



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2016 – 02:36 AM EST

PDB ID : 5L5X
Title : Yeast 20S proteasome with human beta5c (1-138) and human beta6 (97-111; 118-133) in complex with ONX 0914
Authors : Groll, M.; Huber, E.M.
Deposited on : 2016-05-28
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

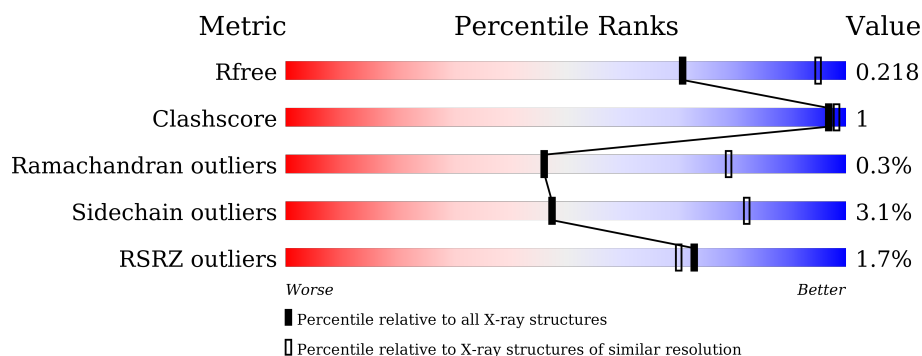
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



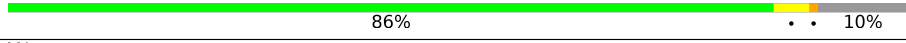

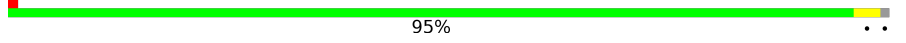
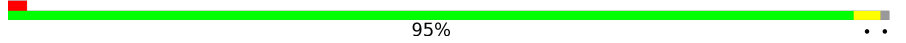






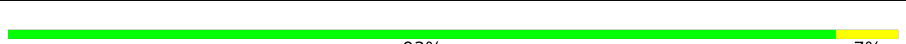
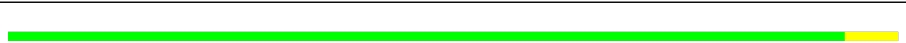




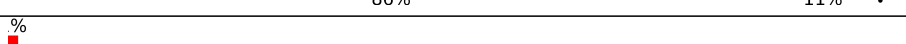
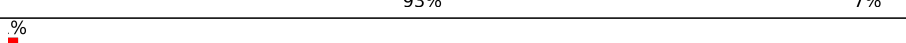
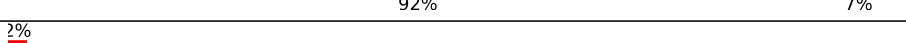
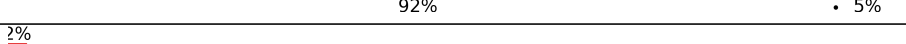
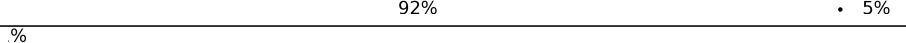
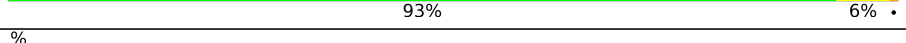
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>2%</div> <div>98%</div> <div>.</div> </div>
1	O	250	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>
2	B	258	<div> <div>3%</div> <div>91%</div> <div>5%</div> </div>
2	P	258	<div> <div>2%</div> <div>91%</div> <div>5%</div> </div>
3	C	254	<div> <div>5%</div> <div>86%</div> <div>7% • 6%</div> </div>
3	Q	254	<div> <div>5%</div> <div>87%</div> <div>6% • 6%</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	211	
11	Y	211	
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	A	301	-	-	-	X
15	MG	J	201	-	-	-	X
15	MG	Z	301	-	-	-	X
17	04C	N	201	-	-	-	X
17	04C	b	201	-	-	-	X
18	MES	H	302	-	-	-	X
18	MES	K	303	-	-	-	X
18	MES	V	302	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49834 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, Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1632	1036	282	306	8			
11	Y	211	Total	C	N	O	S	0	0	0
			1632	1036	282	306	8			

- Molecule 12 is a protein called Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	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			

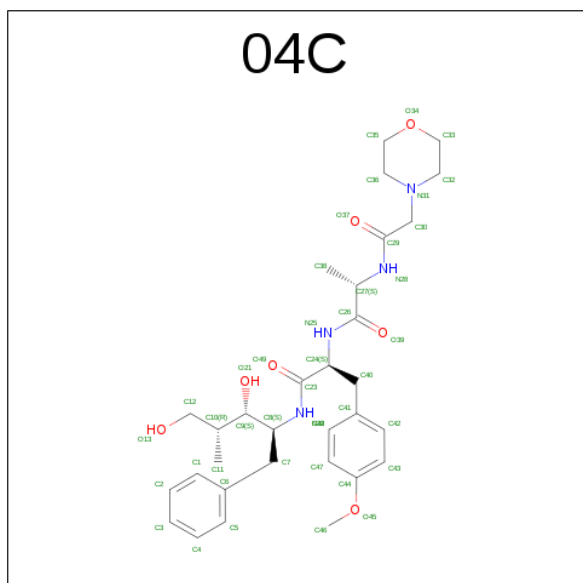
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	Z	1	Total Mg 1 1	0	0
15	A	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0

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

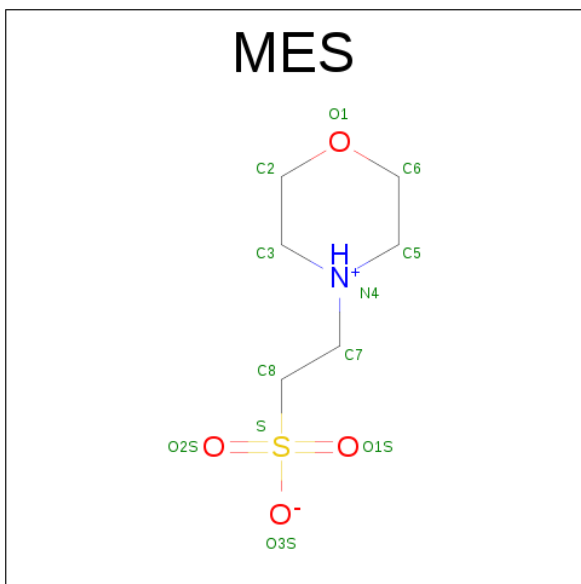
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is 1,2,4-trideoxy-4-methyl-2-{[N-(morpholin-4-ylacetyl)-L-alanyl-O-methyl-L-tyrosyl]amino}-1-phenyl-D-xylitol (three-letter code: 04C) (formula: C₃₁H₄₄N₄O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			42	31	4	7		
17	K	1	Total	C	N	O	0	0
			42	31	4	7		
17	N	1	Total	C	N	O	0	0
			42	31	4	7		
17	V	1	Total	C	N	O	0	0
			42	31	4	7		
17	Y	1	Total	C	N	O	0	0
			42	31	4	7		
17	b	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	X	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	5	Total O 5 5	0	0
19	B	9	Total O 9 9	0	0
19	C	2	Total O 2 2	0	0
19	D	8	Total O 8 8	0	0
19	E	1	Total O 1 1	0	0
19	F	6	Total O 6 6	0	0
19	G	6	Total O 6 6	0	0
19	H	8	Total O 8 8	0	0
19	I	8	Total O 8 8	0	0
19	J	4	Total O 4 4	0	0
19	K	3	Total O 3 3	0	0
19	L	11	Total O 11 11	0	0
19	M	11	Total O 11 11	0	0
19	N	5	Total O 5 5	0	0
19	O	2	Total O 2 2	0	0
19	P	7	Total O 7 7	0	0
19	Q	4	Total O 4 4	0	0
19	R	4	Total O 4 4	0	0
19	S	5	Total O 5 5	0	0
19	T	5	Total O 5 5	0	0
19	U	9	Total O 9 9	0	0
19	V	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	W	5	Total 5	O 5	0	0
19	X	8	Total 8	O 8	0	0
19	Y	6	Total 6	O 6	0	0
19	Z	6	Total 6	O 6	0	0
19	a	8	Total 8	O 8	0	0
19	b	5	Total 5	O 5	0	0

3 Residue-property plots [i](#)

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

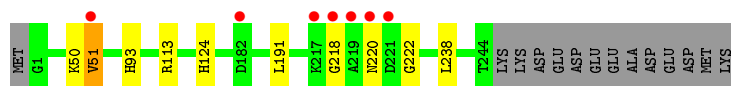
- Molecule 1: Proteasome subunit alpha type-2



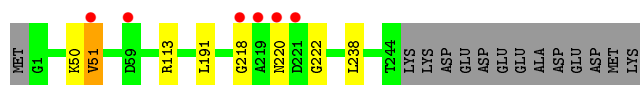
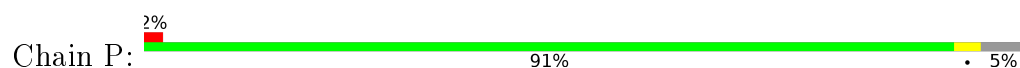
- Molecule 1: Proteasome subunit alpha type-2



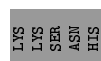
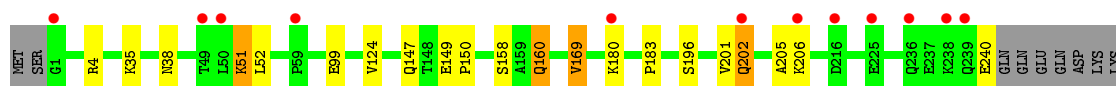
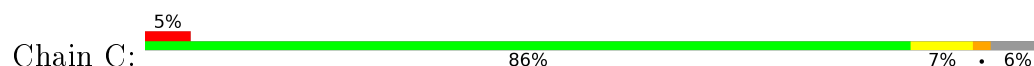
- Molecule 2: Proteasome subunit alpha type-3



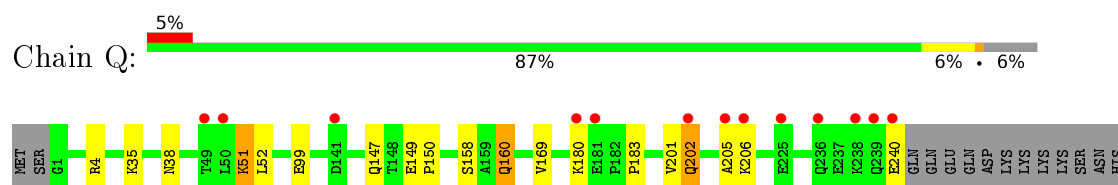
- Molecule 2: Proteasome subunit alpha type-3



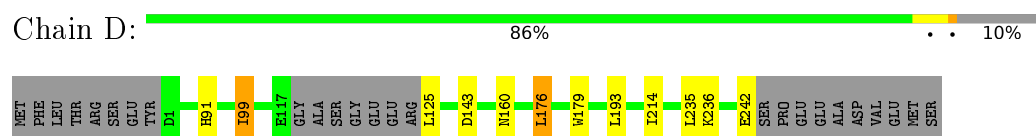
- Molecule 3: Proteasome subunit alpha type-4



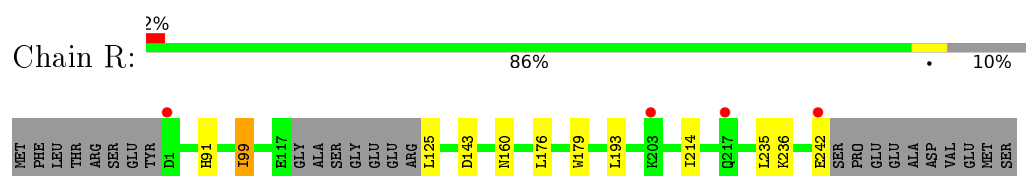
- Molecule 3: Proteasome subunit alpha type-4



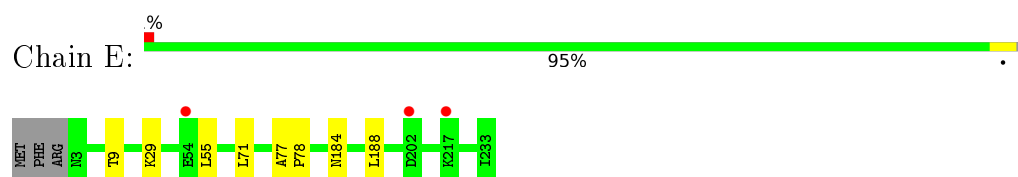
- Molecule 4: Proteasome subunit alpha type-5



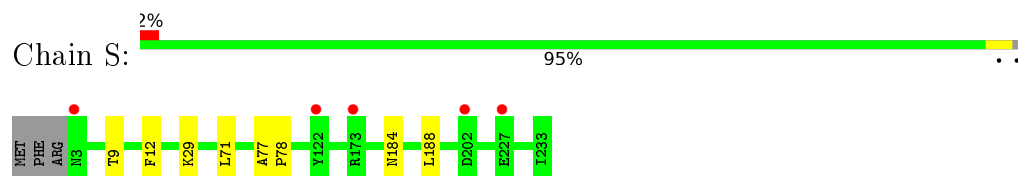
- Molecule 4: Proteasome subunit alpha type-5



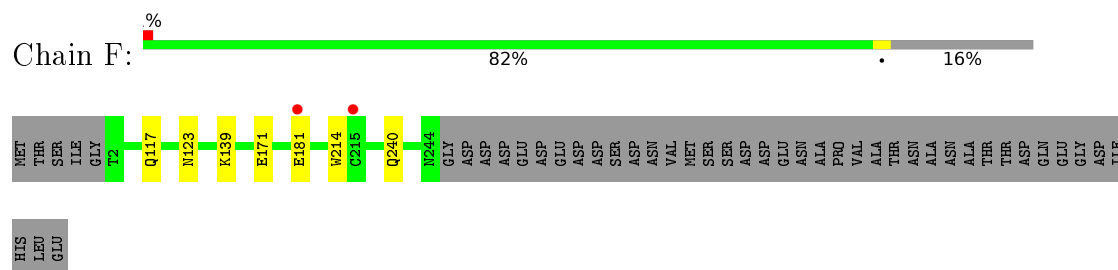
- Molecule 5: Proteasome subunit alpha type-6



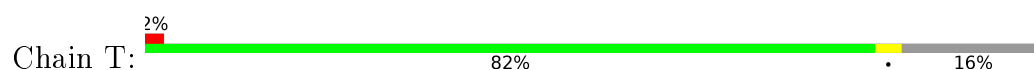
- Molecule 5: Proteasome subunit alpha type-6

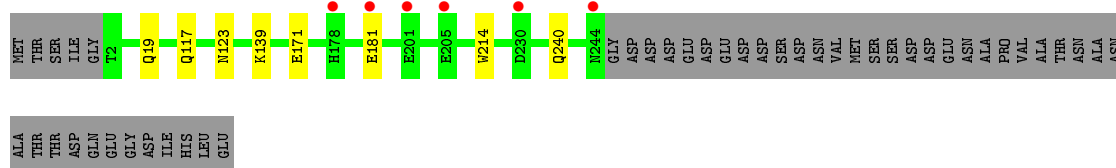


- Molecule 6: Probable proteasome subunit alpha type-7

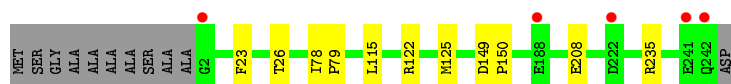


- Molecule 6: Probable proteasome subunit alpha type-7

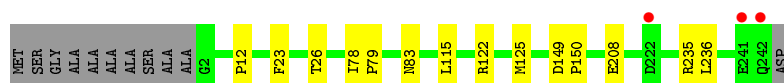
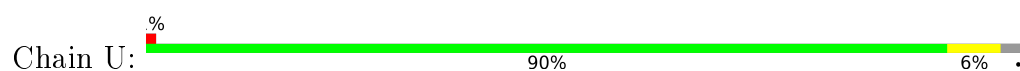




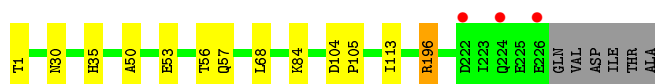
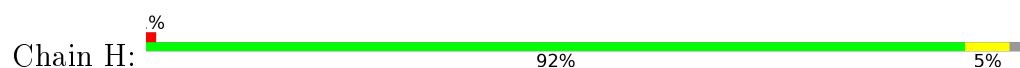
• Molecule 7: Proteasome subunit alpha type-1



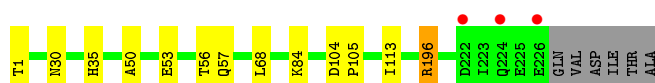
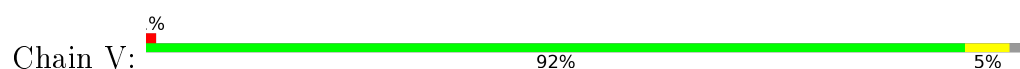
• Molecule 7: Proteasome subunit alpha type-1



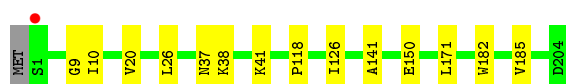
• Molecule 8: Proteasome subunit beta type-2



• Molecule 8: Proteasome subunit beta type-2



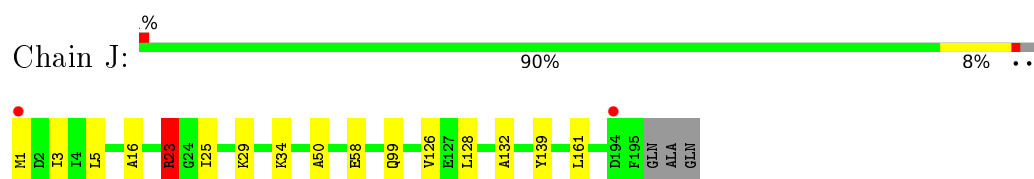
• Molecule 9: Proteasome subunit beta type-3



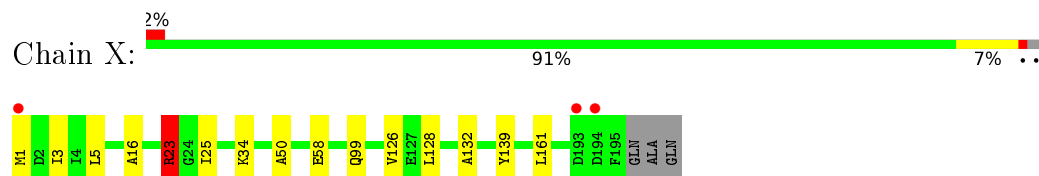
• Molecule 9: Proteasome subunit beta type-3



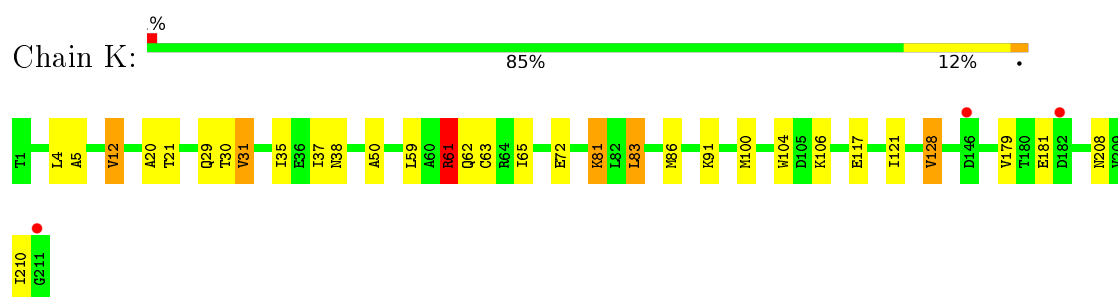
• Molecule 10: Proteasome subunit beta type-4



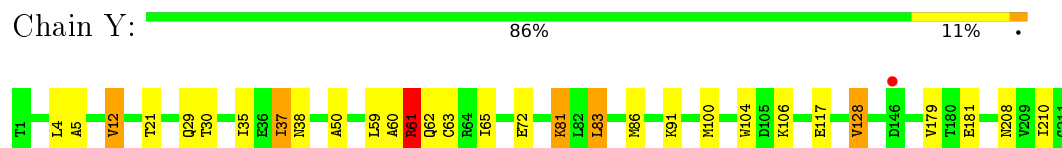
- Molecule 10: Proteasome subunit beta type-4



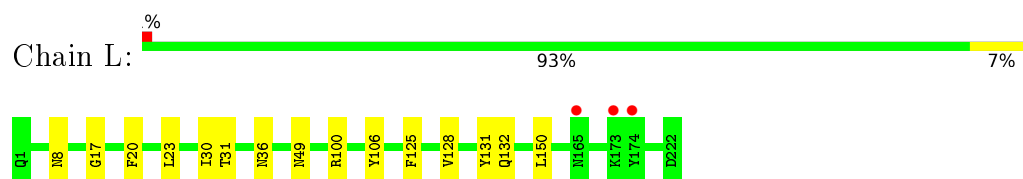
- Molecule 11: Proteasome subunit beta type-5, Proteasome subunit beta type-5



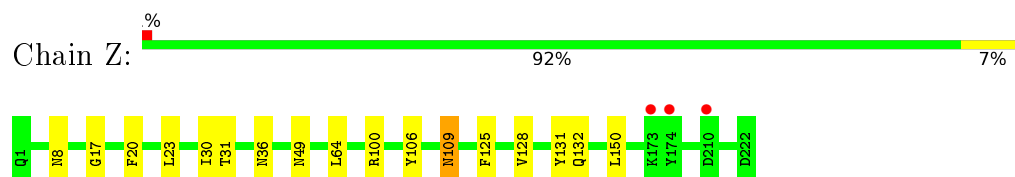
- Molecule 11: Proteasome subunit beta type-5, Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6

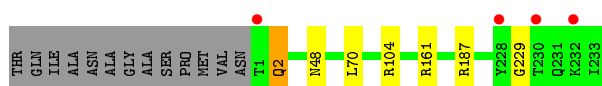


- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6

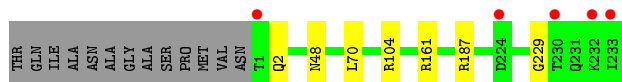
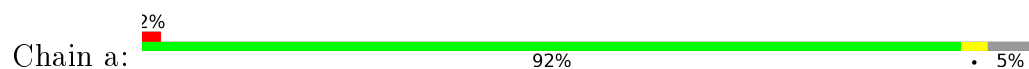


- Molecule 13: Proteasome subunit beta type-7

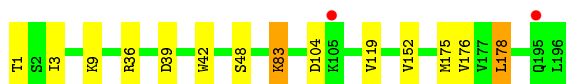
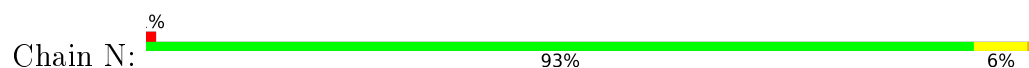




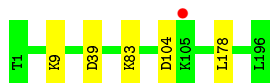
- Molecule 13: Proteasome subunit beta type-7



- 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, α , β , γ	136.02Å 300.51Å 145.45Å 90.00° 112.97° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 14.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (15.00-2.90) 96.9 (14.99-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.179 , 0.215 0.183 , 0.218	Depositor DCC
R_{free} test set	11380 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49834	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 04C, MES, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.48	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.46	0/2475
4	R	0.26	0/1837	0.46	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.25	0/1750	0.50	1/2373 (0.0%)
8	V	0.25	0/1750	0.50	1/2373 (0.0%)
9	I	0.26	0/1611	0.49	0/2174
9	W	0.26	0/1611	0.49	0/2174
10	J	0.26	0/1589	0.74	4/2142 (0.2%)
10	X	0.27	0/1589	0.81	4/2142 (0.2%)
11	K	0.32	0/1668	0.70	4/2253 (0.2%)
11	Y	0.32	0/1668	0.67	3/2253 (0.1%)
12	L	0.31	0/1802	0.78	3/2430 (0.1%)
12	Z	0.31	0/1802	0.75	3/2430 (0.1%)
13	M	0.27	0/1855	0.50	0/2514
13	a	0.27	0/1855	0.50	0/2514
14	N	0.26	0/1541	0.49	0/2087
14	b	0.26	0/1541	0.49	0/2087
All	All	0.27	0/50252	0.54	23/67940 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1
10	X	0	1
11	K	0	1
11	Y	0	1
All	All	0	4

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	23	ARG	NE-CZ-NH2	-21.89	109.35	120.30
12	L	100	ARG	NE-CZ-NH2	-21.82	109.39	120.30
12	Z	100	ARG	NE-CZ-NH1	-20.10	110.25	120.30
12	L	100	ARG	NE-CZ-NH1	17.74	129.17	120.30
12	Z	100	ARG	NE-CZ-NH2	17.60	129.10	120.30
10	J	23	ARG	NE-CZ-NH1	-16.91	111.84	120.30
10	J	23	ARG	NE-CZ-NH2	16.25	128.43	120.30
10	X	23	ARG	NE-CZ-NH1	15.60	128.10	120.30
11	K	61	ARG	NE-CZ-NH1	-14.64	112.98	120.30
11	Y	61	ARG	NE-CZ-NH2	-14.62	112.99	120.30
11	K	61	ARG	NE-CZ-NH2	12.24	126.42	120.30
11	Y	61	ARG	NE-CZ-NH1	10.54	125.57	120.30
11	K	61	ARG	CB-CG-CD	10.50	138.90	111.60
10	X	23	ARG	CD-NE-CZ	10.47	138.26	123.60
12	L	100	ARG	CD-NE-CZ	9.75	137.25	123.60
10	J	23	ARG	CD-NE-CZ	9.20	136.49	123.60
12	Z	100	ARG	CD-NE-CZ	9.14	136.40	123.60
11	Y	61	ARG	CB-CG-CD	8.02	132.45	111.60
10	X	23	ARG	CG-CD-NE	-7.95	95.10	111.80
10	J	23	ARG	CG-CD-NE	5.83	124.04	111.80
8	H	1	THR	N-CA-C	5.27	125.23	111.00
8	V	1	THR	N-CA-C	5.23	125.13	111.00
11	K	61	ARG	CD-NE-CZ	5.10	130.75	123.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	23	ARG	Sidechain
11	K	61	ARG	Sidechain
10	X	23	ARG	Sidechain
11	Y	61	ARG	Sidechain

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	0	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	3	0
2	P	1904	0	1904	2	0
3	C	1881	0	1895	9	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	0	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	1716	7	0
8	V	1719	0	1716	7	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	10	0
10	X	1561	0	1569	9	0
11	K	1632	0	1590	17	0
11	Y	1632	0	1590	15	0
12	L	1764	0	1716	6	0
12	Z	1764	0	1716	7	0
13	M	1824	0	1832	1	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	6	0
14	b	1512	0	1478	0	0
15	A	1	0	0	0	0
15	G	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	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	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	H	42	0	42	0	0
17	K	42	0	42	1	0
17	N	42	0	42	2	0
17	V	42	0	42	0	0
17	Y	42	0	42	1	0
17	b	42	0	42	0	0
18	H	12	0	13	0	0
18	K	12	0	13	0	0
18	V	12	0	13	0	0
18	X	12	0	13	0	0
19	A	5	0	0	0	0
19	B	9	0	0	1	0
19	C	2	0	0	0	0
19	D	8	0	0	0	0
19	E	1	0	0	0	0
19	F	6	0	0	0	0
19	G	6	0	0	0	0
19	H	8	0	0	0	0
19	I	8	0	0	0	0
19	J	4	0	0	0	0
19	K	3	0	0	1	0
19	L	11	0	0	0	0
19	M	11	0	0	1	0
19	N	5	0	0	0	0
19	O	2	0	0	0	0
19	P	7	0	0	0	0
19	Q	4	0	0	0	0
19	R	4	0	0	0	0
19	S	5	0	0	0	0
19	T	5	0	0	0	0
19	U	9	0	0	0	0
19	V	6	0	0	0	0
19	W	5	0	0	0	0
19	X	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Y	6	0	0	0	0
19	Z	6	0	0	0	0
19	a	8	0	0	0	0
19	b	5	0	0	0	0
All	All	49834	0	49422	117	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 (117) 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:Y:72:GLU:OE1	11:Y:106:LYS:NZ	2.18	0.77
11:K:72:GLU:OE1	11:K:106:LYS:NZ	2.18	0.76
11:K:30:THR:O	12:L:132:GLN:NE2	2.28	0.66
11:K:31:VAL:HG12	19:K:402:HOH:O	1.99	0.61
8:H:50:ALA:HB3	9:I:126:ILE:HD12	1.83	0.60
14:N:152:VAL:HA	14:N:175:MET:HE1	1.84	0.59
10:J:25:ILE:O	10:X:139:TYR:OH	2.19	0.59
10:J:139:TYR:OH	10:X:25:ILE:O	2.21	0.58
8:V:50:ALA:HB3	9:W:126:ILE:HD12	1.84	0.58
11:K:208:ASN:O	9:W:38:LYS:NZ	2.36	0.58
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.37	0.57
12:Z:64:LEU:HD23	12:Z:109:ASN:OD1	2.06	0.56
8:H:196:ARG:NH2	9:I:150:GLU:O	2.41	0.54
17:N:201:04C:H24	17:N:201:04C:H6	1.89	0.54
7:G:23:PHE:O	7:G:26:THR:HB	2.07	0.53
7:U:23:PHE:O	7:U:26:THR:HB	2.08	0.53
2:B:93:HIS:HB3	19:B:301:HOH:O	2.07	0.53
14:N:48:SER:HB2	17:N:201:04C:H25	1.89	0.53
8:V:53:GLU:O	8:V:57:GLN:HG2	2.09	0.52
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.92	0.51
10:J:50:ALA:O	11:K:91:LYS:NZ	2.44	0.51
10:X:58:GLU:OE1	11:Y:81:LYS:NZ	2.44	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.50
3:C:99:GLU:HG3	11:K:81:LYS:HE2	1.94	0.50
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.93	0.50
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.93	0.50
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:53:GLU:O	8:H:57:GLN:HG2	2.11	0.49
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.77	0.49
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.77	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.49
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	1.94	0.49
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.93	0.49
11:K:12:VAL:HG13	11:K:179:VAL:HB	1.95	0.49
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.48	0.49
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.94	0.49
17:K:301:04C:O13	17:K:301:04C:H19	2.13	0.49
10:X:1:MET:HB3	10:X:34:LYS:HE3	1.95	0.49
17:Y:301:04C:O13	17:Y:301:04C:H19	2.13	0.49
10:J:1:MET:HB3	10:J:34:LYS:HE3	1.94	0.49
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.48
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.48	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.48
13:M:2:GLN:NE2	19:M:301:HOH:O	2.46	0.48
11:Y:30:THR:O	12:Z:132:GLN:NE2	2.46	0.48
10:J:58:GLU:OE1	11:K:81:LYS:NZ	2.47	0.48
8:H:35:HIS:CB	8:H:56:THR:HG21	2.45	0.47
11:Y:59:LEU:CD2	11:Y:63:CYS:SG	3.03	0.47
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.45	0.47
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.97	0.47
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.97	0.46
8:V:35:HIS:CB	8:V:56:THR:HG21	2.45	0.46
3:Q:99:GLU:HG3	11:Y:81:LYS:HE2	1.96	0.46
8:V:196:ARG:NH2	9:W:150:GLU:O	2.48	0.46
3:C:35:LYS:HG2	3:C:158:SER:O	2.16	0.46
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.48	0.46
11:Y:59:LEU:HD12	11:Y:83:LEU:HG	1.98	0.45
11:K:59:LEU:CD2	11:K:63:CYS:SG	3.04	0.45
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.17	0.45
3:C:201:VAL:O	3:C:202:GLN:HB3	2.16	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.45
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.45
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.98	0.45
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.52	0.45
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.98	0.44
11:K:59:LEU:HD12	11:K:83:LEU:HG	1.98	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.44
3:C:51:LYS:O	3:C:52:LEU:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.47	0.44
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.99	0.44
10:J:29:LYS:HD2	11:K:121:ILE:CG2	2.49	0.43
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.84	0.43
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.53	0.43
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.18	0.43
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.17	0.43
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.43
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.83	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.53	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.19	0.43
11:K:100:MET:SD	11:K:128:VAL:CG1	3.07	0.43
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.48	0.43
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.01	0.43
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.99	0.42
11:K:50:ALA:CB	12:L:128:VAL:HG23	2.49	0.42
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.55	0.42
11:Y:100:MET:SD	11:Y:128:VAL:CG1	3.07	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.42
5:S:12:PHE:H	6:T:19:GLN:HE22	1.67	0.42
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.55	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
14:N:1:THR:CG2	14:N:3:ILE:HG23	2.50	0.42
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.01	0.41
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.01	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.83	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.55	0.41
11:Y:50:ALA:CB	12:Z:128:VAL:HG23	2.50	0.41
11:Y:72:GLU:OE1	11:Y:106:LYS:CE	2.69	0.41
4:D:176:LEU:HA	5:E:55:LEU:HD21	2.02	0.41
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
10:J:5:LEU:HD23	10:J:132:ALA:HB2	2.03	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.02	0.41
11:Y:37:ILE:HG23	11:Y:60:ALA:HA	2.03	0.41
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.03	0.40
11:K:72:GLU:OE1	11:K:106:LYS:CE	2.68	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.91	0.40
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.03	0.40
10:X:5:LEU:HD23	10:X:132:ALA:HB2	2.03	0.40
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.04	0.40
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.03	0.40
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.04	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%)	239 (96%)	8 (3%)	1 (0%)	39	74
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	74
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	11	38
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	11	38
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	15	46
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	15	46
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	221 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	224/232 (97%)	221 (99%)	3 (1%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	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	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
11	Y	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	39	74
13	a	231/246 (94%)	224 (97%)	6 (3%)	1 (0%)	39	74
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6282/6612 (95%)	6126 (98%)	138 (2%)	18 (0%)	46	79

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
3	C	205	ALA
3	Q	205	ALA
2	B	220	ASN
2	P	220	ASN
13	M	229	GLY
13	a	229	GLY
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	93
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	93
2	B	203/216 (94%)	200 (98%)	3 (2%)	72	92
2	P	203/216 (94%)	200 (98%)	3 (2%)	72	92
3	C	212/226 (94%)	203 (96%)	9 (4%)	36	73
3	Q	212/226 (94%)	203 (96%)	9 (4%)	36	73
4	D	194/215 (90%)	185 (95%)	9 (5%)	33	69
4	R	194/215 (90%)	185 (95%)	9 (5%)	33	69
5	E	190/193 (98%)	185 (97%)	5 (3%)	54	85
5	S	190/193 (98%)	185 (97%)	5 (3%)	54	85
6	F	201/239 (84%)	194 (96%)	7 (4%)	43	78
6	T	201/239 (84%)	194 (96%)	7 (4%)	43	78
7	G	206/210 (98%)	201 (98%)	5 (2%)	57	86
7	U	206/210 (98%)	199 (97%)	7 (3%)	44	79
8	H	185/190 (97%)	182 (98%)	3 (2%)	70	91
8	V	185/190 (97%)	182 (98%)	3 (2%)	70	91
9	I	172/173 (99%)	169 (98%)	3 (2%)	68	91
9	W	172/173 (99%)	169 (98%)	3 (2%)	68	91
10	J	173/175 (99%)	170 (98%)	3 (2%)	68	91
10	X	173/175 (99%)	170 (98%)	3 (2%)	68	91
11	K	165/165 (100%)	148 (90%)	17 (10%)	9	26
11	Y	165/165 (100%)	149 (90%)	16 (10%)	10	30
12	L	186/186 (100%)	182 (98%)	4 (2%)	60	88
12	Z	186/186 (100%)	181 (97%)	5 (3%)	52	84
13	M	199/208 (96%)	193 (97%)	6 (3%)	48	83
13	a	199/208 (96%)	193 (97%)	6 (3%)	48	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	157 (97%)	5 (3%)	47	82
14	b	162/162 (100%)	157 (97%)	5 (3%)	47	82
All	All	5314/5534 (96%)	5148 (97%)	166 (3%)	47	82

All (166) 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	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
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	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	171	GLU
6	F	181	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	214	TRP
6	F	240	GLN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
8	H	30	ASN
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	3	ILE
10	J	23	ARG
10	J	99	GLN
11	K	4	LEU
11	K	12	VAL
11	K	21	THR
11	K	29	GLN
11	K	31	VAL
11	K	35	ILE
11	K	37	ILE
11	K	38	ASN
11	K	61	ARG
11	K	62	GLN
11	K	65	ILE
11	K	81	LYS
11	K	83	LEU
11	K	86	MET
11	K	117	GLU
11	K	128	VAL
11	K	210	ILE
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	187	ARG
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	178	LEU
1	O	122	THR
1	O	157	PHE
1	O	250	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	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	143	ASP
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
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	181	GLU
6	T	214	TRP
6	T	240	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	30	ASN
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	3	ILE
10	X	23	ARG
10	X	99	GLN
11	Y	4	LEU
11	Y	12	VAL
11	Y	21	THR
11	Y	29	GLN
11	Y	35	ILE
11	Y	37	ILE
11	Y	38	ASN
11	Y	61	ARG
11	Y	62	GLN
11	Y	65	ILE
11	Y	81	LYS
11	Y	83	LEU
11	Y	86	MET
11	Y	117	GLU
11	Y	128	VAL
11	Y	210	ILE
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
12	Z	109	ASN
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	a	187	ARG
14	b	9	LYS
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	58	GLN
2	B	119	GLN
2	B	123	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
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	66	HIS
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	175	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	207	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	109	ASN
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
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
9	W	37	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	X	55	GLN
11	Y	85	ASN
11	Y	175	ASN
11	Y	207	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN

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 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
17	04C	H	301	8	44,44,44	1.16	3 (6%)	55,58,58	1.18	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	MES	H	302	-	12,12,12	2.14	1 (8%)	15,16,16	1.69	3 (20%)
17	04C	K	301	11	44,44,44	1.31	3 (6%)	55,58,58	1.34	10 (18%)
18	MES	K	303	-	12,12,12	2.20	1 (8%)	15,16,16	1.56	3 (20%)
17	04C	N	201	14	44,44,44	1.21	3 (6%)	55,58,58	1.30	9 (16%)
17	04C	V	301	8	44,44,44	1.15	3 (6%)	55,58,58	1.17	6 (10%)
18	MES	V	302	-	12,12,12	2.11	1 (8%)	15,16,16	1.93	3 (20%)
18	MES	X	201	-	12,12,12	2.16	1 (8%)	15,16,16	1.57	2 (13%)
17	04C	Y	301	11	44,44,44	1.31	3 (6%)	55,58,58	1.33	10 (18%)
17	04C	b	201	14	44,44,44	1.20	3 (6%)	55,58,58	1.32	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	04C	H	301	8	-	0/44/52/52	0/3/3/3
18	MES	H	302	-	-	0/6/14/14	0/1/1/1
17	04C	K	301	11	-	0/44/52/52	0/3/3/3
18	MES	K	303	-	-	0/6/14/14	0/1/1/1
17	04C	N	201	14	-	0/44/52/52	0/3/3/3
17	04C	V	301	8	-	0/44/52/52	0/3/3/3
18	MES	V	302	-	-	0/6/14/14	0/1/1/1
18	MES	X	201	-	-	0/6/14/14	0/1/1/1
17	04C	Y	301	11	-	0/44/52/52	0/3/3/3
17	04C	b	201	14	-	0/44/52/52	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	303	MES	C8-S	-7.38	1.66	1.77
18	X	201	MES	C8-S	-7.17	1.66	1.77
18	H	302	MES	C8-S	-7.14	1.66	1.77
18	V	302	MES	C8-S	-7.03	1.67	1.77
17	K	301	04C	C40-C41	-4.70	1.39	1.51
17	Y	301	04C	C40-C41	-4.63	1.39	1.51
17	H	301	04C	C40-C41	-4.51	1.40	1.51
17	V	301	04C	C40-C41	-4.45	1.40	1.51
17	b	201	04C	C40-C41	-4.34	1.40	1.51
17	N	201	04C	C40-C41	-4.29	1.40	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	04C	C7-C6	-3.84	1.41	1.51
17	N	201	04C	C7-C6	-3.77	1.42	1.51
17	b	201	04C	C7-C6	-3.75	1.42	1.51
17	V	301	04C	C7-C6	-3.72	1.42	1.51
17	Y	301	04C	C7-C6	-3.64	1.42	1.51
17	K	301	04C	C7-C6	-3.59	1.42	1.51
17	V	301	04C	C10-C9	2.89	1.59	1.53
17	H	301	04C	C10-C9	2.89	1.59	1.53
17	b	201	04C	C10-C9	3.30	1.59	1.53
17	N	201	04C	C10-C9	3.48	1.60	1.53
17	K	301	04C	C10-C9	4.92	1.62	1.53
17	Y	301	04C	C10-C9	4.96	1.62	1.53

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	201	04C	C11-C10-C12	-4.72	103.53	109.73
17	N	201	04C	C11-C10-C12	-4.66	103.61	109.73
17	H	301	04C	C29-C30-N31	-3.91	103.48	113.26
17	V	301	04C	C29-C30-N31	-3.91	103.48	113.26
17	b	201	04C	C7-C8-N22	-3.33	106.49	110.17
17	K	301	04C	C7-C8-N22	-3.31	106.51	110.17
17	Y	301	04C	C7-C8-N22	-3.30	106.52	110.17
17	N	201	04C	C7-C8-N22	-3.27	106.55	110.17
17	H	301	04C	O34-C35-C36	-3.25	104.33	111.83
17	Y	301	04C	C30-N31-C32	-3.16	106.49	111.14
17	K	301	04C	C30-N31-C32	-3.14	106.53	111.14
17	V	301	04C	O34-C35-C36	-3.13	104.61	111.83
17	K	301	04C	C41-C40-C24	-2.91	104.84	113.44
17	b	201	04C	C29-C30-N31	-2.89	106.04	113.26
17	Y	301	04C	C41-C40-C24	-2.86	104.98	113.44
17	Y	301	04C	C46-O45-C44	-2.80	111.03	117.51
17	N	201	04C	C29-C30-N31	-2.79	106.28	113.26
17	K	301	04C	C46-O45-C44	-2.77	111.11	117.51
17	K	301	04C	O13-C12-C10	-2.75	105.41	111.16
17	V	301	04C	C41-C40-C24	-2.74	105.36	113.44
17	N	201	04C	C33-C32-N31	-2.72	105.95	110.11
17	b	201	04C	C33-C32-N31	-2.71	105.96	110.11
17	H	301	04C	C41-C40-C24	-2.71	105.44	113.44
17	V	301	04C	C7-C8-N22	-2.62	107.28	110.17
17	Y	301	04C	O13-C12-C10	-2.61	105.70	111.16
17	K	301	04C	C11-C10-C12	-2.55	106.38	109.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	201	04C	O34-C35-C36	-2.55	105.94	111.83
17	H	301	04C	C7-C8-N22	-2.53	107.38	110.17
17	Y	301	04C	C11-C10-C12	-2.51	106.44	109.73
17	b	201	04C	O34-C35-C36	-2.47	106.12	111.83
17	Y	301	04C	O34-C35-C36	-2.40	106.29	111.83
17	K	301	04C	O34-C35-C36	-2.33	106.45	111.83
17	b	201	04C	C41-C40-C24	-2.23	106.85	113.44
17	Y	301	04C	C7-C6-C1	-2.23	116.40	120.91
17	K	301	04C	C7-C6-C1	-2.22	116.42	120.91
17	N	201	04C	C41-C40-C24	-2.16	107.07	113.44
17	b	201	04C	C7-C6-C1	-2.13	116.60	120.91
17	V	301	04C	C7-C6-C1	-2.12	116.63	120.91
17	H	301	04C	C7-C6-C1	-2.07	116.72	120.91
17	N	201	04C	C7-C6-C1	-2.06	116.76	120.91
17	b	201	04C	C9-C8-N22	2.03	114.42	110.06
17	N	201	04C	C9-C8-N22	2.06	114.47	110.06
17	H	301	04C	C7-C6-C5	2.21	125.37	120.91
18	K	303	MES	O1S-S-C8	2.21	108.43	106.87
17	N	201	04C	C7-C6-C5	2.22	125.40	120.91
18	H	302	MES	O3S-S-C8	2.24	109.65	104.99
17	V	301	04C	C7-C6-C5	2.28	125.52	120.91
17	b	201	04C	C7-C6-C5	2.30	125.56	120.91
17	Y	301	04C	C35-C36-N31	2.34	113.69	110.11
18	X	201	MES	O3S-S-C8	2.34	109.85	104.99
18	K	303	MES	O3S-S-C8	2.43	110.03	104.99
17	Y	301	04C	C7-C6-C5	2.44	125.84	120.91
17	K	301	04C	C35-C36-N31	2.44	113.85	110.11
18	V	302	MES	O3S-S-C8	2.45	110.07	104.99
17	K	301	04C	C7-C6-C5	2.47	125.91	120.91
18	H	302	MES	O1S-S-C8	3.00	108.99	106.87
18	V	302	MES	O2S-S-C8	3.98	109.68	106.87
18	K	303	MES	O2S-S-C8	4.04	109.72	106.87
18	X	201	MES	O2S-S-C8	4.50	110.05	106.87
18	H	302	MES	O2S-S-C8	4.59	110.11	106.87
18	V	302	MES	O1S-S-C8	5.10	110.47	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	04C	1	0
17	N	201	04C	2	0
17	Y	301	04C	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.45	4 (1%) 74 72	46, 65, 103, 139	0
1	O	250/250 (100%)	-0.45	4 (1%) 74 72	52, 68, 112, 147	0
2	B	244/258 (94%)	-0.41	7 (2%) 55 49	53, 70, 112, 165	0
2	P	244/258 (94%)	-0.38	6 (2%) 61 55	53, 71, 112, 165	0
3	C	240/254 (94%)	-0.22	12 (5%) 32 26	49, 78, 142, 179	0
3	Q	240/254 (94%)	-0.17	13 (5%) 29 23	54, 84, 159, 197	0
4	D	235/260 (90%)	-0.46	0 100 100	53, 74, 105, 138	0
4	R	235/260 (90%)	-0.36	4 (1%) 73 70	63, 79, 119, 147	0
5	E	231/234 (98%)	-0.34	3 (1%) 79 78	58, 79, 119, 165	0
5	S	231/234 (98%)	-0.34	5 (2%) 65 60	61, 81, 120, 157	0
6	F	243/288 (84%)	-0.51	2 (0%) 87 86	50, 72, 122, 147	0
6	T	243/288 (84%)	-0.42	6 (2%) 61 55	51, 77, 131, 163	0
7	G	241/252 (95%)	-0.47	5 (2%) 67 62	52, 70, 112, 171	0
7	U	241/252 (95%)	-0.49	3 (1%) 81 78	45, 67, 102, 145	0
8	H	226/232 (97%)	-0.55	3 (1%) 79 78	46, 64, 102, 149	0
8	V	226/232 (97%)	-0.51	3 (1%) 79 78	49, 64, 97, 161	0
9	I	204/205 (99%)	-0.70	1 (0%) 91 90	47, 62, 92, 116	0
9	W	204/205 (99%)	-0.68	1 (0%) 91 90	47, 64, 94, 119	0
10	J	195/198 (98%)	-0.51	2 (1%) 84 82	48, 68, 97, 135	0
10	X	195/198 (98%)	-0.50	3 (1%) 76 74	52, 70, 98, 145	0
11	K	211/211 (100%)	-0.44	3 (1%) 78 76	53, 72, 103, 131	0
11	Y	211/211 (100%)	-0.49	1 (0%) 91 90	53, 74, 104, 133	0
12	L	222/222 (100%)	-0.46	3 (1%) 78 76	58, 70, 115, 146	0
12	Z	222/222 (100%)	-0.49	3 (1%) 78 76	55, 72, 115, 145	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.50	4 (1%)	73 70	48, 66, 98, 123	0
13	a	233/246 (94%)	-0.50	5 (2%)	67 62	49, 67, 100, 135	0
14	N	196/196 (100%)	-0.63	2 (1%)	84 82	48, 64, 94, 120	0
14	b	196/196 (100%)	-0.66	1 (0%)	91 90	48, 63, 94, 121	0
All	All	6342/6612 (95%)	-0.46	109 (1%)	73 70	45, 70, 115, 197	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	238	LYS	4.8
10	J	1	MET	4.7
9	W	1	SER	4.6
3	C	206	LYS	4.6
3	C	238	LYS	4.5
3	Q	50	LEU	4.4
10	X	1	MET	4.3
2	P	51	VAL	4.3
5	E	202	ASP	4.3
2	B	221	ASP	4.1
3	Q	236	GLN	4.0
5	S	202	ASP	4.0
10	X	194	ASP	3.8
1	O	249	ALA	3.6
9	I	1	SER	3.5
3	C	50	LEU	3.5
8	V	226	GLU	3.5
2	B	220	ASN	3.4
6	F	181	GLU	3.4
1	A	1	MET	3.4
2	P	220	ASN	3.3
12	L	174	TYR	3.3
4	R	1	ASP	3.2
2	P	219	ALA	3.2
3	C	49	THR	3.2
7	G	242	GLN	3.1
12	Z	174	TYR	3.1
13	a	1	THR	3.1
3	Q	141	ASP	3.1
13	a	233	ILE	3.1
1	O	1	MET	3.1
10	J	194	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	216	ASP	3.0
3	Q	240	GLU	3.0
3	Q	206	LYS	3.0
13	M	230	THR	3.0
11	K	146	ASP	3.0
13	a	232	LYS	3.0
3	C	202	GLN	3.0
6	T	181	GLU	2.9
5	S	173	ARG	2.9
3	Q	239	GLN	2.9
6	T	244	ASN	2.9
7	U	222	ASP	2.9
7	G	188	GLU	2.8
12	L	165	ASN	2.8
12	L	173	LYS	2.8
3	C	236	GLN	2.8
2	B	218	GLY	2.8
2	P	218	GLY	2.7
2	P	221	ASP	2.6
14	N	195	GLN	2.6
1	A	54	PRO	2.6
13	a	224	ASP	2.6
14	b	105	LYS	2.6
6	T	205	GLU	2.6
7	G	2	GLY	2.6
5	E	54	GLU	2.6
8	V	222	ASP	2.6
13	M	1	THR	2.6
3	C	180	LYS	2.5
3	C	239	GLN	2.5
3	Q	202	GLN	2.5
2	B	182	ASP	2.5
13	a	230	THR	2.5
11	K	211	GLY	2.4
2	P	59	ASP	2.4
3	Q	205	ALA	2.4
3	C	225	GLU	2.3
13	M	228	TYR	2.3
8	V	224	GLN	2.3
12	Z	210	ASP	2.3
14	N	105	LYS	2.3
13	M	232	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	215	CYS	2.3
1	A	201	GLU	2.3
8	H	224	GLN	2.3
3	C	59	PRO	2.2
1	A	2	THR	2.2
3	Q	49	THR	2.2
2	B	217	LYS	2.2
11	K	182	ASP	2.2
11	Y	146	ASP	2.2
12	Z	173	LYS	2.2
5	S	227	GLU	2.2
7	G	241	GLU	2.2
1	O	2	THR	2.1
6	T	230	ASP	2.1
7	U	241	GLU	2.1
2	B	51	VAL	2.1
4	R	217	GLN	2.1
3	C	1	GLY	2.1
3	Q	225	GLU	2.1
5	E	217	LYS	2.1
4	R	203	LYS	2.1
2	B	219	ALA	2.1
4	R	242	GLU	2.1
7	G	222	ASP	2.1
3	Q	180	LYS	2.1
10	X	193	ASP	2.0
1	O	248	GLU	2.0
5	S	3	ASN	2.0
5	S	122	TYR	2.0
8	H	226	GLU	2.0
3	Q	181	GLU	2.0
7	U	242	GLN	2.0
6	T	178	HIS	2.0
6	T	201	GLU	2.0
8	H	222	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	MG	A	301	1/1	0.91	0.22	7.82	69,69,69,69	0
15	MG	Z	301	1/1	0.92	0.26	4.22	95,95,95,95	0
18	MES	V	302	12/12	0.93	0.23	4.20	77,84,92,97	0
17	04C	b	201	42/42	0.92	0.23	4.09	71,88,110,113	0
17	04C	N	201	42/42	0.90	0.25	3.72	71,85,104,109	0
18	MES	K	303	12/12	0.88	0.32	3.44	61,66,72,77	12
18	MES	H	302	12/12	0.97	0.24	3.27	80,82,87,90	0
15	MG	J	201	1/1	0.96	0.13	3.21	55,55,55,55	0
18	MES	X	201	12/12	0.94	0.24	1.97	67,70,78,86	12
15	MG	N	202	1/1	0.96	0.18	1.69	60,60,60,60	0
17	04C	Y	301	42/42	0.93	0.23	1.49	62,73,89,90	0
17	04C	K	301	42/42	0.93	0.22	1.39	60,71,86,88	0
17	04C	H	301	42/42	0.95	0.15	0.68	57,66,87,89	0
17	04C	V	301	42/42	0.94	0.16	0.59	56,68,93,97	0
15	MG	G	301	1/1	0.95	0.11	-0.80	78,78,78,78	0
15	MG	I	301	1/1	0.98	0.09	-1.07	59,59,59,59	0
15	MG	I	302	1/1	0.99	0.07	-1.57	60,60,60,60	0
15	MG	K	302	1/1	0.94	0.07	-1.97	57,57,57,57	0
15	MG	L	301	1/1	0.98	0.05	-3.30	77,77,77,77	0
16	CL	U	301	1/1	0.99	0.18	-	49,49,49,49	0
16	CL	G	302	1/1	0.99	0.25	-	52,52,52,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.