



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:01 am BST

PDB ID : 4JSQ  
Title : Yeast 20S proteasome in complex with the dimerized linear mimetic of TMC-95A - yCP:4e  
Authors : Desvergne, A.; Genin, E.; Marechal, X.; Gallastegui, N.; Dufau, L.; Richy, N.; Groll, M.; Vidal, J.; Reboud-Ravaux, M.  
Deposited on : 2013-03-22  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

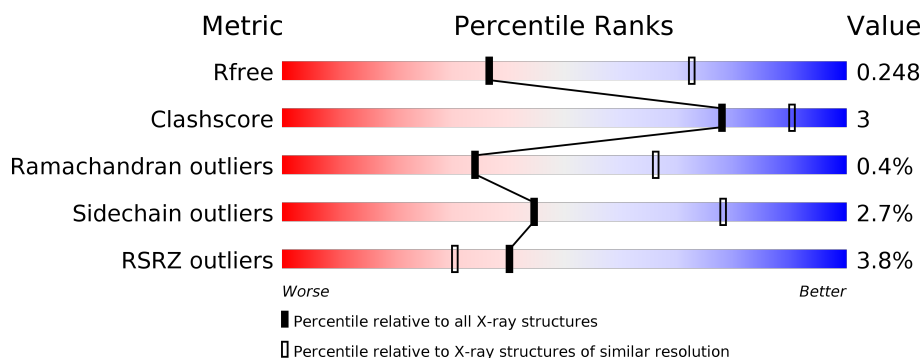
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	O	250	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
2	B	258	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>5%</div> </div> </div>
2	P	258	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>5%</div> </div> </div>
3	C	254	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>5%</div> </div> </div>
3	Q	254	<div> <div>10%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>5%</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	233	
13	a	233	
14	N	196	
14	b	196	
15	c	8	
15	d	8	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	ACA	c	4	-	-	-	X
15	ACA	d	4	-	-	-	X

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 51011 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	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	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	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	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
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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

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

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

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

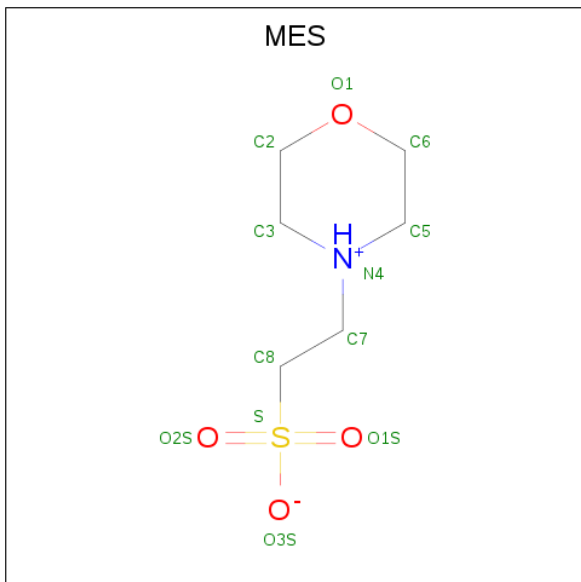
- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called TMC-95A mimic ligand yCP:4e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			56	43	6	7			
15	d	5	Total	C	N	O	0	0	0
			56	43	6	7			

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
16	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	59	Total	O	0	0
			59	59		
17	B	39	Total	O	0	0
			39	39		
17	C	43	Total	O	0	0
			43	43		
17	D	36	Total	O	0	0
			36	36		
17	E	21	Total	O	0	0
			21	21		
17	F	47	Total	O	0	0
			47	47		
17	G	60	Total	O	0	0
			60	60		
17	H	52	Total	O	0	0
			52	52		

*Continued on next page...*



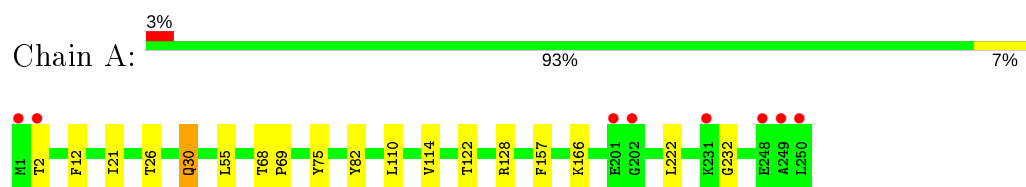
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	I	64	Total 64	O 64	0	0
17	J	53	Total 53	O 53	0	0
17	K	48	Total 48	O 48	0	0
17	L	54	Total 54	O 54	0	0
17	M	81	Total 81	O 81	0	0
17	N	58	Total 58	O 58	0	0
17	O	34	Total 34	O 34	0	0
17	P	30	Total 30	O 30	0	0
17	Q	29	Total 29	O 29	0	0
17	R	27	Total 27	O 27	0	0
17	S	18	Total 18	O 18	0	0
17	T	43	Total 43	O 43	0	0
17	U	55	Total 55	O 55	0	0
17	V	50	Total 50	O 50	0	0
17	W	62	Total 62	O 62	0	0
17	X	41	Total 41	O 41	0	0
17	Y	50	Total 50	O 50	0	0
17	Z	49	Total 49	O 49	0	0
17	a	78	Total 78	O 78	0	0
17	b	56	Total 56	O 56	0	0

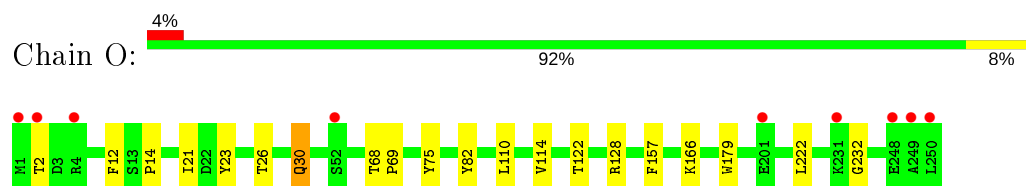
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

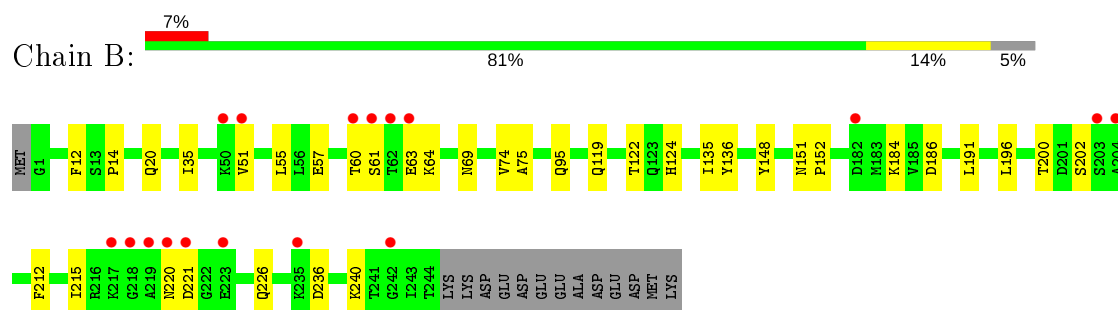
- Molecule 1: Proteasome subunit alpha type-2



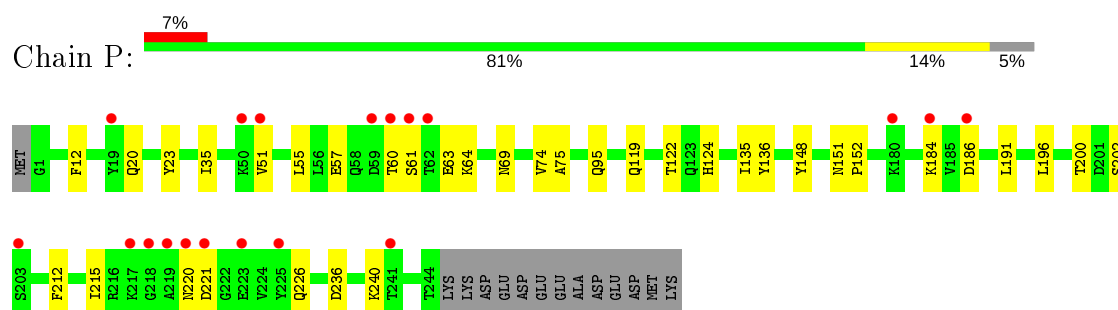
- Molecule 1: Proteasome subunit alpha type-2



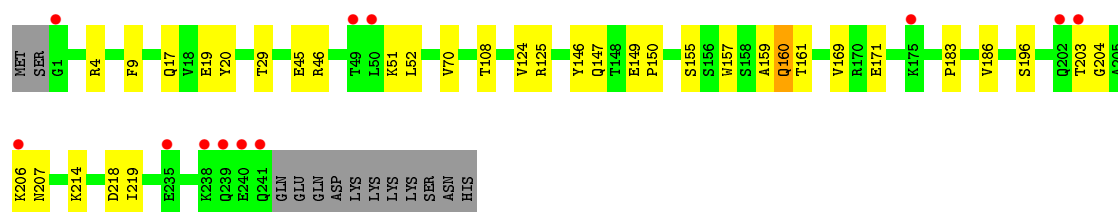
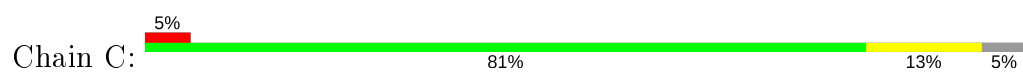
- Molecule 2: Proteasome subunit alpha type-3



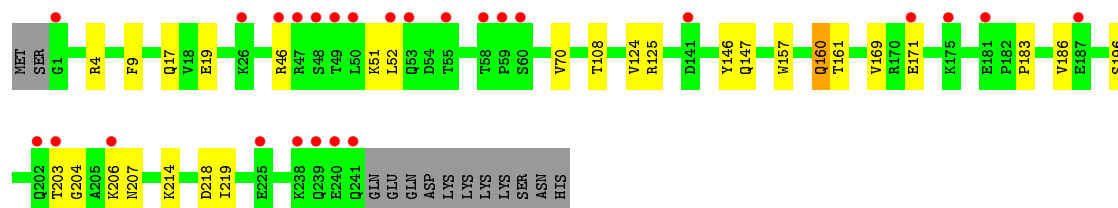
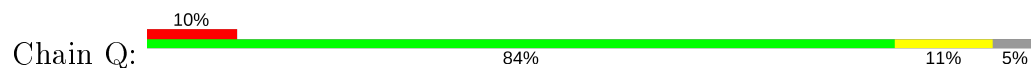
- Molecule 2: Proteasome subunit alpha type-3



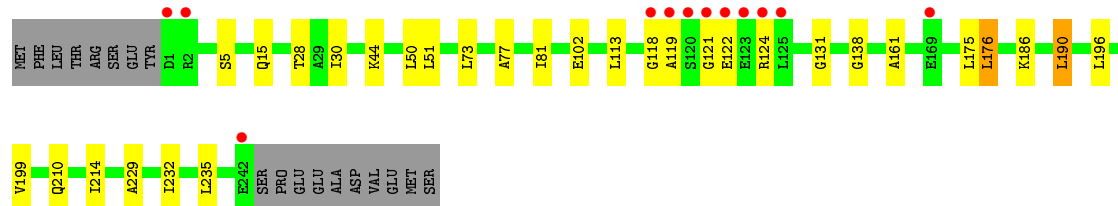
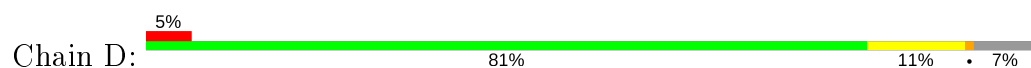
- Molecule 3: Proteasome subunit alpha type-4



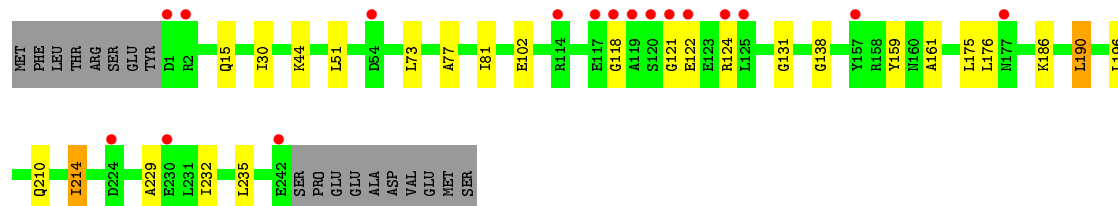
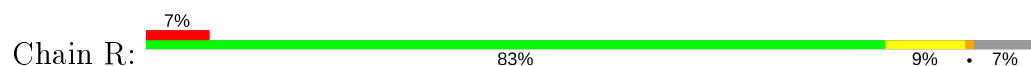
• Molecule 3: Proteasome subunit alpha type-4



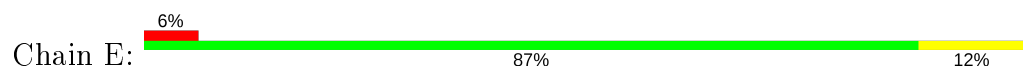
• Molecule 4: Proteasome subunit alpha type-5



• Molecule 4: Proteasome subunit alpha type-5

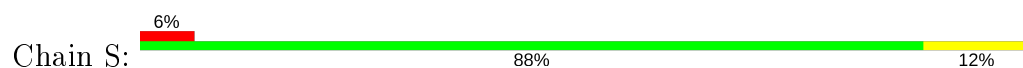


• Molecule 5: Proteasome subunit alpha type-6

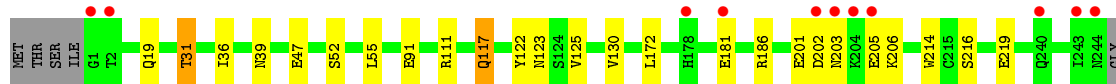
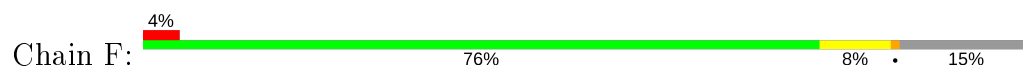




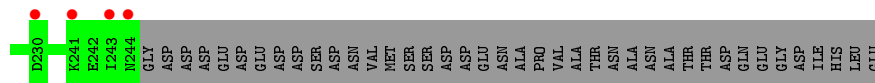
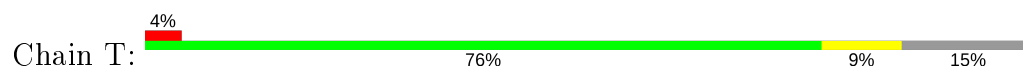
- Molecule 5: Proteasome subunit alpha type-6



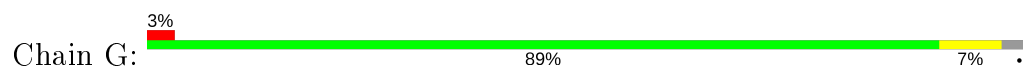
- Molecule 6: Probable proteasome subunit alpha type-7



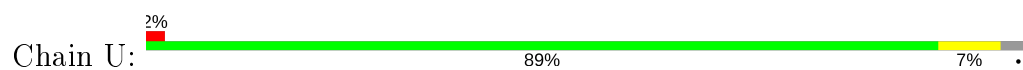
- Molecule 6: Probable proteasome subunit alpha type-7



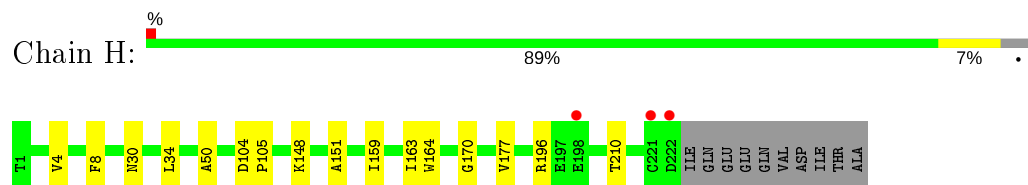
- Molecule 7: Proteasome subunit alpha type-1



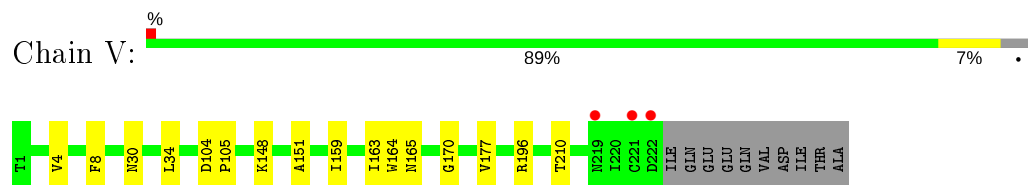
- Molecule 7: Proteasome subunit alpha type-1



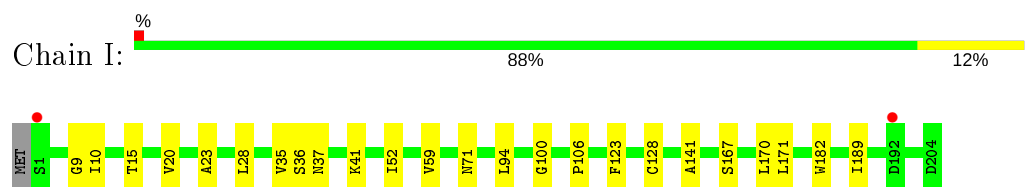
- Molecule 8: Proteasome subunit beta type-2



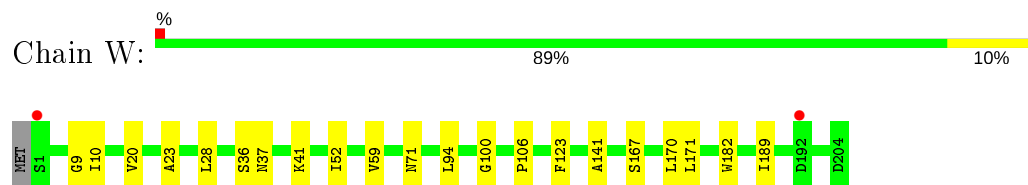
- Molecule 8: Proteasome subunit beta type-2



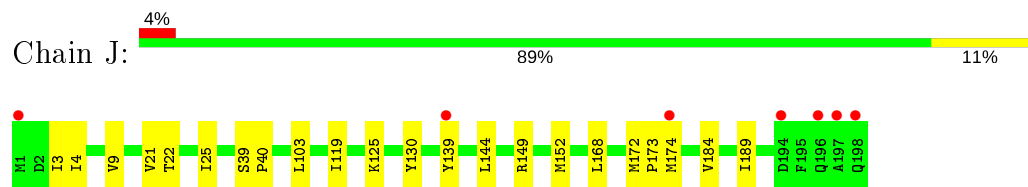
- Molecule 9: Proteasome subunit beta type-3



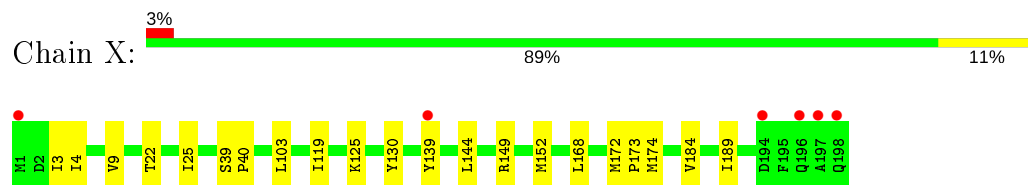
- Molecule 9: Proteasome subunit beta type-3



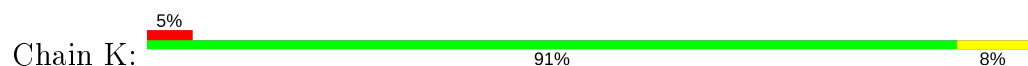
- Molecule 10: Proteasome subunit beta type-4

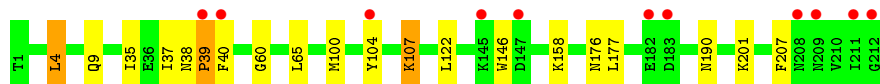


- Molecule 10: Proteasome subunit beta type-4

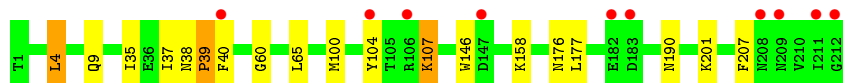
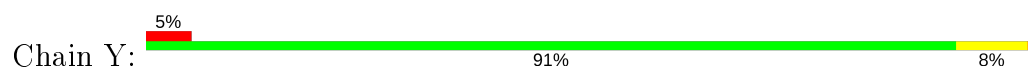


- Molecule 11: Proteasome subunit beta type-5

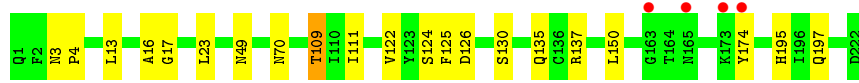
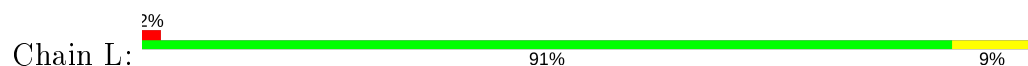




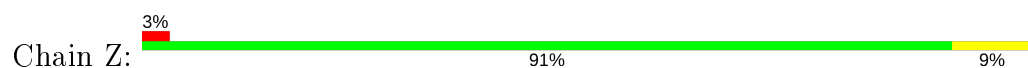
- Molecule 11: Proteasome subunit beta type-5



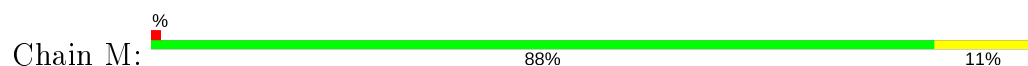
- Molecule 12: Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7



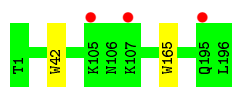
- Molecule 13: Proteasome subunit beta type-7



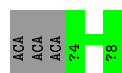
- Molecule 14: Proteasome subunit beta type-1



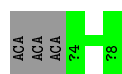
- Molecule 14: Proteasome subunit beta type-1



- Molecule 15: TMC-95A mimic ligand yCP:4e



- Molecule 15: TMC-95A mimic ligand yCP:4e



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.77Å 300.22Å 144.26Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-2.80) 99.3 (15.00-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.235 , 0.241 0.241 , 0.248	Depositor DCC
$R_{free}$ test set	12835 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.1	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	51011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: TY5, ACA, RE0, ABN, MES

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	0.37	0/1952	0.47	0/2642
1	O	0.37	1/1952 (0.1%)	0.47	0/2642
2	B	0.33	0/1934	0.46	0/2618
2	P	0.34	0/1934	0.47	0/2618
3	C	0.34	0/1919	0.48	0/2598
3	Q	0.34	0/1919	0.48	0/2598
4	D	0.36	0/1886	0.49	0/2541
4	R	0.36	0/1886	0.49	0/2541
5	E	0.31	0/1823	0.46	0/2463
5	S	0.31	0/1823	0.46	0/2463
6	F	0.41	0/1936	0.45	0/2614
6	T	0.41	0/1936	0.45	0/2614
7	G	0.35	0/1959	0.46	0/2652
7	U	0.34	0/1959	0.46	0/2652
8	H	0.44	1/1715 (0.1%)	0.47	0/2326
8	V	0.44	1/1715 (0.1%)	0.47	0/2326
9	I	0.34	0/1611	0.47	0/2174
9	W	0.34	0/1611	0.47	0/2174
10	J	0.31	0/1613	0.46	0/2173
10	X	0.31	0/1613	0.46	0/2173
11	K	0.50	1/1681 (0.1%)	0.50	1/2274 (0.0%)
11	Y	0.50	1/1681 (0.1%)	0.50	1/2274 (0.0%)
12	L	0.36	0/1795	0.46	0/2420
12	Z	0.36	0/1795	0.46	0/2420
13	M	0.36	0/1855	0.48	0/2514
13	a	0.36	0/1855	0.48	0/2514
14	N	0.39	0/1541	0.45	0/2087
14	b	0.39	2/1541 (0.1%)	0.45	0/2087
15	c	0.79	0/4	0.50	0/4
15	d	0.80	0/4	0.46	0/4
All	All	0.37	7/50448 (0.0%)	0.47	2/68200 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	146	TRP	CD2-CE2	5.07	1.47	1.41
11	K	146	TRP	CD2-CE2	5.06	1.47	1.41
1	O	179	TRP	CD2-CE2	5.03	1.47	1.41
8	H	164	TRP	CD2-CE2	5.03	1.47	1.41
14	b	42	TRP	CD2-CE2	5.01	1.47	1.41
14	b	165	TRP	CD2-CE2	5.01	1.47	1.41
8	V	164	TRP	CD2-CE2	5.00	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.34	127.59	115.30
11	K	4	LEU	CA-CB-CG	5.33	127.56	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	10	0
1	O	1915	0	1929	10	0
2	B	1904	0	1904	16	0
2	P	1904	0	1904	16	0
3	C	1890	0	1903	19	0
3	Q	1890	0	1903	14	0
4	D	1861	0	1839	17	0
4	R	1861	0	1839	12	0
5	E	1795	0	1800	17	0
5	S	1795	0	1800	15	0
6	F	1896	0	1889	11	0
6	T	1896	0	1889	11	0
7	G	1921	0	1913	8	0
7	U	1921	0	1913	9	0
8	H	1684	0	1688	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	V	1684	0	1688	7	0
9	I	1581	0	1574	13	0
9	W	1581	0	1574	10	0
10	J	1585	0	1590	16	0
10	X	1585	0	1590	14	0
11	K	1644	0	1595	8	0
11	Y	1644	0	1595	7	0
12	L	1757	0	1711	13	0
12	Z	1757	0	1711	14	0
13	M	1824	0	1832	17	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	1	0
14	b	1512	0	1481	0	0
15	c	56	0	48	0	0
15	d	56	0	48	0	0
16	K	12	0	13	0	0
16	Y	12	0	13	0	0
17	A	59	0	0	0	0
17	B	39	0	0	0	0
17	C	43	0	0	0	0
17	D	36	0	0	0	0
17	E	21	0	0	0	0
17	F	47	0	0	0	0
17	G	60	0	0	0	0
17	H	52	0	0	0	0
17	I	64	0	0	0	0
17	J	53	0	0	2	0
17	K	48	0	0	0	0
17	L	54	0	0	0	0
17	M	81	0	0	0	0
17	N	58	0	0	0	0
17	O	34	0	0	0	0
17	P	30	0	0	0	0
17	Q	29	0	0	0	0
17	R	27	0	0	0	0
17	S	18	0	0	0	0
17	T	43	0	0	0	0
17	U	55	0	0	0	0
17	V	50	0	0	0	0
17	W	62	0	0	0	0
17	X	41	0	0	0	0
17	Y	50	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Z	49	0	0	0	0
17	a	78	0	0	0	0
17	b	56	0	0	0	0
All	All	51011	0	49418	264	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 3.

All (264) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:PHE:H	4:D:15:GLN:HE22	1.33	0.77
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.67	0.76
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.51	0.76
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.51	0.75
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.67	0.74
12:Z:109:THR:HG23	12:Z:125:PHE:HB2	1.72	0.72
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.40	0.70
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.71	0.70
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.75	0.69
5:S:12:PHE:H	6:T:19:GLN:HE22	1.41	0.69
13:M:161:ARG:HH11	13:M:161:ARG:HG3	1.57	0.69
1:O:12:PHE:H	2:P:20:GLN:HE22	1.42	0.67
5:E:12:PHE:H	6:F:19:GLN:HE22	1.44	0.65
13:M:48:ASN:H	13:M:48:ASN:HD22	1.45	0.64
10:X:4:ILE:HG22	10:X:103:LEU:HD12	1.80	0.62
10:J:4:ILE:HG22	10:J:103:LEU:HD12	1.80	0.62
2:B:12:PHE:H	3:C:17:GLN:HE22	1.47	0.61
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.82	0.61
1:A:12:PHE:H	2:B:20:GLN:HE22	1.49	0.61
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.48	0.61
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.84	0.60
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.82	0.60
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.82	0.60
2:P:200:THR:HG22	2:P:202:SER:H	1.67	0.59
2:B:200:THR:HG22	2:B:202:SER:H	1.67	0.59
11:K:107:LYS:H	11:K:107:LYS:HD2	1.68	0.59
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.51	0.58
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.68	0.58
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.86	0.58
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.86	0.57
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.86	0.57
10:X:168:LEU:O	10:X:172:MET:HB2	2.05	0.57
4:D:44:LYS:HE3	4:D:210:GLN:HB2	1.86	0.57
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.86	0.57
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.86	0.57
10:J:168:LEU:O	10:J:172:MET:HB2	2.04	0.57
4:D:73:LEU:HD12	4:D:131:GLY:HA3	1.87	0.56
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.87	0.56
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.86	0.56
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.87	0.56
4:R:44:LYS:HE3	4:R:210:GLN:HB2	1.86	0.56
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.54	0.56
4:R:73:LEU:HD12	4:R:131:GLY:HA3	1.88	0.56
9:I:28:LEU:HB3	9:I:36:SER:HB3	1.88	0.56
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.87	0.56
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.86	0.56
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.87	0.55
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.87	0.55
4:D:77:ALA:O	4:D:81:ILE:HG12	2.07	0.55
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.87	0.55
4:R:77:ALA:O	4:R:81:ILE:HG12	2.06	0.55
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.88	0.55
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.53	0.55
9:W:28:LEU:HB3	9:W:36:SER:HB3	1.88	0.55
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.89	0.54
12:L:195:HIS:HD2	12:L:197:GLN:H	1.56	0.54
2:P:63:GLU:HG3	2:P:64:LYS:HG3	1.90	0.54
2:P:75:ALA:HB3	2:P:135:ILE:HB	1.89	0.54
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.89	0.54
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.55	0.54
2:B:75:ALA:HB3	2:B:135:ILE:HB	1.89	0.54
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.89	0.54
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.54	0.54
13:M:43:ILE:HG12	13:M:64:GLU:HG2	1.91	0.53
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.90	0.53
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.91	0.53
6:T:91:GLU:HG3	6:T:111:ARG:HH11	1.74	0.53
2:B:63:GLU:HG3	2:B:64:LYS:HG3	1.90	0.53
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.90	0.53
10:J:173:PRO:HB2	10:X:174:MET:HE1	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.89	0.53
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.43	0.53
10:J:174:MET:HE1	10:X:173:PRO:HB2	1.90	0.53
4:D:119:ALA:HA	5:E:124:GLY:HA2	1.91	0.53
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.90	0.52
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.90	0.52
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.07	0.52
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.91	0.52
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.73	0.52
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.90	0.52
5:E:231:LYS:H	5:E:231:LYS:HD2	1.76	0.51
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.07	0.51
10:J:139:TYR:OH	10:X:25:ILE:HG12	2.10	0.51
5:S:231:LYS:HD2	5:S:231:LYS:H	1.76	0.51
1:A:110:LEU:O	1:A:114:VAL:HG23	2.11	0.51
1:O:110:LEU:O	1:O:114:VAL:HG23	2.11	0.51
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.93	0.51
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.93	0.51
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.93	0.51
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.93	0.51
7:G:63:ILE:HD12	7:G:215:GLU:HG2	1.93	0.51
6:T:31:THR:HG21	6:T:47:GLU:O	2.11	0.51
6:F:31:THR:HG21	6:F:47:GLU:O	2.11	0.50
9:I:35:VAL:HG13	17:J:241:HOH:O	2.10	0.50
10:J:3:ILE:HD13	10:J:168:LEU:HD13	1.94	0.50
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.46	0.50
3:C:186:VAL:HG21	3:C:214:LYS:HE2	1.94	0.50
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.93	0.50
8:V:148:LYS:HE3	8:V:177:VAL:HG11	1.93	0.50
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.93	0.50
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	1.94	0.50
7:G:78:ILE:N	7:G:79:PRO:HD2	2.27	0.50
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.93	0.50
8:H:148:LYS:HE3	8:H:177:VAL:HG11	1.94	0.50
1:O:26:THR:O	1:O:30:GLN:HG2	2.12	0.50
10:X:3:ILE:HD13	10:X:168:LEU:HD13	1.94	0.50
3:Q:186:VAL:HG21	3:Q:214:LYS:HE2	1.94	0.49
10:J:139:TYR:HD1	17:J:227:HOH:O	1.95	0.49
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.93	0.49
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.94	0.49
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:63:ILE:HD12	7:U:215:GLU:HG2	1.93	0.49
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.94	0.49
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.94	0.49
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.93	0.49
10:J:119:ILE:HG12	10:J:125:LYS:HG3	1.94	0.49
12:L:126:ASP:HB2	12:L:130:SER:HB3	1.94	0.49
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.48	0.49
7:U:78:ILE:N	7:U:79:PRO:HD2	2.27	0.49
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.78	0.49
3:Q:70:VAL:HG13	3:Q:219:ILE:HD13	1.95	0.49
1:A:21:ILE:HD11	1:A:122:THR:HG21	1.95	0.49
10:J:25:ILE:HG12	10:X:139:TYR:OH	2.12	0.49
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.76	0.48
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.94	0.48
1:A:26:THR:O	1:A:30:GLN:HG2	2.12	0.48
12:Z:17:GLY:HA2	12:Z:174:TYR:HE1	1.78	0.48
3:C:70:VAL:HG13	3:C:219:ILE:HD13	1.95	0.48
1:O:21:ILE:HD11	1:O:122:THR:HG21	1.95	0.48
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.96	0.48
12:L:17:GLY:HA2	12:L:174:TYR:HE1	1.78	0.48
8:V:210:THR:HG21	9:W:167:SER:HB3	1.96	0.47
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.94	0.47
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.12	0.47
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.49	0.47
1:A:68:THR:HB	1:A:69:PRO:HD2	1.96	0.47
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.49	0.47
12:Z:124:SER:HB3	12:Z:137:ARG:HG2	1.96	0.47
13:M:209:LYS:HB3	13:M:212:LEU:HD11	1.96	0.47
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.45	0.47
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.96	0.47
12:Z:135:GLN:HG3	12:Z:174:TYR:OH	2.15	0.47
5:E:227:GLU:CD	5:E:227:GLU:H	2.18	0.47
4:D:113:LEU:HD12	5:E:78:PRO:HB2	1.96	0.47
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.80	0.47
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.63	0.47
5:S:227:GLU:CD	5:S:227:GLU:H	2.18	0.47
2:B:236:ASP:O	2:B:240:LYS:HG2	2.15	0.47
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	1.97	0.47
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.97	0.46
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.96	0.46
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.13	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.96	0.46
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.98	0.46
2:P:236:ASP:O	2:P:240:LYS:HG2	2.15	0.46
12:L:135:GLN:HG3	12:L:174:TYR:OH	2.15	0.46
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.45	0.46
4:D:5:SER:HB2	5:E:125:ARG:HD3	1.97	0.46
12:L:124:SER:HB3	12:L:137:ARG:HG2	1.96	0.46
1:O:68:THR:HB	1:O:69:PRO:HD2	1.96	0.46
6:F:122:TYR:HB2	6:F:125:VAL:HG22	1.98	0.46
13:M:96:LEU:O	13:M:100:MET:HG2	2.16	0.46
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.98	0.46
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.97	0.46
4:D:176:LEU:HD22	5:E:55:LEU:HD13	1.99	0.45
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.99	0.45
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.97	0.45
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.80	0.45
6:T:122:TYR:HB2	6:T:125:VAL:HG22	1.99	0.45
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.97	0.45
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.80	0.45
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.98	0.45
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.98	0.45
5:S:131:LEU:HB2	5:S:146:PHE:HB3	1.98	0.45
2:B:136:TYR:HB2	2:B:148:TYR:HB2	1.99	0.45
10:J:184:VAL:HG22	10:J:189:ILE:HG12	1.99	0.45
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.52	0.45
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.97	0.45
11:Y:201:LYS:HG3	11:Y:207:PHE:HB2	1.98	0.45
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.99	0.45
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.99	0.45
11:K:201:LYS:HG3	11:K:207:PHE:HB2	1.98	0.44
13:M:129:TYR:HE1	13:M:144:THR:HG22	1.81	0.44
13:M:15:LYS:HB3	13:M:20:VAL:HG12	1.98	0.44
3:C:155:SER:HB2	4:D:51:LEU:HD21	1.99	0.44
3:C:108:THR:HG21	3:C:146:TYR:HB3	1.99	0.44
4:D:229:ALA:HA	4:D:232:ILE:HD12	1.99	0.44
12:Z:111:ILE:HG12	12:Z:125:PHE:HE1	1.83	0.44
13:M:161:ARG:NH1	13:M:161:ARG:HG3	2.28	0.44
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.99	0.44
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.52	0.44
13:M:48:ASN:HD22	13:M:48:ASN:N	2.07	0.44
2:P:136:TYR:HB2	2:P:148:TYR:HB2	1.98	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:111:ILE:HG12	12:L:125:PHE:HE1	1.82	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.43
3:C:204:GLY:HA3	3:C:207:ASN:HB2	2.00	0.43
5:E:131:LEU:HB2	5:E:146:PHE:HB3	1.98	0.43
10:J:173:PRO:HB3	10:X:22:THR:HG21	2.00	0.43
10:J:22:THR:HG21	10:X:173:PRO:HB3	2.01	0.43
10:X:184:VAL:HG22	10:X:189:ILE:HG12	1.99	0.43
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.99	0.43
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.00	0.43
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.99	0.43
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.54	0.43
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.99	0.43
4:R:229:ALA:HA	4:R:232:ILE:HD12	1.99	0.43
5:S:134:ILE:HD12	5:S:215:VAL:HG12	2.01	0.43
8:V:4:VAL:HG22	8:V:159:ILE:HD11	2.01	0.43
9:W:106:PRO:HD2	9:W:123:PHE:HB2	2.01	0.43
13:M:227:GLY:HA3	13:M:231:GLN:HB3	2.00	0.43
6:T:52:SER:H	6:T:55:LEU:HD13	1.83	0.43
7:G:7:ILE:HG13	7:G:9:ILE:HG12	2.01	0.43
5:S:230:ALA:HA	5:S:233:ILE:HD12	2.01	0.43
7:U:7:ILE:HG13	7:U:9:ILE:HG12	2.01	0.43
2:P:57:GLU:O	2:P:61:SER:HB2	2.19	0.42
3:Q:204:GLY:HA3	3:Q:207:ASN:HB2	2.00	0.42
2:P:122:THR:HG22	3:Q:125:ARG:HH21	1.84	0.42
4:D:161:ALA:HB1	4:D:175:LEU:HD22	2.00	0.42
5:E:230:ALA:HA	5:E:233:ILE:HD12	2.01	0.42
5:S:127:TYR:O	5:S:148:PRO:HB3	2.18	0.42
3:C:46:ARG:HB2	3:C:207:ASN:HA	2.01	0.42
3:Q:46:ARG:HB2	3:Q:207:ASN:HA	2.01	0.42
4:D:186:LYS:O	4:D:190:LEU:HD22	2.20	0.42
9:I:106:PRO:HD2	9:I:123:PHE:HB2	2.01	0.42
5:E:134:ILE:HD12	5:E:215:VAL:HG12	2.01	0.42
6:T:205:GLU:HG3	6:T:206:LYS:HG3	2.02	0.42
5:E:127:TYR:O	5:E:148:PRO:HB3	2.19	0.42
2:B:57:GLU:O	2:B:61:SER:HB2	2.19	0.42
4:R:161:ALA:HB1	4:R:175:LEU:HD22	2.01	0.42
6:F:205:GLU:HG3	6:F:206:LYS:HG3	2.01	0.42
9:I:23:ALA:HB1	9:I:170:LEU:HD22	2.01	0.42
13:M:193:ARG:HG3	13:M:214:VAL:HB	2.02	0.42
13:M:27:LEU:HD11	13:M:34:LEU:HB3	2.01	0.42
6:T:36:ILE:HG12	6:T:172:LEU:HD11	2.02	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:52:SER:H	6:F:55:LEU:HD13	1.83	0.41
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.02	0.41
11:Y:38:ASN:C	11:Y:40:PHE:H	2.24	0.41
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.85	0.41
6:F:36:ILE:HG12	6:F:172:LEU:HD11	2.02	0.41
8:H:4:VAL:HG22	8:H:159:ILE:HD11	2.01	0.41
4:R:186:LYS:O	4:R:190:LEU:HD22	2.20	0.41
3:C:29:THR:HB	3:C:45:GLU:HG3	2.02	0.41
11:K:38:ASN:C	11:K:40:PHE:H	2.24	0.41
10:X:130:TYR:HB2	10:X:144:LEU:HD13	2.02	0.41
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.56	0.41
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.03	0.41
3:C:159:ALA:HB3	4:D:50:LEU:HD22	2.03	0.41
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.69	0.41
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.56	0.41
9:W:23:ALA:HB1	9:W:170:LEU:HD22	2.01	0.41
5:E:205:LEU:HD23	5:E:205:LEU:H	1.86	0.41
8:H:210:THR:HG21	9:I:167:SER:HB3	2.03	0.41
9:I:15:THR:HG22	9:I:20:VAL:HG12	2.04	0.40
4:D:28:THR:HG21	4:D:199:VAL:HG21	2.04	0.40
11:Y:176:ASN:HD21	11:Y:190:ASN:HD22	1.69	0.40
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.03	0.40
8:H:50:ALA:HB2	9:I:128:CYS:HB2	2.04	0.40
5:S:205:LEU:HD23	5:S:205:LEU:H	1.86	0.40
12:Z:17:GLY:HA2	12:Z:174:TYR:CE1	2.57	0.40
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.04	0.40
6:F:117:GLN:HB3	6:F:117:GLN:HE21	1.69	0.40
10:J:130:TYR:HB2	10:J:144:LEU:HD13	2.02	0.40
1:O:14:PRO:HA	2:P:23:TYR:CD1	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%)	240 (97%)	6 (2%)	2 (1%)	19	49
1	O	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	19	49
2	B	242/258 (94%)	235 (97%)	5 (2%)	2 (1%)	19	49
2	P	242/258 (94%)	235 (97%)	5 (2%)	2 (1%)	19	49
3	C	239/254 (94%)	233 (98%)	3 (1%)	3 (1%)	12	36
3	Q	239/254 (94%)	233 (98%)	3 (1%)	3 (1%)	12	36
4	D	240/260 (92%)	235 (98%)	2 (1%)	3 (1%)	12	36
4	R	240/260 (92%)	235 (98%)	2 (1%)	3 (1%)	12	36
5	E	231/234 (99%)	224 (97%)	6 (3%)	1 (0%)	34	66
5	S	231/234 (99%)	224 (97%)	6 (3%)	1 (0%)	34	66
6	F	242/288 (84%)	233 (96%)	9 (4%)	0	100	100
6	T	242/288 (84%)	233 (96%)	9 (4%)	0	100	100
7	G	241/252 (96%)	236 (98%)	5 (2%)	0	100	100
7	U	241/252 (96%)	236 (98%)	5 (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%)	194 (96%)	7 (4%)	1 (0%)	29	61
9	W	202/205 (98%)	194 (96%)	7 (4%)	1 (0%)	29	61
10	J	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	29	61
10	X	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	29	61
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	29	61
11	Y	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	29	61
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
13	a	231/233 (99%)	221 (96%)	10 (4%)	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
15	c	1/8 (12%)	1 (100%)	0	0	100	100
15	d	1/8 (12%)	1 (100%)	0	0	100	100
All	All	6314/6604 (96%)	6120 (97%)	166 (3%)	28 (0%)	34	66

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	52	LEU
3	Q	52	LEU
1	A	2	THR
1	A	166	LYS
4	D	122	GLU
11	K	39	PRO
1	O	166	LYS
4	R	122	GLU
11	Y	39	PRO
2	B	51	VAL
2	B	221	ASP
3	C	183	PRO
3	C	203	THR
4	D	121	GLY
5	E	201	ARG
1	O	2	THR
2	P	51	VAL
2	P	221	ASP
3	Q	183	PRO
3	Q	203	THR
4	R	121	GLY
5	S	201	ARG
4	D	118	GLY
4	R	118	GLY
9	I	100	GLY
9	W	100	GLY
10	J	9	VAL
10	X	9	VAL

### 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%)	207 (99%)	2 (1%)	76	93
1	O	209/209 (100%)	207 (99%)	2 (1%)	76	93
2	B	203/216 (94%)	193 (95%)	10 (5%)	25	57

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	203/216 (94%)	193 (95%)	10 (5%)	25	57
3	C	213/226 (94%)	206 (97%)	7 (3%)	38	72
3	Q	213/226 (94%)	206 (97%)	7 (3%)	38	72
4	D	198/215 (92%)	193 (98%)	5 (2%)	47	80
4	R	198/215 (92%)	192 (97%)	6 (3%)	41	75
5	E	192/193 (100%)	183 (95%)	9 (5%)	26	59
5	S	192/193 (100%)	183 (95%)	9 (5%)	26	59
6	F	201/239 (84%)	190 (94%)	11 (6%)	21	52
6	T	201/239 (84%)	190 (94%)	11 (6%)	21	52
7	G	207/210 (99%)	202 (98%)	5 (2%)	49	81
7	U	207/210 (99%)	202 (98%)	5 (2%)	49	81
8	H	181/190 (95%)	178 (98%)	3 (2%)	60	87
8	V	181/190 (95%)	178 (98%)	3 (2%)	60	87
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	87
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	87
10	J	175/175 (100%)	175 (100%)	0	100	100
10	X	175/175 (100%)	175 (100%)	0	100	100
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	64
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30	64
12	L	185/185 (100%)	182 (98%)	3 (2%)	62	88
12	Z	185/185 (100%)	182 (98%)	3 (2%)	62	88
13	M	199/199 (100%)	193 (97%)	6 (3%)	41	75
13	a	199/199 (100%)	193 (97%)	6 (3%)	41	75
14	N	162/162 (100%)	162 (100%)	0	100	100
14	b	162/162 (100%)	162 (100%)	0	100	100
All	All	5332/5522 (97%)	5189 (97%)	143 (3%)	44	78

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	157	PHE
2	B	55	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	60	THR
2	B	69	ASN
2	B	74	VAL
2	B	119	GLN
2	B	184	LYS
2	B	186	ASP
2	B	191	LEU
2	B	212	PHE
2	B	220	ASN
3	C	4	ARG
3	C	19	GLU
3	C	51	LYS
3	C	147	GLN
3	C	160	GLN
3	C	171	GLU
3	C	206	LYS
4	D	102	GLU
4	D	124	ARG
4	D	176	LEU
4	D	190	LEU
4	D	235	LEU
5	E	8	ASP
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	198	GLN
5	E	231	LYS
6	F	31	THR
6	F	39	ASN
6	F	117	GLN
6	F	123	ASN
6	F	130	VAL
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	202	ASP
6	F	203	ASN
6	F	214	TRP
7	G	115	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	G	117	GLN
7	G	166	GLN
7	G	221	LYS
7	G	235	ARG
8	H	30	ASN
8	H	34	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	65	LEU
11	K	100	MET
11	K	104	TYR
11	K	107	LYS
12	L	23	LEU
12	L	49	ASN
12	L	109	THR
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE
13	M	161	ARG
13	M	226	LYS
1	O	30	GLN
1	O	157	PHE
2	P	55	LEU
2	P	60	THR
2	P	69	ASN
2	P	74	VAL
2	P	119	GLN
2	P	184	LYS
2	P	186	ASP
2	P	191	LEU
2	P	212	PHE
2	P	220	ASN
3	Q	4	ARG
3	Q	19	GLU
3	Q	51	LYS
3	Q	147	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	Q	160	GLN
3	Q	171	GLU
3	Q	206	LYS
4	R	102	GLU
4	R	124	ARG
4	R	176	LEU
4	R	190	LEU
4	R	214	ILE
4	R	235	LEU
5	S	8	ASP
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	198	GLN
5	S	231	LYS
6	T	31	THR
6	T	39	ASN
6	T	117	GLN
6	T	123	ASN
6	T	130	VAL
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	202	ASP
6	T	203	ASN
6	T	214	TRP
7	U	115	LEU
7	U	117	GLN
7	U	166	GLN
7	U	221	LYS
7	U	235	ARG
8	V	30	ASN
8	V	34	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
11	Y	4	LEU
11	Y	9	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
11	Y	35	ILE
11	Y	65	LEU
11	Y	100	MET
11	Y	104	TYR
11	Y	107	LYS
12	Z	23	LEU
12	Z	49	ASN
12	Z	109	THR
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	146	PHE
13	a	161	ARG
13	a	226	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
2	B	20	GLN
2	B	69	ASN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
3	C	17	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	241	GLN
4	D	15	GLN
4	D	100	ASN
4	D	210	GLN
4	D	225	ASN
5	E	30	GLN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
5	E	198	GLN
5	E	209	ASN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
7	G	6	HIS
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
7	G	231	ASN
8	H	30	ASN
8	H	141	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	88	GLN
10	J	55	GLN
10	J	118	GLN
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	165	ASN
12	L	195	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	171	GLN
13	M	179	ASN
13	M	213	GLN
14	N	161	GLN
1	O	30	GLN
2	P	20	GLN
2	P	69	ASN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
3	Q	17	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	100	ASN
4	R	210	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
5	S	198	GLN
5	S	209	ASN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	T	203	ASN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
7	U	231	ASN
8	V	30	ASN
8	V	141	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	88	GLN
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	165	ASN
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	171	GLN
13	a	179	ASN
13	a	213	GLN
14	b	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	ACA	d	4	15	7,7,8	0.70	0	6,6,8	0.59	0
15	TY5	c	5	15	19,20,21	1.02	0	22,25,27	0.55	0
15	RE0	c	7	15	15,17,18	1.25	1 (6%)	19,25,27	2.03	5 (26%)
15	RE0	d	7	15	15,17,18	1.19	1 (6%)	19,25,27	2.02	5 (26%)
15	TY5	d	5	15	19,20,21	1.01	0	22,25,27	0.49	0
15	ACA	c	4	15	7,7,8	0.72	0	6,6,8	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ACA	d	4	15	-	3/4/5/6	-
15	TY5	c	5	15	-	4/10/11/13	0/2/2/2
15	RE0	c	7	15	-	0/6/23/25	0/2/2/2
15	RE0	d	7	15	-	0/6/23/25	0/2/2/2
15	TY5	d	5	15	-	5/10/11/13	0/2/2/2
15	ACA	c	4	15	-	3/4/5/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	7	RE0	CG-CD2	3.28	1.54	1.51
15	d	7	RE0	CG-CD2	3.05	1.54	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	7	RE0	CG-CD2-CE2	-4.37	107.11	108.86
15	d	7	RE0	CG-CD2-CE2	-4.23	107.16	108.86
15	d	7	RE0	CE2-NE1-CD1	-3.60	109.70	111.86
15	c	7	RE0	CE2-NE1-CD1	-3.52	109.75	111.86
15	c	7	RE0	CD2-CE2-NE1	3.42	111.89	109.59
15	d	7	RE0	CD2-CE2-NE1	3.42	111.89	109.59
15	c	7	RE0	CG-CD1-NE1	3.32	110.43	108.41
15	d	7	RE0	CG-CD1-NE1	3.22	110.37	108.41
15	c	7	RE0	CZ2-CE2-NE1	-2.80	125.16	130.87
15	d	7	RE0	CZ2-CE2-NE1	-2.77	125.23	130.87

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	4	ACA	C1-C2-C3-C4
15	c	5	TY5	CE2-CZ-OH-C49
15	d	5	TY5	CE1-CZ-OH-C49
15	c	5	TY5	CE1-CZ-OH-C49
15	d	5	TY5	CE2-CZ-OH-C49
15	d	4	ACA	C2-C3-C4-C5
15	c	4	ACA	C2-C3-C4-C5
15	c	4	ACA	C3-C4-C5-C6
15	d	5	TY5	N-CA-CB-CG
15	d	4	ACA	C1-C2-C3-C4
15	c	5	TY5	CA-CB-CG-CD1
15	c	5	TY5	CA-CB-CG-CD2
15	d	5	TY5	CA-CB-CG-CD2
15	d	5	TY5	CA-CB-CG-CD1
15	d	4	ACA	C4-C5-C6-N6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	MES	K	301	-	12,12,12	1.29	1 (8%)	14,16,16	1.65	2 (14%)
16	MES	Y	301	-	12,12,12	1.37	1 (8%)	14,16,16	2.01	5 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MES	K	301	-	-	5/6/14/14	0/1/1/1
16	MES	Y	301	-	-	4/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	301	MES	C8-S	3.00	1.81	1.77
16	K	301	MES	C8-S	2.89	1.81	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	MES	O2S-S-C8	-4.00	102.10	106.92
16	K	301	MES	O2S-S-C8	-3.58	102.60	106.92
16	K	301	MES	O3S-S-O1S	3.00	118.62	111.27
16	Y	301	MES	O3S-S-O1S	3.00	118.60	111.27
16	Y	301	MES	C6-C5-N4	2.54	113.96	110.10
16	Y	301	MES	C5-N4-C3	2.38	114.18	108.83
16	Y	301	MES	C2-C3-N4	2.36	113.69	110.10

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Y	301	MES	C7-C8-S-O2S
16	Y	301	MES	C7-C8-S-O3S
16	Y	301	MES	N4-C7-C8-S
16	K	301	MES	C8-C7-N4-C3
16	K	301	MES	C8-C7-N4-C5
16	K	301	MES	C7-C8-S-O3S
16	K	301	MES	C7-C8-S-O1S
16	K	301	MES	C7-C8-S-O2S
16	Y	301	MES	C8-C7-N4-C5

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.07	8 (3%) 47 37	58, 71, 92, 109	0
1	O	250/250 (100%)	-0.03	9 (3%) 42 32	61, 77, 101, 118	0
2	B	244/258 (94%)	0.21	17 (6%) 16 9	58, 75, 111, 120	0
2	P	244/258 (94%)	0.25	19 (7%) 13 7	64, 79, 109, 124	0
3	C	241/254 (94%)	0.13	12 (4%) 28 19	56, 75, 112, 143	0
3	Q	241/254 (94%)	0.40	26 (10%) 5 3	69, 92, 139, 169	0
4	D	242/260 (93%)	0.12	12 (4%) 28 19	61, 76, 103, 120	0
4	R	242/260 (93%)	0.21	17 (7%) 16 9	65, 84, 114, 129	0
5	E	233/234 (99%)	0.06	13 (5%) 24 16	64, 79, 99, 112	0
5	S	233/234 (99%)	0.17	15 (6%) 19 12	65, 86, 112, 124	0
6	F	244/288 (84%)	-0.02	11 (4%) 33 23	59, 74, 102, 125	0
6	T	244/288 (84%)	0.05	11 (4%) 33 23	61, 78, 112, 134	0
7	G	243/252 (96%)	-0.02	8 (3%) 46 36	56, 73, 96, 130	0
7	U	243/252 (96%)	0.01	6 (2%) 57 47	60, 72, 91, 116	0
8	H	222/232 (95%)	-0.14	3 (1%) 75 70	56, 67, 81, 98	0
8	V	222/232 (95%)	-0.20	3 (1%) 75 70	55, 66, 81, 105	0
9	I	204/205 (99%)	-0.37	2 (0%) 82 77	53, 63, 79, 83	0
9	W	204/205 (99%)	-0.25	2 (0%) 82 77	59, 66, 82, 91	0
10	J	198/198 (100%)	-0.08	7 (3%) 44 34	54, 66, 83, 116	0
10	X	198/198 (100%)	-0.07	6 (3%) 50 40	59, 68, 83, 116	0
11	K	212/212 (100%)	-0.05	11 (5%) 27 18	52, 66, 85, 91	0
11	Y	212/212 (100%)	-0.07	10 (4%) 31 22	58, 69, 88, 96	0
12	L	222/222 (100%)	-0.19	4 (1%) 68 61	55, 65, 89, 96	0
12	Z	222/222 (100%)	-0.17	7 (3%) 47 37	56, 66, 88, 95	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	233/233 (100%)	-0.29	2 (0%) 84 80	53, 64, 77, 80	0
13	a	233/233 (100%)	-0.29	1 (0%) 92 91	53, 65, 76, 80	0
14	N	196/196 (100%)	-0.32	0 100 100	55, 62, 78, 86	0
14	b	196/196 (100%)	-0.30	3 (1%) 73 68	54, 62, 77, 85	0
15	c	1/8 (12%)	-0.23	0 100 100	58, 58, 58, 58	0
15	d	1/8 (12%)	-0.02	0 100 100	56, 56, 56, 56	0
All	All	6370/6604 (96%)	-0.04	245 (3%) 40 30	52, 71, 104, 169	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	119	ALA	10.6
4	D	119	ALA	10.0
2	P	219	ALA	9.3
4	D	120	SER	9.3
2	B	220	ASN	8.9
10	X	198	GLN	8.5
4	R	120	SER	8.5
4	D	118	GLY	8.4
4	R	121	GLY	8.4
2	P	218	GLY	8.2
2	B	219	ALA	8.1
2	P	220	ASN	7.5
4	R	118	GLY	7.5
7	U	243	ASP	7.5
5	E	1	PHE	7.4
3	C	49	THR	7.4
10	J	198	GLN	6.7
1	A	1	MET	6.6
10	J	197	ALA	6.5
7	G	1	ALA	6.4
3	Q	48	SER	6.2
2	B	218	GLY	6.1
7	G	243	ASP	5.9
10	X	197	ALA	5.9
7	U	1	ALA	5.9
3	C	50	LEU	5.7
12	L	174	TYR	5.7
3	Q	240	GLU	5.7
8	V	222	ASP	5.6

Continued on next page...

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	W	1	SER	5.6
8	V	221	CYS	5.5
11	Y	104	TYR	5.5
3	Q	49	THR	5.5
4	D	121	GLY	5.5
1	A	2	THR	5.4
2	P	223	GLU	5.4
12	Z	173	LYS	5.4
3	Q	50	LEU	5.4
2	P	61	SER	5.3
3	Q	203	THR	5.3
12	Z	174	TYR	5.1
5	S	202	ASP	5.1
7	G	242	GLN	4.9
5	S	2	ARG	4.9
5	S	1	PHE	4.8
5	E	202	ASP	4.7
4	D	125	LEU	4.7
13	M	1	THR	4.7
1	O	2	THR	4.6
8	H	221	CYS	4.6
4	D	124	ARG	4.5
3	Q	239	GLN	4.5
4	R	1	ASP	4.4
11	K	104	TYR	4.4
3	C	241	GLN	4.4
8	H	222	ASP	4.4
10	X	194	ASP	4.4
10	J	196	GLN	4.4
6	F	1	GLY	4.4
11	K	208	ASN	4.4
6	F	243	ILE	4.2
6	T	2	THR	4.2
6	F	202	ASP	4.1
10	J	1	MET	4.1
5	S	52	ALA	4.1
11	K	183	ASP	4.1
2	B	221	ASP	4.0
3	C	203	THR	4.0
2	B	51	VAL	3.9
5	S	3	ASN	3.9
5	S	173	ARG	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	O	1	MET	3.9
4	R	124	ARG	3.8
2	P	221	ASP	3.8
4	D	122	GLU	3.8
3	Q	241	GLN	3.8
9	I	1	SER	3.8
2	B	203	SER	3.8
2	B	223	GLU	3.8
1	A	250	LEU	3.7
2	P	50	LYS	3.7
5	E	2	ARG	3.6
4	R	125	LEU	3.6
1	O	201	GLU	3.6
2	P	51	VAL	3.6
6	T	178	HIS	3.6
11	K	209	ASN	3.6
2	B	61	SER	3.5
12	L	165	ASN	3.5
2	P	60	THR	3.5
11	K	40	PHE	3.5
6	F	2	THR	3.5
11	Y	182	GLU	3.5
5	E	204	SER	3.5
4	R	177	ASN	3.5
3	C	206	LYS	3.4
6	T	1	GLY	3.4
6	T	244	ASN	3.4
1	O	250	LEU	3.4
1	O	249	ALA	3.4
3	C	1	GLY	3.4
5	S	30	GLN	3.4
2	P	225	TYR	3.4
1	A	201	GLU	3.3
11	Y	212	GLY	3.3
10	X	196	GLN	3.3
11	Y	209	ASN	3.3
13	a	1	THR	3.3
4	R	157	TYR	3.3
11	K	182	GLU	3.3
3	C	239	GLN	3.3
5	E	3	ASN	3.2
5	E	30	GLN	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	60	THR	3.2
1	O	248	GLU	3.2
4	D	123	GLU	3.2
11	Y	183	ASP	3.2
7	G	2	GLY	3.2
11	Y	208	ASN	3.2
13	M	47	ASP	3.1
7	G	188	GLU	3.1
6	F	178	HIS	3.1
2	P	203	SER	3.1
3	C	202	GLN	3.1
2	P	180	LYS	3.1
5	S	51	ASN	3.1
6	T	243	ILE	3.1
8	V	219	ASN	3.1
10	X	1	MET	3.1
5	S	54	GLU	3.1
6	T	207	ASP	3.0
3	Q	202	GLN	3.0
4	R	122	GLU	3.0
3	C	238	LYS	3.0
2	P	59	ASP	3.0
6	T	241	LYS	2.9
3	Q	52	LEU	2.9
5	E	54	GLU	2.9
4	D	1	ASP	2.9
6	F	181	GLU	2.9
11	K	212	GLY	2.9
4	D	2	ARG	2.9
7	U	222	ASP	2.9
12	L	173	LYS	2.8
6	F	205	GLU	2.8
9	W	192	ASP	2.8
5	S	58	TYR	2.8
3	Q	206	LYS	2.8
1	A	231	LYS	2.7
11	K	147	ASP	2.7
14	b	107	LYS	2.7
1	O	52	SER	2.7
2	B	204	ALA	2.7
10	X	139	TYR	2.7
5	S	204	SER	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	E	173	ARG	2.6
6	T	205	GLU	2.6
3	Q	46	ARG	2.6
6	T	230	ASP	2.6
12	Z	210	ASP	2.6
3	Q	55	THR	2.6
3	Q	53	GLN	2.6
5	E	233	ILE	2.6
2	B	235	LYS	2.6
10	J	139	TYR	2.6
10	J	194	ASP	2.6
1	A	202	GLY	2.6
6	F	244	ASN	2.6
10	J	174	MET	2.5
11	Y	40	PHE	2.5
1	A	248	GLU	2.5
12	L	163	GLY	2.5
4	R	230	GLU	2.5
1	O	231	LYS	2.5
5	S	180	LYS	2.5
14	b	195	GLN	2.5
5	S	209	ASN	2.5
3	Q	171	GLU	2.5
3	Q	47	ARG	2.5
2	B	62	THR	2.4
5	S	207	VAL	2.4
6	F	240	GLN	2.4
2	P	241	THR	2.4
3	C	240	GLU	2.4
3	Q	58	THR	2.4
5	E	203	GLU	2.4
1	A	249	ALA	2.4
11	Y	106	ARG	2.4
7	G	240	ALA	2.4
3	C	175	LYS	2.4
14	b	105	LYS	2.4
4	D	242	GLU	2.4
5	S	201	ARG	2.4
7	U	188	GLU	2.4
12	Z	116	GLU	2.4
5	E	180	LYS	2.4
7	U	2	GLY	2.3

*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	141	ASP	2.3
3	Q	26	LYS	2.3
7	G	179	LYS	2.3
3	Q	238	LYS	2.3
9	I	192	ASP	2.3
12	Z	171	PRO	2.3
2	B	63	GLU	2.3
3	C	235	GLU	2.3
3	Q	60	SER	2.3
4	R	54	ASP	2.3
4	R	224	ASP	2.3
11	K	211	ILE	2.3
4	R	242	GLU	2.3
7	U	242	GLN	2.3
12	Z	80	ASN	2.3
1	O	4	ARG	2.3
11	Y	147	ASP	2.3
3	Q	1	GLY	2.3
2	B	217	LYS	2.2
3	Q	175	LYS	2.2
6	F	203	ASN	2.2
12	Z	165	ASN	2.2
4	R	114	ARG	2.2
2	P	19	TYR	2.2
7	G	181	LYS	2.2
3	Q	181	GLU	2.2
8	H	198	GLU	2.2
5	E	201	ARG	2.2
6	T	187	GLU	2.2
3	Q	59	PRO	2.2
6	F	204	LYS	2.1
3	Q	187	GLU	2.1
4	R	2	ARG	2.1
2	B	50	LYS	2.1
2	P	184	LYS	2.1
5	E	52	ALA	2.1
11	Y	211	ILE	2.1
11	K	145	LYS	2.1
6	T	166	GLN	2.1
2	P	62	THR	2.1
2	P	186	ASP	2.1
4	R	117	GLU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	P	217	LYS	2.1
2	B	182	ASP	2.1
2	B	242	GLY	2.0
4	D	169	GLU	2.0
11	K	39	PRO	2.0
3	Q	225	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
15	ACA	d	4	8/9	0.61	0.45	61,63,64,64	0
15	ACA	c	4	8/9	0.78	0.47	63,64,65,65	0
15	TY5	c	5	19/20	0.87	0.29	60,62,63,63	0
15	TY5	d	5	19/20	0.88	0.26	58,60,61,61	0
15	RE0	c	7	16/17	0.89	0.20	56,57,58,58	0
15	RE0	d	7	16/17	0.91	0.20	56,57,57,58	0

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
16	MES	Y	301	12/12	0.87	0.33	60,64,66,66	0
16	MES	K	301	12/12	0.91	0.27	61,62,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.