q	237	GLU	2.9
6	T	205	GLU	2.9
4	R	1	ASP	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	C	225	GLU	2.9
1	O	250	LEU	2.9
4	R	125	LEU	2.9
13	M	47	ASP	2.9
3	C	236	GLN	2.9
3	C	239	GLN	2.9
6	F	215	CYS	2.8
2	B	59	ASP	2.8
3	Q	223	SER	2.8
12	Z	173	LYS	2.8
9	I	1	SER	2.8
3	Q	187	GLU	2.7
3	Q	55	THR	2.7
2	B	203	SER	2.7
1	O	50	LYS	2.7
6	T	201	GLU	2.7
6	F	204	LYS	2.7
3	C	180	LYS	2.7
5	S	203	GLU	2.7
6	F	229	GLY	2.7
3	Q	203	THR	2.7
2	B	50	LYS	2.6
11	Y	106	ARG	2.6
1	O	201	GLU	2.6
4	R	230	GLU	2.6
7	U	2	GLY	2.6
1	O	53	SER	2.6
5	E	201	ARG	2.6
14	N	195	GLN	2.6
4	D	1	ASP	2.5
1	A	182	GLU	2.5
8	H	198	GLU	2.5
2	P	52	THR	2.5
3	C	47	ARG	2.5
7	U	188	GLU	2.5
2	P	225	TYR	2.5
1	A	203	GLU	2.5
1	A	250	LEU	2.5
5	S	57	SER	2.5
2	B	217	LYS	2.5
7	G	68	ARG	2.5
2	P	230	LYS	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	248	GLU	2.4
6	T	181	GLU	2.4
4	R	201	GLU	2.4
8	H	225	GLU	2.4
6	T	215	CYS	2.4
13	M	1	THR	2.4
2	P	50	LYS	2.4
2	P	60	THR	2.4
5	S	54	GLU	2.4
7	U	183	ASP	2.4
3	Q	59	PRO	2.4
3	Q	216	ASP	2.4
9	W	133	LYS	2.4
3	C	202	GLN	2.4
3	C	240	GLU	2.4
3	Q	225	GLU	2.4
7	U	230	GLU	2.4
3	C	216	ASP	2.3
7	G	222	ASP	2.3
6	F	2	THR	2.3
4	D	217	GLN	2.3
7	U	206	GLY	2.3
11	Y	212	GLY	2.3
5	E	218	ASP	2.3
14	b	104	ASP	2.3
3	Q	180	LYS	2.3
2	B	52	THR	2.3
1	O	231	LYS	2.3
1	A	166	LYS	2.2
4	R	242	GLU	2.2
8	V	145	ASP	2.2
2	P	61	SER	2.2
7	U	241	GLU	2.2
3	C	27	ARG	2.2
4	R	54	ASP	2.2
11	K	212	GLY	2.2
6	T	230	ASP	2.2
6	T	206	LYS	2.1
4	D	2	ARG	2.1
1	O	203	GLU	2.1
5	E	54	GLU	2.1
6	T	2	THR	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	222	GLY	2.1
3	Q	60	SER	2.1
4	R	116	GLY	2.1
11	K	106	ARG	2.1
1	A	52	SER	2.1
5	S	3	ASN	2.1
4	D	224	ASP	2.1
9	W	192	ASP	2.1
6	T	58	GLN	2.1
8	H	221	CYS	2.1
5	E	122	TYR	2.1
14	N	105	LYS	2.1
3	Q	221	ALA	2.1
1	O	229	THR	2.1
3	C	3	ASP	2.0
4	R	224	ASP	2.0
6	F	202	ASP	2.0
5	S	165	GLN	2.0
4	D	125	LEU	2.0
5	E	173	ARG	2.0
3	Q	179	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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	302	1/1	0.95	0.42	16.01	52,52,52,52	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	Z	301	1/1	0.91	0.28	5.77	64,64,64,64	0
15	MG	I	301	1/1	0.95	0.28	4.96	57,57,57,57	0
15	MG	N	201	1/1	0.96	0.10	0.04	48,48,48,48	0
15	MG	J	201	1/1	0.98	0.09	-0.16	52,52,52,52	0
15	MG	V	301	1/1	0.99	0.12	-0.50	44,44,44,44	0
15	MG	G	301	1/1	0.99	0.05	-1.46	45,45,45,45	0
15	MG	Y	301	1/1	0.99	0.06	-1.77	43,43,43,43	0
15	MG	K	301	1/1	0.97	0.07	-2.11	38,38,38,38	0
15	MG	H	301	1/1	0.85	0.14	-	57,57,57,57	0
16	CL	U	301	1/1	0.99	0.16	-	43,43,43,43	0
16	CL	G	302	1/1	0.99	0.06	-	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.