



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:22 AM GMT

PDB ID : 3OEV
Title : Structure of yeast 20S open-gate proteasome with Compound 25
Authors : Sintchak, M.D.
Deposited on : 2010-08-13
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

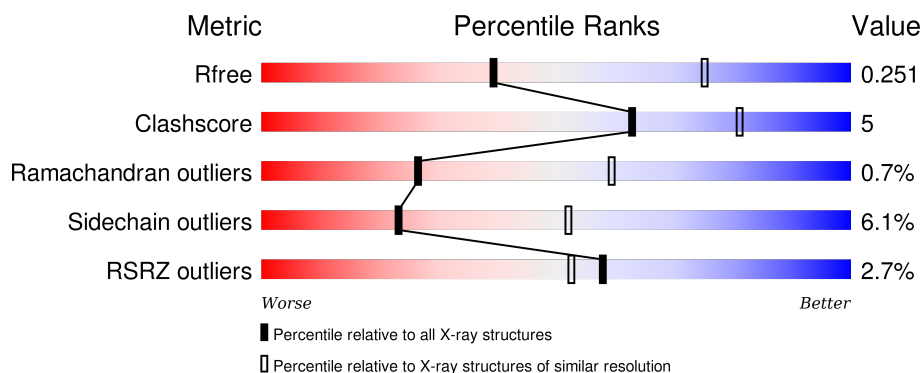
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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.





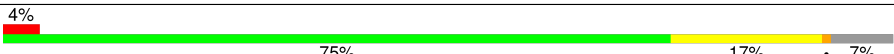
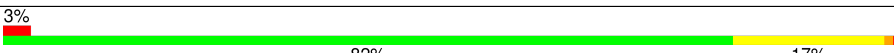
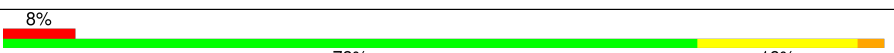
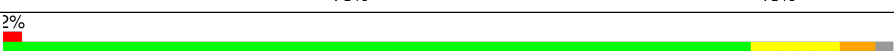

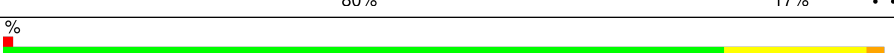
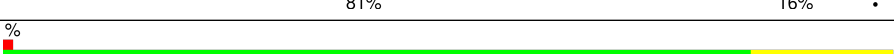
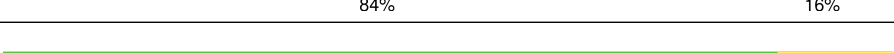
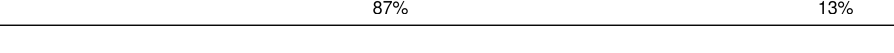
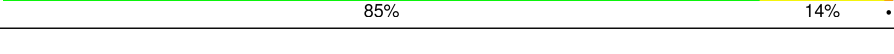
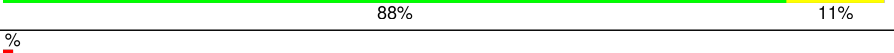




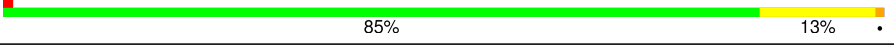

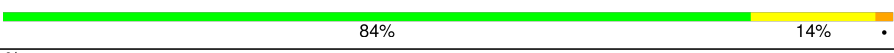



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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>0%</div> <div>87%</div> <div>11%</div> <div>•</div> </div>
1	O	250	<div> <div>2%</div> <div>84%</div> <div>14%</div> <div>•</div> </div>
2	B	235	<div> <div>3%</div> <div>81%</div> <div>18%</div> <div>•</div> </div>
2	P	235	<div> <div>2%</div> <div>80%</div> <div>17%</div> <div>•</div> </div>
3	C	241	<div> <div>10%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	241	
4	D	260	
4	R	260	
5	E	233	
5	S	233	
6	F	242	
6	T	242	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	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	F	243	-	-	-	X
15	MG	H	224	-	-	-	X
15	MG	I	196	-	-	-	X
15	MG	K	212	-	-	-	X
16	3OE	Y	212	-	-	-	X
17	MES	K	214	-	-	-	X
17	MES	Y	213	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49398 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 component Y7.

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 component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1829	1158	303	365	3			
2	P	235	Total	C	N	O	S	0	0	0
			1829	1158	303	365	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called Proteasome component PUP2.

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 component PRE5.

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
			1788	1123	312	349	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	237	Total	C	N	O	S	0	0	0
			1848	1175	323	346	4			
6	T	237	Total	C	N	O	S	0	0	0
			1848	1175	323	346	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

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 component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

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 component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1582	1003	269	305	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	197	Total	C	N	O	S	0	0	0
			1577	1000	268	304	5			

- Molecule 11 is a protein called Proteasome component PRE2.

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 component C5.

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 component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

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

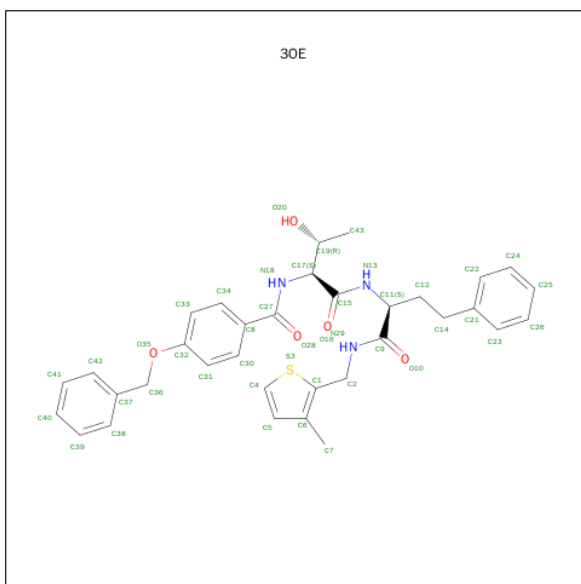
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

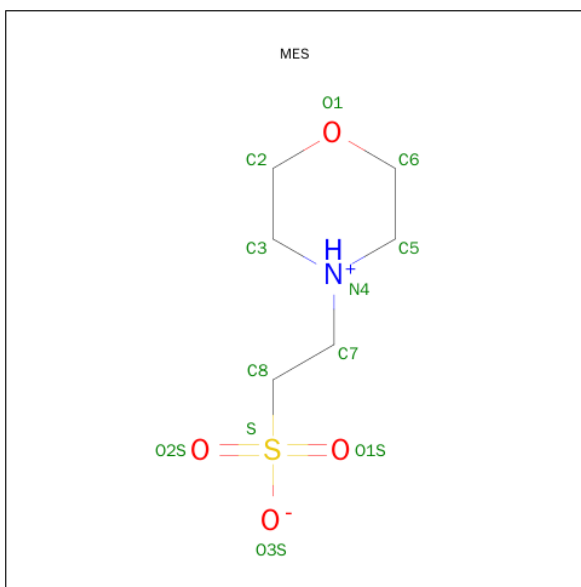
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total	Mg	0	0
			1	1		
15	I	2	Total	Mg	0	0
			2	2		
15	N	1	Total	Mg	0	0
			1	1		
15	L	2	Total	Mg	0	0
			2	2		
15	F	2	Total	Mg	0	0
			2	2		

- Molecule 16 is 4-(BENZYLOXY)-N-[(2S,3R)-3-HYDROXY-1-{[(2S)-1-{[(3-METHYLTHIO PHEN-2-YL)METHYL]AMINO}-1-OXO-4-PHENYLBUTAN-2-YL]AMINO}-1-OXOBUT AN-2-YL]BENZAMIDE (three-letter code: 3OE) (formula: C₃₄H₃₇N₃O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	K	1	Total	C	N	O	S	0	0
			43	34	3	5	1		
16	Y	1	Total	C	N	O	S	0	0
			43	34	3	5	1		

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).

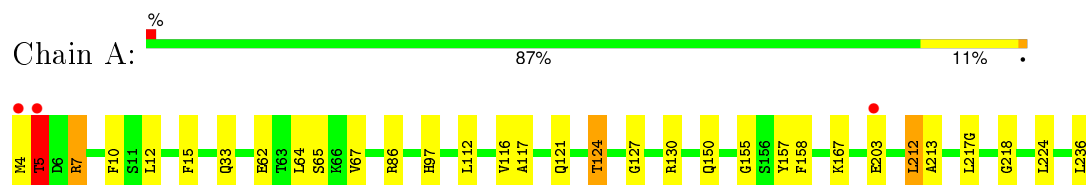


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

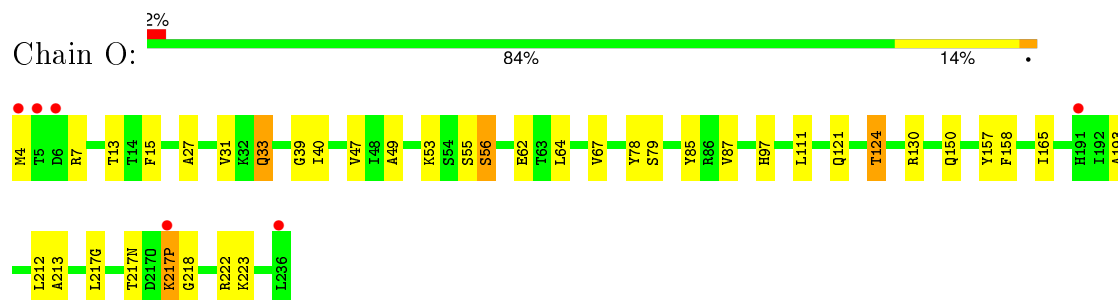
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

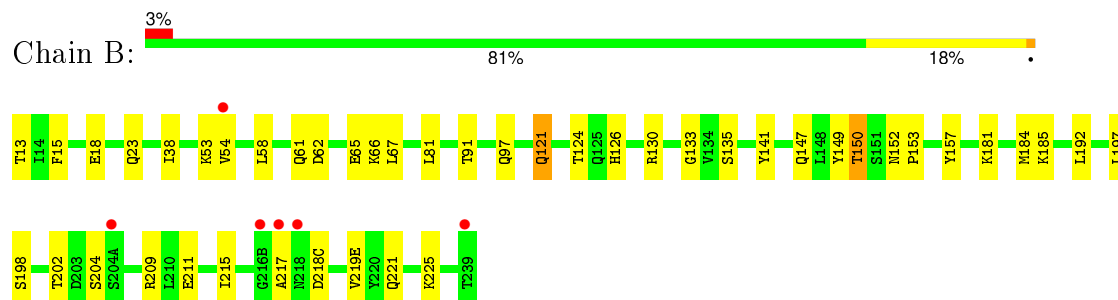
- Molecule 1: Proteasome component Y7



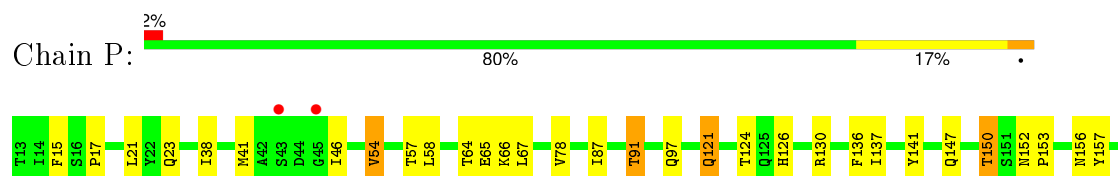
- Molecule 1: Proteasome component Y7

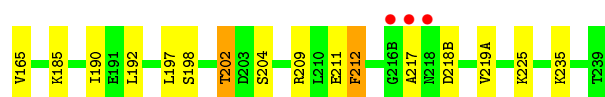


- Molecule 2: Proteasome component Y13

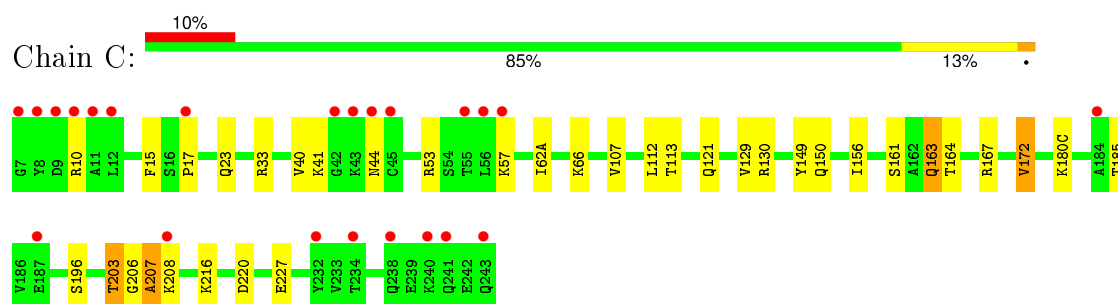


- Molecule 2: Proteasome component Y13

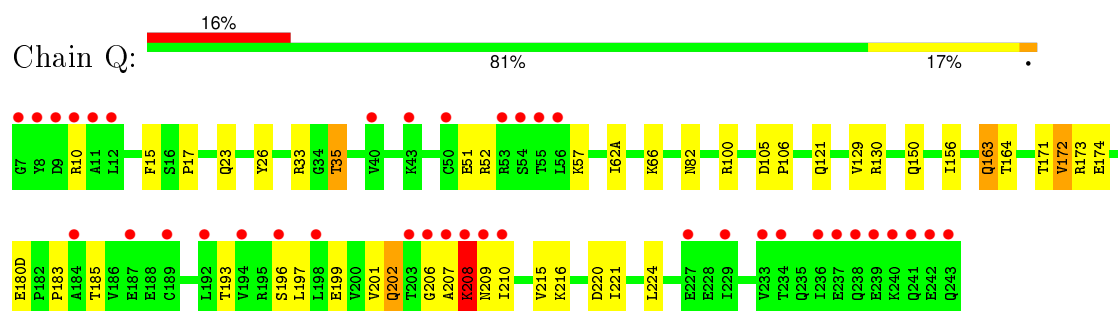




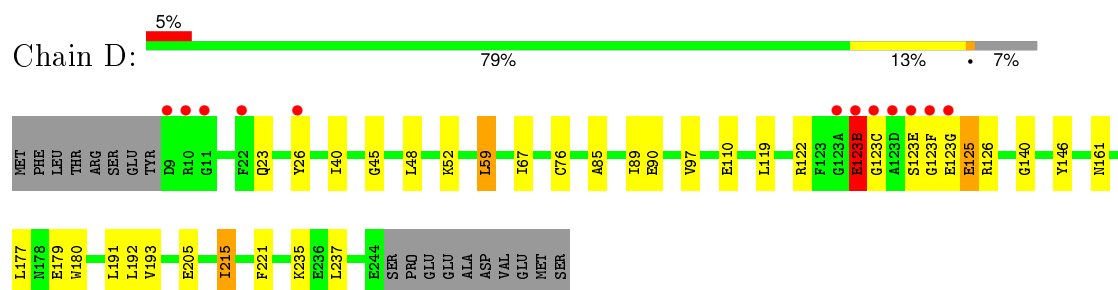
• Molecule 3: Proteasome component PRE6



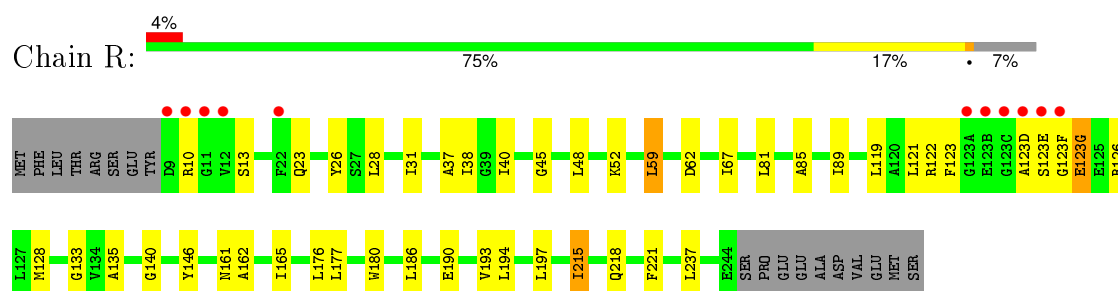
• Molecule 3: Proteasome component PRE6



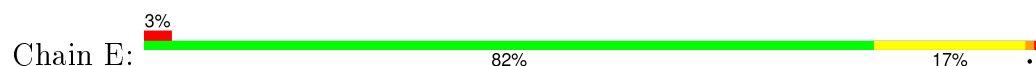
• Molecule 4: Proteasome component PUP2

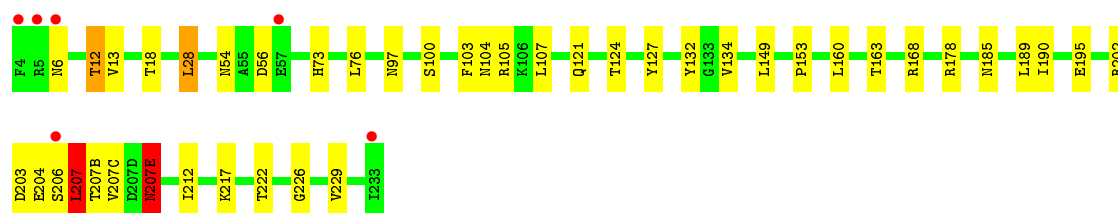


• Molecule 4: Proteasome component PUP2

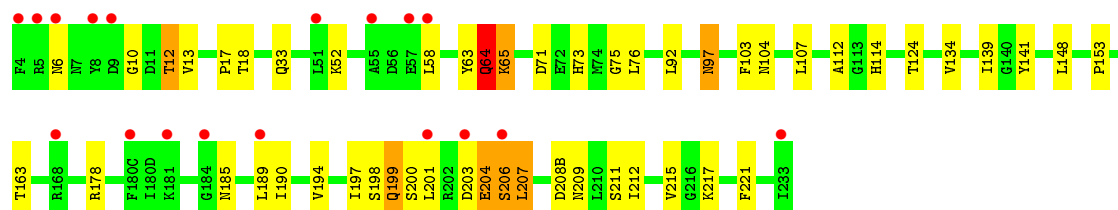
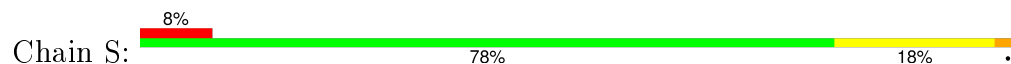


• Molecule 5: Proteasome component PRE5

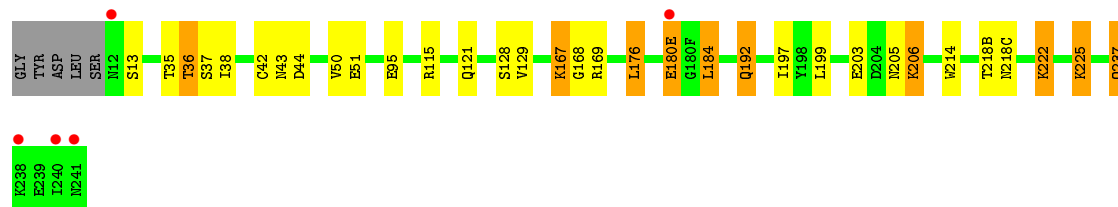
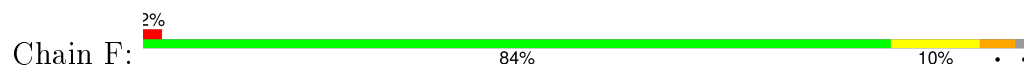




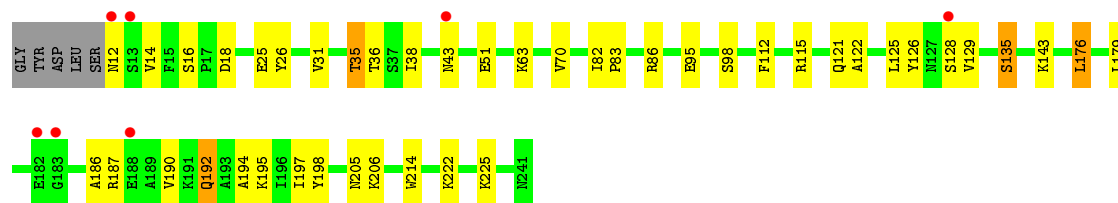
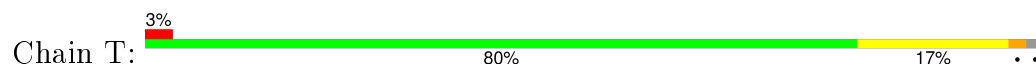
• Molecule 5: Proteasome component PRE5



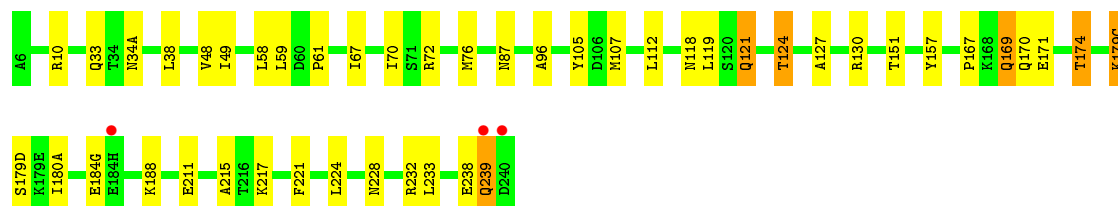
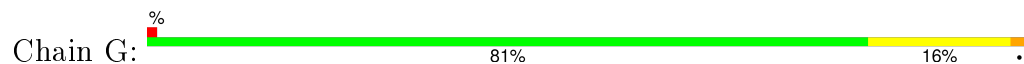
• Molecule 6: Proteasome component C1



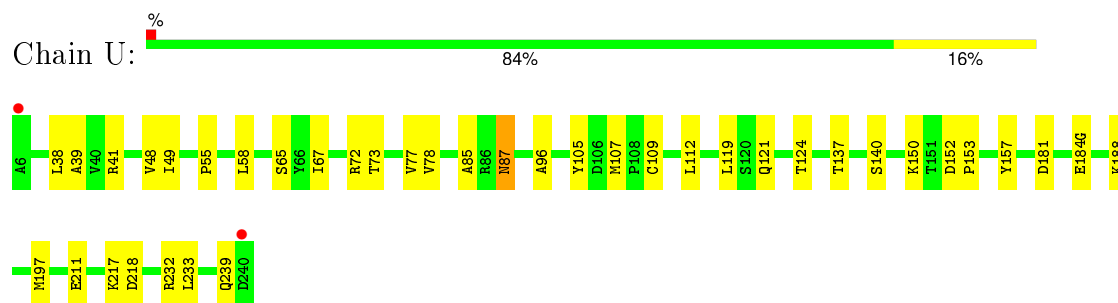
• Molecule 6: Proteasome component C1



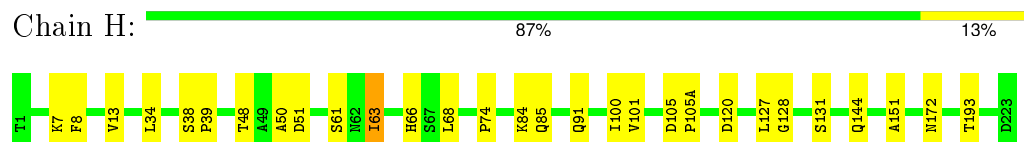
• Molecule 7: Proteasome component C7-alpha



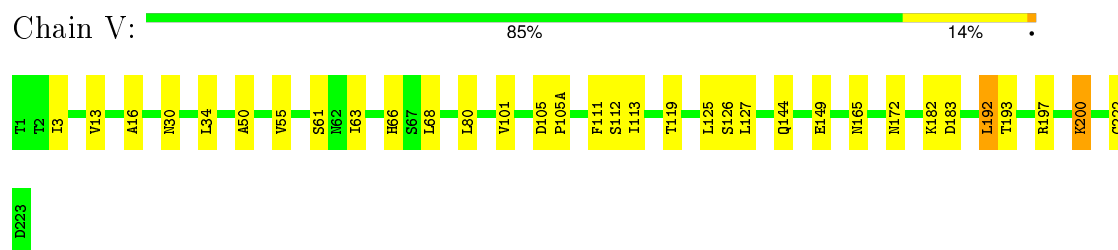
• Molecule 7: Proteasome component C7-alpha



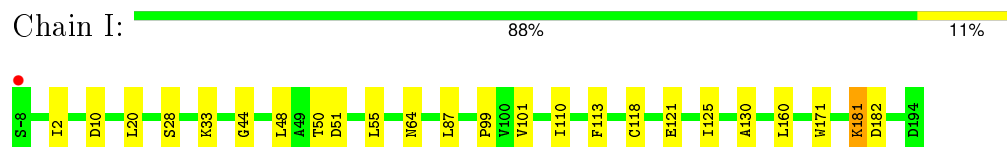
- Molecule 8: Proteasome component PUP1



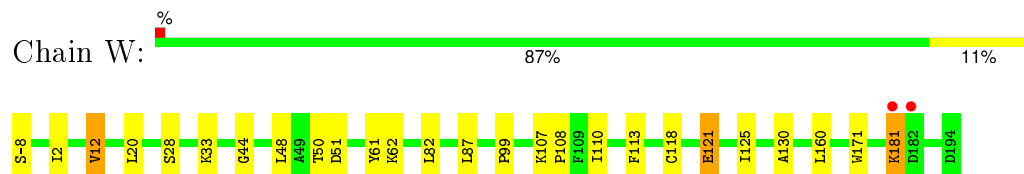
- Molecule 8: Proteasome component PUP1



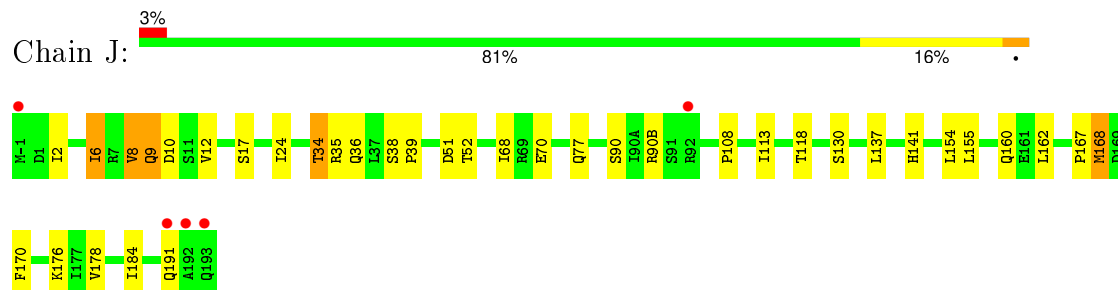
- Molecule 9: Proteasome component PUP3



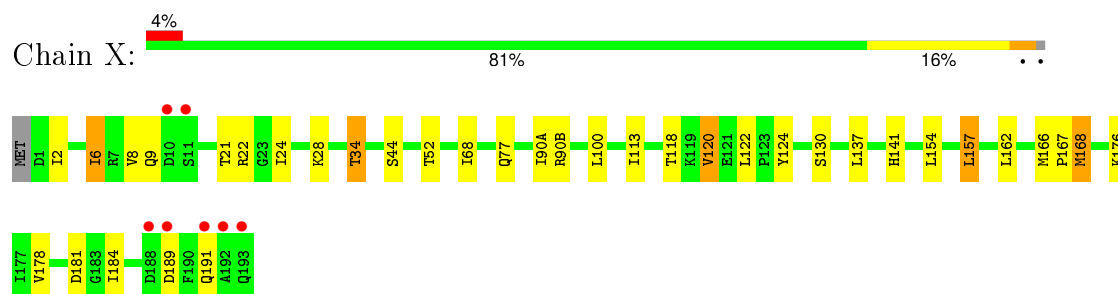
- Molecule 9: Proteasome component PUP3



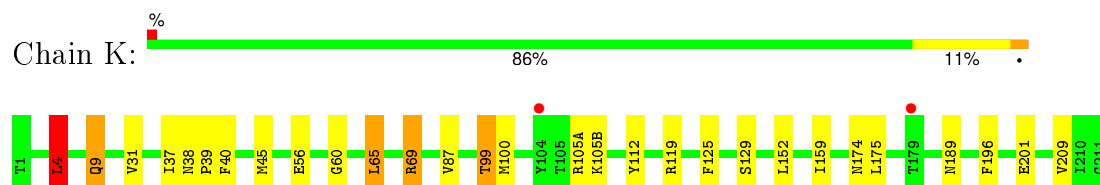
- Molecule 10: Proteasome component C11



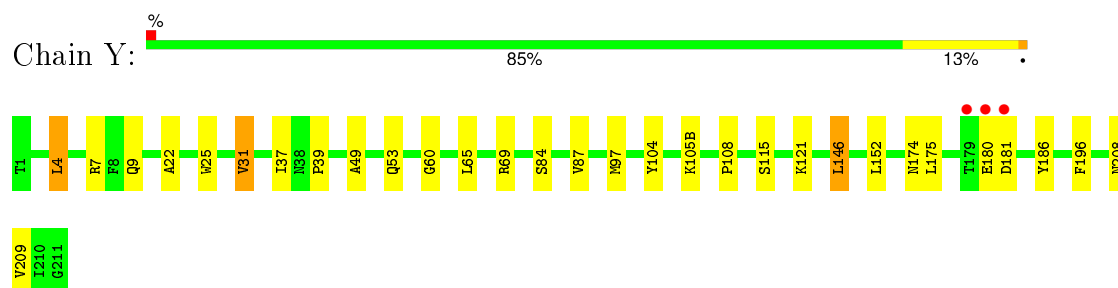
- Molecule 10: Proteasome component C11



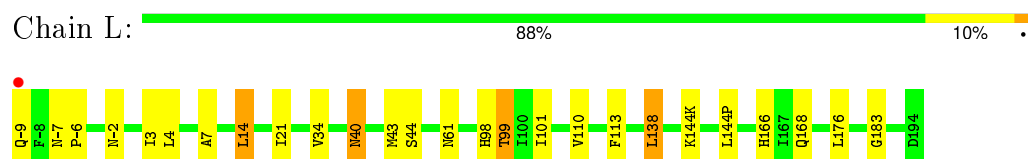
- Molecule 11: Proteasome component PRE2



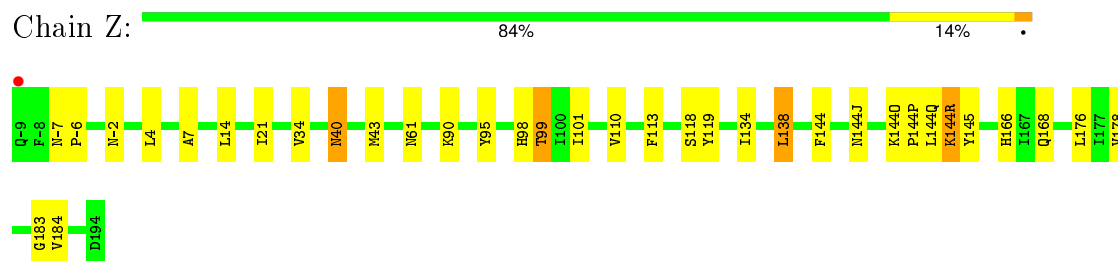
- Molecule 11: Proteasome component PRE2



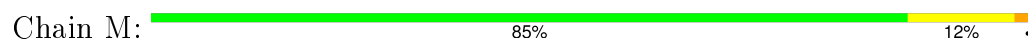
- Molecule 12: Proteasome component C5

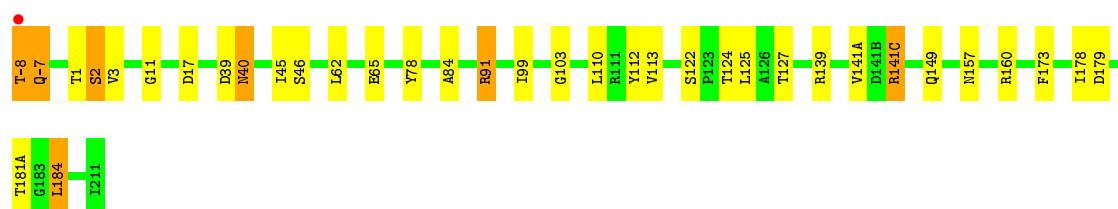


- Molecule 12: Proteasome component C5

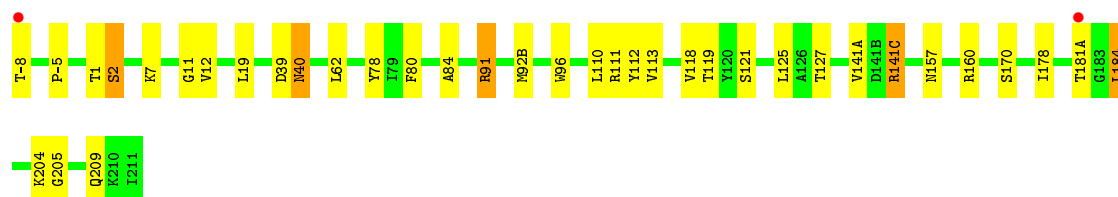
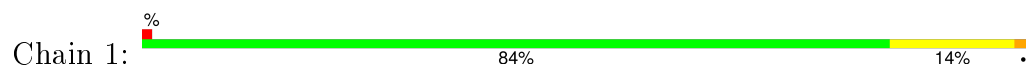


- Molecule 13: Proteasome component PRE4

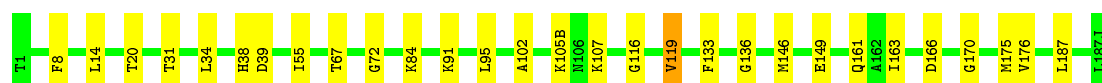
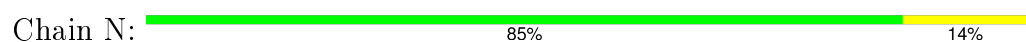




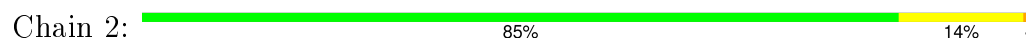
• Molecule 13: Proteasome component PRE4



• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.07Å 299.95Å 145.62Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 49.00 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.85) 98.3 (49.00-2.84)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.257 0.215 , 0.251	Depositor DCC
R_{free} test set	4944 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 22.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 247474 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	49398	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 3OE, 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	0.39	0/1952	0.55	0/2642
1	O	0.42	0/1952	0.56	0/2642
2	B	0.38	0/1858	0.55	0/2516
2	P	0.39	0/1858	0.55	0/2516
3	C	0.39	0/1920	0.55	0/2598
3	Q	0.45	1/1920 (0.1%)	0.56	0/2598
4	D	0.39	0/1886	0.57	1/2541 (0.0%)
4	R	0.43	0/1886	0.88	4/2541 (0.2%)
5	E	0.50	1/1823 (0.1%)	0.77	3/2463 (0.1%)
5	S	0.44	1/1815 (0.1%)	0.55	0/2452
6	F	0.40	0/1887	0.53	0/2546
6	T	0.41	0/1887	0.55	0/2546
7	G	0.41	0/1959	0.55	0/2652
7	U	0.41	0/1959	0.55	0/2652
8	H	0.41	0/1716	0.55	0/2326
8	V	0.46	0/1716	0.55	0/2326
9	I	0.50	0/1611	0.56	0/2174
9	W	0.49	0/1611	0.56	0/2174
10	J	0.41	0/1610	0.57	0/2170
10	X	0.39	0/1605	0.56	0/2163
11	K	0.40	0/1681	0.56	1/2274 (0.0%)
11	Y	0.39	0/1681	0.57	1/2274 (0.0%)
12	L	0.44	0/1795	0.56	0/2420
12	Z	0.44	0/1795	0.57	0/2420
13	1	0.45	0/1855	0.61	0/2514
13	M	0.44	0/1855	0.61	0/2514
14	2	0.51	0/1541	0.55	0/2087
14	N	0.50	0/1541	0.54	0/2087
All	All	0.43	3/50175 (0.0%)	0.58	10/67828 (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
1	O	0	1
4	R	0	1
5	E	0	2
5	S	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	207	LEU	CA-C	-10.54	1.25	1.52
3	Q	180(D)	GLU	C-O	6.35	1.35	1.23
5	S	206	SER	CA-CB	5.61	1.61	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	123(G)	GLU	CA-C-N	-21.19	70.59	117.20
4	R	123(G)	GLU	O-C-N	-18.41	93.24	122.70
4	R	123(G)	GLU	CA-C-O	17.94	157.78	120.10
5	E	207(E)	ASN	CA-C-N	-16.08	81.83	117.20
5	E	207(E)	ASN	O-C-N	-15.68	97.62	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	204	GLU	Peptide
5	E	207(E)	ASN	Mainchain
1	O	217(N)	THR	Peptide
4	R	123(G)	GLU	Mainchain
5	S	204	GLU	Peptide

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	1926	23	0
1	O	1915	0	1926	25	0
2	B	1829	0	1829	23	0
2	P	1829	0	1829	28	0
3	C	1891	0	1900	28	0
3	Q	1891	0	1900	29	0
4	D	1861	0	1836	15	0
4	R	1861	0	1835	21	0
5	E	1795	0	1797	24	0
5	S	1788	0	1790	27	0
6	F	1848	0	1844	20	0
6	T	1848	0	1844	27	0
7	G	1921	0	1910	28	0
7	U	1921	0	1910	28	0
8	H	1685	0	1688	12	0
8	V	1685	0	1688	17	0
9	I	1581	0	1574	17	0
9	W	1581	0	1574	14	0
10	J	1582	0	1583	18	0
10	X	1577	0	1581	18	0
11	K	1644	0	1595	16	0
11	Y	1644	0	1595	14	0
12	L	1757	0	1711	16	0
12	Z	1757	0	1711	27	0
13	1	1824	0	1832	24	0
13	M	1824	0	1832	25	0
14	2	1512	0	1481	14	0
14	N	1512	0	1481	18	0
15	F	2	0	0	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	2	0	0	0	0
15	N	1	0	0	0	0
16	K	43	0	37	2	0
16	Y	43	0	37	1	0
17	K	12	0	13	1	0
17	Y	12	0	13	0	0
All	All	49398	0	49102	519	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 5.

The worst 5 of 519 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)
5:S:52:LYS:HB3	5:S:63:TYR:O	1.35	1.24
3:C:203:THR:HG22	3:C:206:GLY:N	1.65	1.06
12:Z:144(P):PRO:O	12:Z:144(R):LYS:HG2	1.53	1.05
1:O:7:ARG:HG3	6:T:128:SER:HB3	1.38	1.03
7:U:96:ALA:HA	7:U:107:MET:HE2	1.42	1.01

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%)	238 (96%)	8 (3%)	2 (1%)	24	56
1	O	248/250 (99%)	236 (95%)	10 (4%)	2 (1%)	24	56
2	B	233/235 (99%)	223 (96%)	7 (3%)	3 (1%)	15	42
2	P	233/235 (99%)	219 (94%)	11 (5%)	3 (1%)	15	42
3	C	239/241 (99%)	231 (97%)	6 (2%)	2 (1%)	24	56
3	Q	239/241 (99%)	226 (95%)	9 (4%)	4 (2%)	11	35
4	D	240/260 (92%)	222 (92%)	14 (6%)	4 (2%)	11	35
4	R	240/260 (92%)	227 (95%)	11 (5%)	2 (1%)	24	56
5	E	231/233 (99%)	217 (94%)	10 (4%)	4 (2%)	11	35
5	S	231/233 (99%)	212 (92%)	14 (6%)	5 (2%)	8	27
6	F	235/242 (97%)	224 (95%)	10 (4%)	1 (0%)	39	71
6	T	235/242 (97%)	225 (96%)	10 (4%)	0	100	100
7	G	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	39	71
7	U	241/243 (99%)	234 (97%)	5 (2%)	2 (1%)	24	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	34	67
8	V	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
9	I	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
9	W	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
10	J	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	34	67
10	X	195/198 (98%)	184 (94%)	9 (5%)	2 (1%)	19	49
11	K	210/212 (99%)	204 (97%)	4 (2%)	2 (1%)	19	49
11	Y	210/212 (99%)	201 (96%)	7 (3%)	2 (1%)	19	49
12	L	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
12	Z	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	34	67
13	1	231/233 (99%)	220 (95%)	11 (5%)	0	100	100
13	M	231/233 (99%)	220 (95%)	10 (4%)	1 (0%)	39	71
14	2	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6279/6382 (98%)	5988 (95%)	246 (4%)	45 (1%)	26	59

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	217	ALA
3	C	203	THR
3	C	207	ALA
4	D	123(E)	SER
5	E	203	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	197 (94%)	12 (6%)	25	56
1	O	209/209 (100%)	199 (95%)	10 (5%)	31	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	195/195 (100%)	181 (93%)	14 (7%)	18	43
2	P	195/195 (100%)	182 (93%)	13 (7%)	20	47
3	C	213/213 (100%)	196 (92%)	17 (8%)	15	38
3	Q	213/213 (100%)	200 (94%)	13 (6%)	23	52
4	D	198/215 (92%)	184 (93%)	14 (7%)	18	44
4	R	198/215 (92%)	185 (93%)	13 (7%)	21	48
5	E	192/192 (100%)	178 (93%)	14 (7%)	17	42
5	S	191/192 (100%)	173 (91%)	18 (9%)	11	29
6	F	196/200 (98%)	179 (91%)	17 (9%)	13	33
6	T	196/200 (98%)	180 (92%)	16 (8%)	14	36
7	G	207/207 (100%)	190 (92%)	17 (8%)	14	36
7	U	207/207 (100%)	198 (96%)	9 (4%)	35	69
8	H	181/181 (100%)	173 (96%)	8 (4%)	35	68
8	V	181/181 (100%)	170 (94%)	11 (6%)	23	52
9	I	172/172 (100%)	168 (98%)	4 (2%)	58	85
9	W	172/172 (100%)	165 (96%)	7 (4%)	37	71
10	J	174/175 (99%)	158 (91%)	16 (9%)	11	30
10	X	174/175 (99%)	162 (93%)	12 (7%)	19	45
11	K	169/169 (100%)	160 (95%)	9 (5%)	28	60
11	Y	169/169 (100%)	159 (94%)	10 (6%)	24	54
12	L	185/185 (100%)	178 (96%)	7 (4%)	40	74
12	Z	185/185 (100%)	177 (96%)	8 (4%)	35	69
13	1	199/199 (100%)	191 (96%)	8 (4%)	38	72
13	M	199/199 (100%)	190 (96%)	9 (4%)	34	67
14	2	162/162 (100%)	150 (93%)	12 (7%)	17	42
14	N	162/162 (100%)	157 (97%)	5 (3%)	47	79
All	All	5303/5348 (99%)	4980 (94%)	323 (6%)	23	52

5 of 323 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	99	THR
2	P	192	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Z	99	THR
13	M	2	SER
1	O	33	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 147 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	161	GLN
4	R	141	HIS
12	Z	166	HIS
1	O	97	HIS
3	Q	82	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 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	3OE	K	213	-	43,46,46	1.04	2 (4%)	53,61,61	0.75	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	MES	K	214	-	11,12,12	0.63	0	14,16,16	1.17	1 (7%)
16	3OE	Y	212	-	43,46,46	1.00	1 (2%)	53,61,61	0.84	1 (1%)
17	MES	Y	213	-	11,12,12	0.65	0	14,16,16	1.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	3OE	K	213	-	-	0/37/39/39	0/4/4/4
17	MES	K	214	-	-	0/6/14/14	0/1/1/1
16	3OE	Y	212	-	-	0/37/39/39	0/4/4/4
17	MES	Y	213	-	-	0/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	213	3OE	C36-C37	-4.78	1.39	1.50
16	Y	212	3OE	C36-C37	-4.44	1.40	1.50
16	K	213	3OE	C2-C1	2.12	1.54	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	213	3OE	C2-C1-S3	2.10	124.18	120.56
16	K	213	3OE	O35-C36-C37	2.49	116.68	109.21
17	K	214	MES	O1S-S-C8	2.49	109.03	106.91
16	Y	212	3OE	O35-C36-C37	4.02	121.27	109.21

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
16	K	213	3OE	2	0
17	K	214	MES	1	0
16	Y	212	3OE	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%)	-0.09	3 (1%) 81 78	35, 51, 76, 102	0
1	O	250/250 (100%)	-0.11	6 (2%) 62 57	35, 52, 78, 104	0
2	B	235/235 (100%)	-0.01	6 (2%) 59 54	33, 56, 86, 101	0
2	P	235/235 (100%)	0.00	5 (2%) 67 62	32, 56, 89, 101	0
3	C	241/241 (100%)	0.38	23 (9%) 10 6	39, 67, 108, 124	0
3	Q	241/241 (100%)	0.53	38 (15%) 3 1	39, 68, 109, 129	0
4	D	242/260 (93%)	0.04	12 (4%) 32 26	36, 59, 95, 111	0
4	R	242/260 (93%)	0.10	11 (4%) 37 31	37, 59, 98, 116	0
5	E	233/233 (100%)	0.07	6 (2%) 59 54	39, 59, 88, 110	0
5	S	233/233 (100%)	0.26	18 (7%) 16 11	39, 59, 92, 115	0
6	F	237/242 (97%)	-0.13	5 (2%) 67 62	34, 51, 83, 95	0
6	T	237/242 (97%)	-0.06	7 (2%) 54 47	34, 52, 81, 98	0
7	G	243/243 (100%)	-0.16	3 (1%) 81 78	31, 45, 72, 102	0
7	U	243/243 (100%)	-0.28	2 (0%) 87 86	31, 46, 70, 99	0
8	H	222/222 (100%)	-0.26	0 100 100	33, 43, 63, 92	0
8	V	222/222 (100%)	-0.33	0 100 100	33, 44, 64, 94	0
9	I	204/204 (100%)	-0.36	1 (0%) 91 90	31, 43, 60, 74	0
9	W	204/204 (100%)	-0.32	2 (0%) 84 81	31, 43, 60, 75	0
10	J	198/198 (100%)	-0.12	5 (2%) 61 56	32, 46, 61, 113	0
10	X	197/198 (99%)	-0.12	7 (3%) 46 39	33, 46, 61, 111	0
11	K	212/212 (100%)	-0.16	2 (0%) 85 84	31, 46, 72, 81	0
11	Y	212/212 (100%)	-0.24	3 (1%) 78 75	31, 46, 73, 80	0
12	L	222/222 (100%)	-0.32	1 (0%) 91 90	31, 44, 72, 80	0
12	Z	222/222 (100%)	-0.27	1 (0%) 91 90	31, 44, 70, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.28	2 (0%) 85 84	29, 43, 56, 63	0
13	M	233/233 (100%)	-0.34	1 (0%) 93 92	29, 42, 56, 63	0
14	2	196/196 (100%)	-0.36	0 100 100	30, 40, 57, 66	0
14	N	196/196 (100%)	-0.35	0 100 100	31, 40, 57, 66	0
All	All	6335/6382 (99%)	-0.11	170 (2%) 58 52	29, 49, 85, 129	0

The worst 5 of 170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	7	GLY	9.5
4	R	123(C)	GLY	8.9
5	S	4	PHE	8.1
4	D	123(E)	SER	8.0
3	Q	55	THR	7.6

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	F	243	1/1	0.83	0.69	10.23	105,105,105,105	0
17	MES	K	214	12/12	0.92	0.24	4.32	92,93,93,93	0
15	MG	K	212	1/1	0.98	0.25	4.14	47,47,47,47	0
15	MG	I	196	1/1	0.96	0.25	4.11	46,46,46,46	0
17	MES	Y	213	12/12	0.91	0.25	3.44	101,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	MG	H	224	1/1	0.91	0.20	2.74	68,68,68,68	0
16	3OE	Y	212	43/43	0.91	0.24	2.01	71,72,74,75	0
16	3OE	K	213	43/43	0.91	0.23	1.75	55,60,68,68	0
15	MG	N	188	1/1	0.98	0.15	-0.70	36,36,36,36	0
15	MG	L	196	1/1	0.96	0.15	-0.82	50,50,50,50	0
15	MG	L	195	1/1	0.69	0.12	-1.08	56,56,56,56	0
15	MG	G	1	1/1	0.96	0.05	-2.93	41,41,41,41	0
15	MG	I	195	1/1	0.73	0.32	-	57,57,57,57	0
15	MG	F	242	1/1	0.89	0.40	-	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.