



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 10:33 pm GMT

PDB ID : 4Y8N
Title : Yeast 20S proteasome beta7-delta7_Cter mutant in complex with Ac-PAE-ep
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-16
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

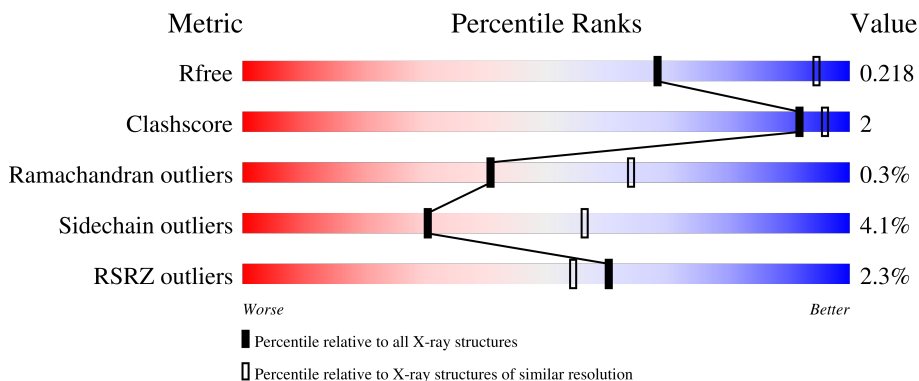
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 98%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 0.5%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 0.5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2% 98% .</p>
1	O	250	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 97%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 0.5%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 0.5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3% 97% .</p>
2	B	258	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3% 85% 10% 5%</p>
2	P	258	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">4% 86% 9% 5%</p>
3	C	254	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">6% 84% 9% 6%</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	7% 86% 7% • 6%
4	D	260	% 85% 5% • 10%
4	R	260	2% 85% 5% 10%
5	E	234	3% 91% 8% •
5	S	234	3% 91% 7% •
6	F	288	2% 80% 5% 16%
6	T	288	3% 81% • 16%
7	G	252	2% 87% 8% •
7	U	252	2% 88% 7% •
8	H	232	3% 91% 6% •
8	V	232	3% 91% 6% •
9	I	205	94% 5%
9	W	205	% 93% 6%
10	J	198	% 90% 8% ••
10	X	198	2% 91% 7% ••
11	K	212	92% 7% •
11	Y	212	92% 6% •
12	L	222	% 97% •
12	Z	222	% 96% •
13	M	239	2% 88% 5% • 6%
13	a	239	2% 90% • 7%
14	N	196	% 94% 5% •
14	b	196	% 97% •
15	c	5	60% 40%
15	d	5	60% 20% 20%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49891 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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
5	E	231	Total 1773	C 1114	N 307	O 348	S 4	0	0	0
5	S	231	Total 1773	C 1114	N 307	O 348	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	243	Total 1892	C 1203	N 329	O 356	S 4	0	0	0
6	T	243	Total 1892	C 1203	N 329	O 356	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	241	Total 1907	C 1214	N 320	O 365	S 8	0	0	0
7	U	241	Total 1907	C 1214	N 320	O 365	S 8	0	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	226	Total 1719	C 1082	N 298	O 332	S 7	0	0	0
8	V	226	Total 1719	C 1082	N 298	O 332	S 7	0	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	Total 1581	C 1010	N 258	O 305	S 8	0	0	0
9	W	204	Total 1581	C 1010	N 258	O 305	S 8	0	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	195	Total 1561	C 992	N 264	O 299	S 6	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	X	195	1561	992	264	299	6	0	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	212	1644	1045	280	312	7	0	0	0
11	Y	212	1644	1045	280	312	7	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	224	1753	1108	300	338	7	0	0	0
13	a	223	1745	1104	299	335	7	0	0	0

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

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

- Molecule 15 is a protein called Ac-PAE-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	c	5	28	18	3	7	0	0	0
15	d	5	28	18	3	7	0	0	0

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	Mg 1	0	0
16	I	2	Total 2	Mg 2	0	0
16	K	1	Total 1	Mg 1	0	0
16	L	1	Total 1	Mg 1	0	0
16	N	1	Total 1	Mg 1	0	0
16	Z	1	Total 1	Mg 1	0	0

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total 1	Cl 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	28	Total 28	O 28	0	0
18	B	23	Total 23	O 23	0	0
18	C	19	Total 19	O 19	0	0
18	D	16	Total 16	O 16	0	0
18	E	9	Total 9	O 9	0	0
18	F	26	Total 26	O 26	0	0
18	G	30	Total 30	O 30	0	0
18	H	25	Total 25	O 25	0	0
18	I	24	Total 24	O 24	0	0
18	J	22	Total 22	O 22	0	0

Continued on next page...

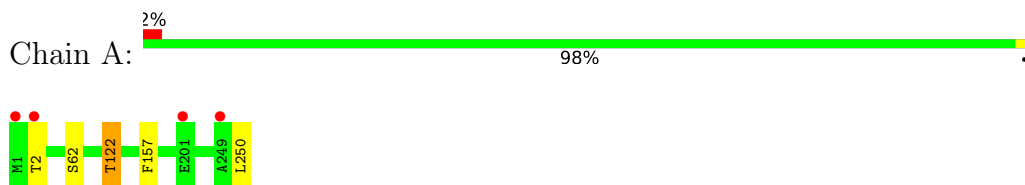
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	K	20	Total O 20 20	0	0
18	L	31	Total O 31 31	0	0
18	M	27	Total O 27 27	0	0
18	N	19	Total O 19 19	0	0
18	O	15	Total O 15 15	0	0
18	P	18	Total O 18 18	0	0
18	Q	15	Total O 15 15	0	0
18	R	21	Total O 21 21	0	0
18	S	9	Total O 9 9	0	0
18	T	19	Total O 19 19	0	0
18	U	26	Total O 26 26	0	0
18	V	20	Total O 20 20	0	0
18	W	16	Total O 16 16	0	0
18	X	19	Total O 19 19	0	0
18	Y	31	Total O 31 31	0	0
18	Z	27	Total O 27 27	0	0
18	a	27	Total O 27 27	0	0
18	b	24	Total O 24 24	0	0
18	c	3	Total O 3 3	0	0
18	d	2	Total O 2 2	0	0

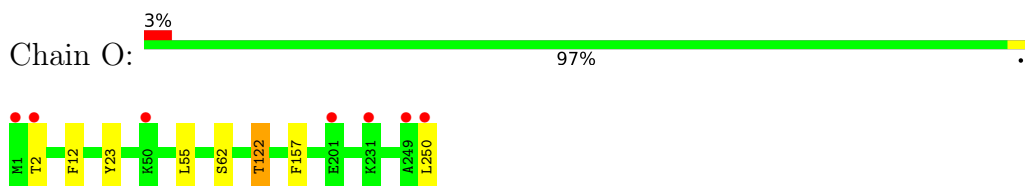
3 Residue-property plots [i](#)

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

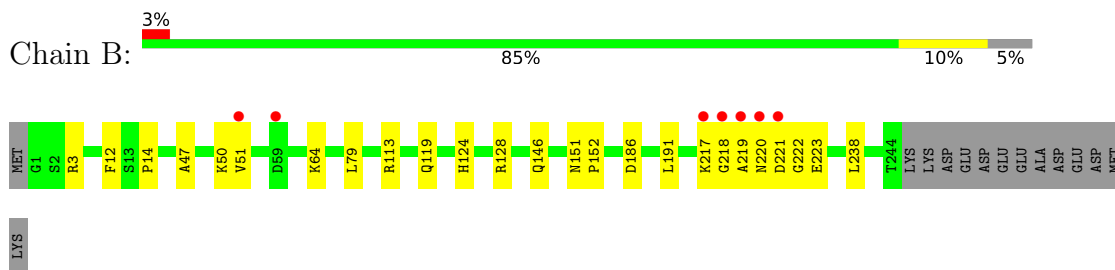
- Molecule 1: Proteasome subunit alpha type-2



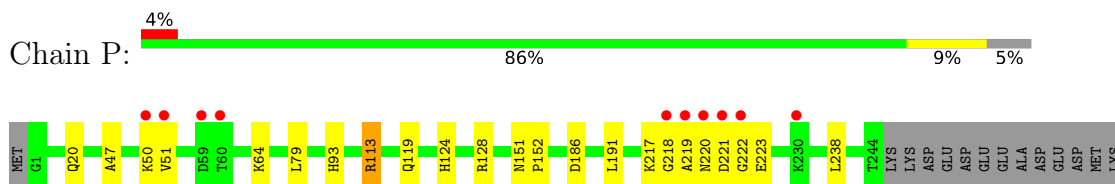
- Molecule 1: Proteasome subunit alpha type-2



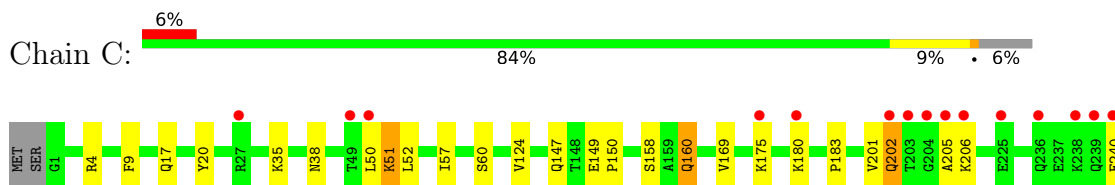
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

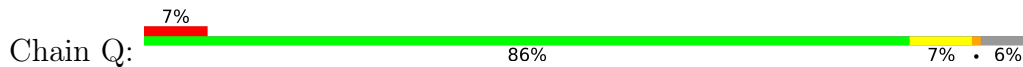


- Molecule 3: Proteasome subunit alpha type-4



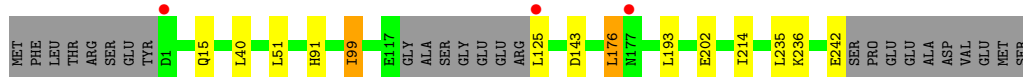
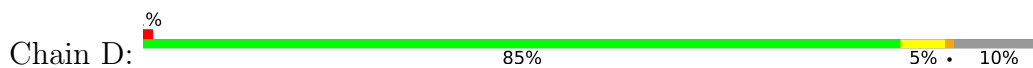
GLN
GLN
GLU
GLN
GLN
ASP
LYS
LYS
LYS
LYS
SER
SER
ASN
HIS

• Molecule 3: Proteasome subunit alpha type-4

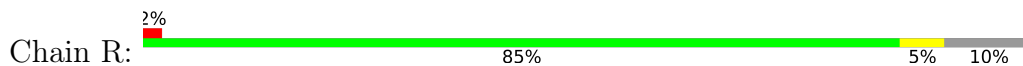


E240
GLN
GLN
GLU
GLN
GLN
ASP
LYS
LYS
LYS
SER
SER
ASN
HIS

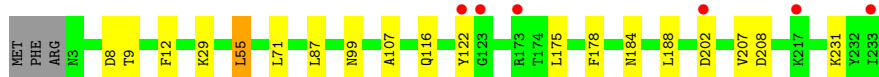
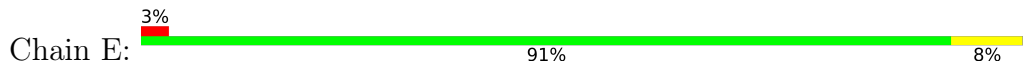
• Molecule 4: Proteasome subunit alpha type-5



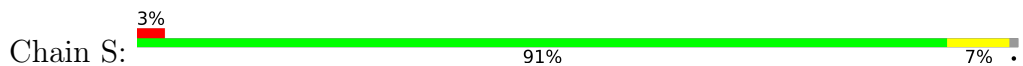
• Molecule 4: Proteasome subunit alpha type-5



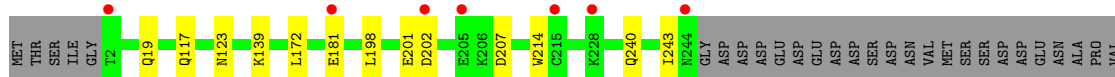
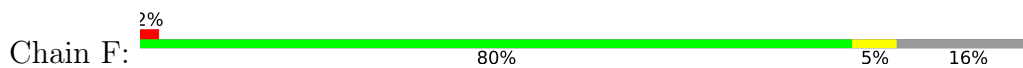
• Molecule 5: Proteasome subunit alpha type-6



• Molecule 5: Proteasome subunit alpha type-6

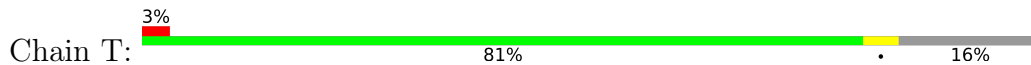


• Molecule 6: Probable proteasome subunit alpha type-7



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

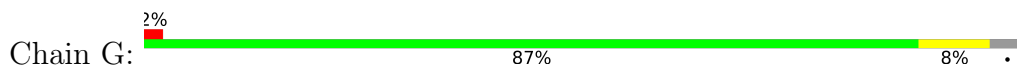
● Molecule 6: Probable proteasome subunit alpha type-7



MET THR SER ILE GLY T2 Q19 Q117 N123 K139 L172 H178 E181 E201 D202 N203 K204 E205 K206 D207 W214 K239 Q240 K241 E242 I243 N244 GLY ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP VAL MET SER SER ASP ASP ASP ASP ASP ASP ASP ASP ASP

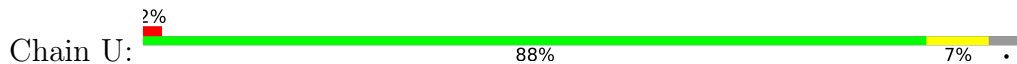
ALA
THR
THR
ASN
ALA
ALA
ASN
ALA
THR
THR
ASP
GLN
GLU
GLY
ASP
ILE
HIS
LEU
GLU

● Molecule 7: Proteasome subunit alpha type-1



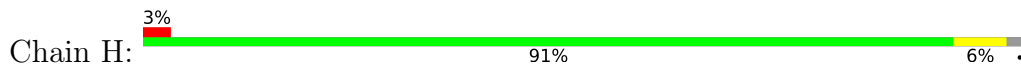
MET SER GLY ALA ALA ALA SER ALA ALA G2 Y3 F23 T26 I63 R68 V73 V74 N75 I78 P79 N83 L115 S116 Q117 R122 M125 T133 T133 K165 K178 L205 E208 E215 D222 R235 L236 K240 E241 Q242 ASP

● Molecule 7: Proteasome subunit alpha type-1



MET SER GLY ALA ALA ALA SER ALA ALA G2 Y3 P12 F23 T26 V73 V74 N75 I78 P79 N83 L115 S116 Q117 R122 M125 T133 A159 K178 K181 G206 T207 E208 D222 R235 L236 Q242 ASP

● Molecule 8: Proteasome subunit beta type-2



TI Q22 A27 N30 H35 E53 T56 Q57 L68 D104 P105 S112 I113 T119 L125 R196 E197 E198 G221 D222 I223 Q224 E225 E226 GLN VAL ASP ILE THR ALA

● Molecule 8: Proteasome subunit beta type-2



TI N30 H35 E53 T56 Q57 L68 D104 P105 S112 I113 T119 Y123 Y124 L125 R196 V218 N219 I220 C221 D222 I223 Q224 E225 E226 GLN VAL ASP ILE THR ALA

● Molecule 9: Proteasome subunit beta type-3

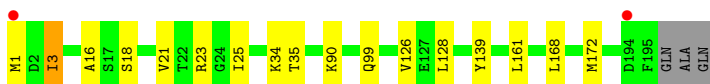
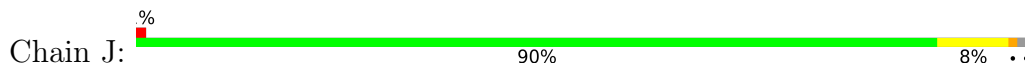


MET SI G9 I10 V20 S36 N37 K41 R98 P101 P118 I126 A141 L171 E204

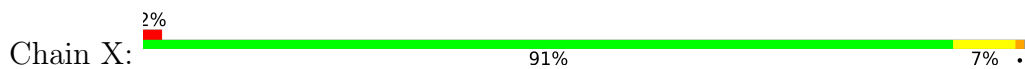
● Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



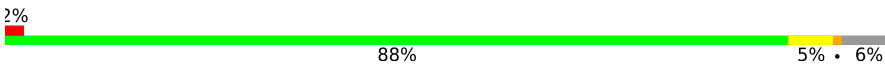
- Molecule 12: Proteasome subunit beta type-6

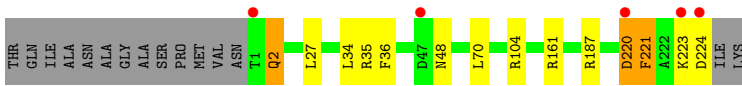


- Molecule 12: Proteasome subunit beta type-6

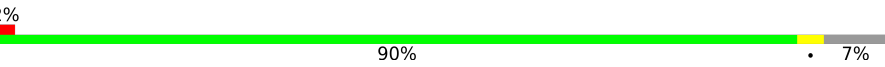


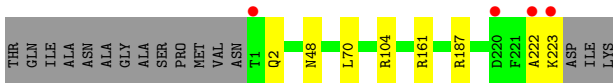
- Molecule 13: Proteasome subunit beta type-7

Chain M:  2% 88% 5% • 6%



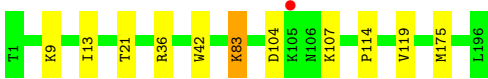
- Molecule 13: Proteasome subunit beta type-7

Chain a:  2% 90% • 7%



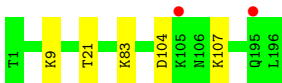
- Molecule 14: Proteasome subunit beta type-1

Chain N:  1% 94% 5% •



- Molecule 14: Proteasome subunit beta type-1

Chain b:  1% 97% •



- Molecule 15: Ac-PAE-ep

Chain c:  60% 40%



- Molecule 15: Ac-PAE-ep

Chain d:  60% 20% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.41Å 301.59Å 145.62Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.5 (15.00-2.60) 95.5 (15.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.197 , 0.215 0.199 , 0.218	Depositor DCC
R_{free} test set	15717 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49891	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: ACE, MG, CL, GAU, POL

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	0.28	0/1952	0.47	0/2642
1	O	0.28	0/1952	0.47	0/2642
2	B	0.28	0/1934	0.50	0/2618
2	P	0.28	0/1934	0.50	0/2618
3	C	0.28	0/1910	0.51	0/2586
3	Q	0.28	0/1910	0.51	0/2586
4	D	0.27	0/1837	0.48	0/2475
4	R	0.27	0/1837	0.48	0/2475
5	E	0.28	0/1800	0.48	0/2433
5	S	0.28	0/1800	0.48	0/2433
6	F	0.28	0/1932	0.45	0/2609
6	T	0.28	0/1932	0.45	0/2609
7	G	0.28	0/1945	0.47	0/2634
7	U	0.28	0/1945	0.47	0/2634
8	H	0.29	0/1750	0.48	0/2373
8	V	0.26	0/1750	0.48	0/2373
9	I	0.32	0/1611	0.49	0/2174
9	W	0.28	0/1611	0.48	0/2174
10	J	0.28	0/1589	0.49	0/2142
10	X	0.27	0/1589	0.48	0/2142
11	K	0.29	0/1681	0.51	1/2274 (0.0%)
11	Y	0.27	0/1681	0.50	1/2274 (0.0%)
12	L	0.28	0/1795	0.50	1/2420 (0.0%)
12	Z	0.29	0/1795	0.50	0/2420
13	M	0.33	0/1783	0.52	0/2420
13	a	0.34	0/1775	0.52	0/2409
14	N	0.37	0/1541	0.51	0/2087
14	b	0.34	0/1541	0.49	0/2087
15	c	2.43	1/13 (7.7%)	1.11	0/18
15	d	2.67	1/13 (7.7%)	1.24	0/18
All	All	0.29	2/50138 (0.0%)	0.49	3/67799 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	d	2	PRO	CA-C	-7.62	1.37	1.52
15	c	2	PRO	CA-C	-7.24	1.38	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
12	L	132	GLU	CA-CB-CG	5.21	124.87	113.40
11	Y	4	LEU	CA-CB-CG	5.13	127.09	115.30
11	K	4	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	4	0
2	B	1904	0	1904	12	0
2	P	1904	0	1904	10	0
3	C	1881	0	1895	10	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	5	0
8	H	1719	0	1719	9	0
8	V	1719	0	1719	9	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	X	1561	0	1569	9	0
11	K	1644	0	1595	7	0
11	Y	1644	0	1595	6	0
12	L	1757	0	1711	0	0
12	Z	1757	0	1711	1	0
13	M	1753	0	1754	10	0
13	a	1745	0	1750	0	0
14	N	1512	0	1478	7	0
14	b	1512	0	1478	0	0
15	c	28	0	26	0	0
15	d	28	0	26	0	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
18	A	28	0	0	0	0
18	B	23	0	0	0	0
18	C	19	0	0	0	0
18	D	16	0	0	0	0
18	E	9	0	0	0	0
18	F	26	0	0	1	0
18	G	30	0	0	0	0
18	H	25	0	0	0	0
18	I	24	0	0	0	0
18	J	22	0	0	0	0
18	K	20	0	0	0	0
18	L	31	0	0	0	0
18	M	27	0	0	1	0
18	N	19	0	0	0	0
18	O	15	0	0	0	0
18	P	18	0	0	2	0
18	Q	15	0	0	0	0
18	R	21	0	0	0	0
18	S	9	0	0	0	0
18	T	19	0	0	0	0
18	U	26	0	0	0	0
18	V	20	0	0	0	0
18	W	16	0	0	0	0
18	X	19	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Y	31	0	0	0	0
18	Z	27	0	0	0	0
18	a	27	0	0	0	0
18	b	24	0	0	0	0
18	c	3	0	0	0	0
18	d	2	0	0	0	0
All	All	49891	0	49016	132	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 2.

All (132) 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)
8:V:53:GLU:OE1	8:V:57:GLN:NE2	2.21	0.73
8:H:53:GLU:OE1	8:H:57:GLN:NE2	2.21	0.72
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.46	0.63
13:M:220:ASP:O	13:M:223:LYS:HG2	2.00	0.61
13:M:224:ASP:OD2	8:V:123:TYR:OH	2.17	0.61
14:N:13:ILE:HG21	14:N:175:MET:CE	2.31	0.61
13:M:35:ARG:HH12	14:N:114:PRO:HB3	1.67	0.60
5:S:12:PHE:H	6:T:19:GLN:HE22	1.50	0.59
2:B:12:PHE:H	3:C:17:GLN:HE22	1.51	0.59
8:H:113:ILE:HG13	8:H:119:THR:HG22	1.86	0.58
8:V:113:ILE:HG13	8:V:119:THR:HG22	1.85	0.58
2:P:93:HIS:HB3	18:P:301:HOH:O	2.04	0.57
2:B:221:ASP:O	2:B:223:GLU:N	2.38	0.56
2:P:221:ASP:O	2:P:223:GLU:N	2.39	0.56
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.86	0.56
13:M:223:LYS:O	13:M:224:ASP:HB3	2.06	0.56
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.05	0.55
5:E:12:PHE:H	6:F:19:GLN:HE22	1.56	0.54
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.91	0.53
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.08	0.53
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.91	0.53
3:C:51:LYS:O	3:C:52:LEU:HB2	2.08	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
11:K:53:GLN:O	11:K:57:THR:HG23	2.11	0.51
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.76	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.77	0.50
2:P:217:LYS:C	2:P:219:ALA:H	2.15	0.50
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.11	0.50
8:H:113:ILE:CG1	8:H:119:THR:HG22	2.41	0.50
13:M:224:ASP:O	13:M:224:ASP:OD1	2.28	0.50
8:H:35:HIS:CE1	8:H:53:GLU:OE2	2.65	0.50
13:M:35:ARG:NH1	14:N:114:PRO:HB3	2.26	0.50
8:V:113:ILE:CG1	8:V:119:THR:HG22	2.41	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.49
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.49
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.77	0.49
2:B:217:LYS:C	2:B:219:ALA:H	2.14	0.49
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.95	0.49
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.95	0.49
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.95	0.49
1:O:12:PHE:H	2:P:20:GLN:HE22	1.61	0.49
13:M:35:ARG:HD3	13:M:36:PHE:CZ	2.48	0.48
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.48
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.95	0.48
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.95	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.96	0.48
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.96	0.48
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.96	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.95	0.48
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.49	0.47
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.95	0.47
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.96	0.47
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.44	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.46
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.97	0.46
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.97	0.46
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.81	0.46
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.16	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.46
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.97	0.46
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.98	0.46
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.46	0.46
3:C:9:PHE:H	4:D:15:GLN:HE22	1.64	0.45
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.96	0.45
11:K:116:ASP:HB2	11:K:120:THR:HB	1.99	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.45
13:M:221:PHE:O	13:M:224:ASP:OD1	2.35	0.45
1:O:55:LEU:HB3	7:U:159:ALA:O	2.17	0.45
8:H:22:GLN:NE2	8:H:27:ALA:HB2	2.32	0.45
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.99	0.44
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.00	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.47	0.44
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.47	0.44
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.98	0.44
10:J:23:ARG:HA	10:J:23:ARG:HD3	1.76	0.44
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.47	0.44
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.52	0.44
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.54	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.00	0.43
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.00	0.43
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.00	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.43
9:W:98:ARG:O	9:W:126:ILE:HD11	2.19	0.43
12:Z:137:ARG:HD3	12:Z:138:ALA:O	2.19	0.43
9:I:98:ARG:O	9:I:126:ILE:HD11	2.18	0.43
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.43
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.49	0.43
10:X:1:MET:HB3	10:X:34:LYS:HE3	2.01	0.43
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.00	0.43
6:F:19:GLN:NE2	18:F:301:HOH:O	2.49	0.42
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.01	0.42
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.99	0.42
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.54	0.42
2:P:113:ARG:NE	18:P:301:HOH:O	2.45	0.42
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.01	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.49	0.42
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.00	0.42
9:I:101:PRO:HB3	9:I:126:ILE:HD12	2.02	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.02	0.42
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.50	0.42
2:B:3:ARG:CB	5:E:122:TYR:OH	2.68	0.42
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.01	0.42
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.01	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.41
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.02	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:1:MET:CB	10:X:34:LYS:HE3	2.50	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.50	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.55	0.41
10:J:1:MET:HB3	10:J:34:LYS:HE3	2.02	0.41
11:Y:128:CYS:SG	11:Y:136:ALA:HB3	2.61	0.41
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.51	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
10:J:25:ILE:O	10:X:139:TYR:OH	2.39	0.41
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.56	0.41
10:J:1:MET:CB	10:J:34:LYS:HE3	2.51	0.41
7:G:73:VAL:HG12	7:G:133:THR:HB	2.01	0.41
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.41
11:K:128:CYS:SG	11:K:136:ALA:HB3	2.61	0.41
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.03	0.40
13:M:2:GLN:NE2	18:M:301:HOH:O	2.54	0.40
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.03	0.40
7:G:63:ILE:HD12	7:G:215:GLU:HG2	2.04	0.40
10:J:139:TYR:OH	10:X:25:ILE:O	2.40	0.40
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.04	0.40
10:J:168:LEU:O	10:J:172:MET:HB2	2.21	0.40
7:U:73:VAL:HG12	7:U:133:THR:HB	2.02	0.40
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.04	0.40
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.52	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%)	238 (96%)	9 (4%)	1 (0%)	34 57
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34 57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	18
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	18
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	24
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	24
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%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	217 (97%)	7 (3%)	0	100	100
8	V	224/232 (97%)	217 (97%)	7 (3%)	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%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	52
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	222/239 (93%)	212 (96%)	9 (4%)	1 (0%)	29	52
13	a	221/239 (92%)	211 (96%)	9 (4%)	1 (0%)	29	52
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
15	c	2/5 (40%)	2 (100%)	0	0	100	100
15	d	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6269/6610 (95%)	6116 (98%)	134 (2%)	19 (0%)	41	64

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN
2	P	51	VAL
2	P	222	GLY
3	Q	202	GLN
13	a	222	ALA
1	A	2	THR
2	B	218	GLY
1	O	2	THR
2	P	218	GLY
2	B	220	ASN
3	C	205	ALA
13	M	221	PHE
2	P	220	ASN
3	Q	205	ALA
10	X	24	GLY
3	C	183	PRO
3	Q	183	PRO

5.3.2 Protein sidechains [i](#)

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%)	205 (98%)	4 (2%)	57 79
1	O	209/209 (100%)	205 (98%)	4 (2%)	57 79
2	B	203/216 (94%)	196 (97%)	7 (3%)	37 63
2	P	203/216 (94%)	196 (97%)	7 (3%)	37 63
3	C	212/226 (94%)	200 (94%)	12 (6%)	20 41
3	Q	212/226 (94%)	200 (94%)	12 (6%)	20 41
4	D	194/215 (90%)	182 (94%)	12 (6%)	18 37
4	R	194/215 (90%)	182 (94%)	12 (6%)	18 37
5	E	190/193 (98%)	177 (93%)	13 (7%)	16 32
5	S	190/193 (98%)	178 (94%)	12 (6%)	18 36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	47
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	47
7	G	206/210 (98%)	195 (95%)	11 (5%)	22	45
7	U	206/210 (98%)	195 (95%)	11 (5%)	22	45
8	H	185/190 (97%)	181 (98%)	4 (2%)	52	76
8	V	185/190 (97%)	181 (98%)	4 (2%)	52	76
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	81
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	81
10	J	173/175 (99%)	169 (98%)	4 (2%)	50	75
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	68
11	K	169/169 (100%)	161 (95%)	8 (5%)	26	50
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	50
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	59
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29	54
13	M	192/203 (95%)	185 (96%)	7 (4%)	35	61
13	a	191/203 (94%)	184 (96%)	7 (4%)	34	60
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	66
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	66
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	0	1 (100%)	0	0
All	All	5307/5532 (96%)	5091 (96%)	216 (4%)	30	56

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	79	LEU
2	B	113	ARG
2	B	119	GLN
2	B	186	ASP
2	B	191	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	50	LEU
3	C	51	LYS
3	C	60	SER
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	207	VAL
5	E	208	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	178	LYS
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	68	LEU
8	H	113	ILE
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	69	ARG
11	K	104	TYR
11	K	107	LYS
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	132	GLU
12	L	136	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	220	ASP
14	N	9	LYS
14	N	21	THR
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	62	SER
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	79	LEU
2	P	113	ARG
2	P	119	GLN
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	50	LEU
3	Q	51	LYS
3	Q	60	SER
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	R	193	LEU
4	R	202	GLU
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	55	LEU
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	207	VAL
5	S	208	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	178	LYS
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	68	LEU
8	V	113	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	69	ARG
11	Y	104	TYR
11	Y	107	LYS
11	Y	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	3	ASN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	132	GLU
12	Z	136	CYS
12	Z	137	ARG
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	223	LYS
14	b	9	LYS
14	b	21	THR
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS
15	d	2	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	92	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	6	HIS
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
8	H	22	GLN
8	H	35	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	66	HIS
8	H	165	ASN
9	I	37	ASN
10	J	55	GLN
10	J	146	HIS
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	158	ASN
13	M	18	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
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
8	V	35	HIS
8	V	165	ASN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
10	X	146	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	GAU	c	4	15,14	8,8,8	1.63	2 (25%)	8,9,9	1.29	1 (12%)
15	GAU	d	4	15,14	8,8,8	1.50	2 (25%)	8,9,9	1.30	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GAU	c	4	15,14	-	1/7/7/7	-
15	GAU	d	4	15,14	-	0/7/7/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	4	GAU	C-CA	3.86	1.58	1.52
15	d	4	GAU	C-CA	2.90	1.57	1.52
15	d	4	GAU	OE2-CD	-2.32	1.22	1.30
15	c	4	GAU	OE2-CD	-2.03	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	4	GAU	CB-CA-N	-2.32	102.29	109.03
15	c	4	GAU	CB-CA-N	-2.04	103.12	109.03

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	4	GAU	O-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.44	4 (1%) 72 68	41, 53, 85, 125	0
1	O	250/250 (100%)	-0.30	7 (2%) 53 46	46, 63, 105, 133	0
2	B	244/258 (94%)	-0.29	7 (2%) 51 45	42, 60, 101, 150	0
2	P	244/258 (94%)	-0.20	10 (4%) 37 30	47, 64, 110, 155	0
3	C	240/254 (94%)	-0.13	15 (6%) 20 15	42, 65, 125, 150	0
3	Q	240/254 (94%)	0.07	19 (7%) 12 9	47, 75, 151, 175	0
4	D	235/260 (90%)	-0.35	3 (1%) 77 73	47, 66, 99, 138	0
4	R	235/260 (90%)	-0.24	5 (2%) 63 58	48, 69, 109, 144	0
5	E	231/234 (98%)	-0.20	6 (2%) 56 50	50, 69, 106, 150	0
5	S	231/234 (98%)	-0.12	6 (2%) 56 50	52, 75, 118, 164	0
6	F	243/288 (84%)	-0.37	7 (2%) 51 45	44, 61, 109, 139	0
6	T	243/288 (84%)	-0.23	8 (3%) 46 39	46, 72, 126, 156	0
7	G	241/252 (95%)	-0.46	4 (1%) 70 66	37, 55, 89, 136	0
7	U	241/252 (95%)	-0.39	6 (2%) 57 51	45, 60, 91, 135	0
8	H	226/232 (97%)	-0.31	6 (2%) 54 48	38, 54, 87, 148	0
8	V	226/232 (97%)	-0.28	7 (3%) 49 42	45, 58, 90, 163	0
9	I	204/205 (99%)	-0.64	1 (0%) 91 89	39, 51, 78, 100	0
9	W	204/205 (99%)	-0.62	3 (1%) 73 70	42, 54, 84, 107	0
10	J	195/198 (98%)	-0.48	2 (1%) 82 80	40, 55, 81, 134	0
10	X	195/198 (98%)	-0.45	3 (1%) 73 70	41, 56, 80, 143	0
11	K	212/212 (100%)	-0.52	1 (0%) 91 89	38, 56, 78, 99	0
11	Y	212/212 (100%)	-0.54	0 100 100	42, 56, 79, 100	0
12	L	222/222 (100%)	-0.51	2 (0%) 84 82	40, 56, 87, 121	0
12	Z	222/222 (100%)	-0.53	2 (0%) 84 82	38, 55, 86, 120	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	224/239 (93%)	-0.53	5 (2%) 62 56	25, 55, 79, 98	0
13	a	223/239 (93%)	-0.51	4 (1%) 68 64	24, 53, 75, 93	0
14	N	196/196 (100%)	-0.54	1 (0%) 91 89	40, 51, 79, 107	0
14	b	196/196 (100%)	-0.51	2 (1%) 82 80	40, 53, 79, 113	0
15	c	2/5 (40%)	-0.87	0 100 100	66, 66, 66, 67	0
15	d	2/5 (40%)	-0.80	0 100 100	57, 57, 57, 63	0
All	All	6329/6610 (95%)	-0.37	146 (2%) 60 54	24, 59, 103, 175	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	6.8
3	C	206	LYS	6.6
3	Q	50	LEU	6.3
2	P	220	ASN	6.0
10	J	1	MET	5.9
10	X	1	MET	5.9
3	C	205	ALA	5.8
2	B	218	GLY	5.4
8	V	224	GLN	5.2
13	M	224	ASP	5.1
3	C	49	THR	5.1
2	B	221	ASP	5.0
2	B	51	VAL	5.0
3	Q	206	LYS	5.0
5	S	202	ASP	5.0
8	V	226	GLU	4.9
10	X	194	ASP	4.7
2	B	219	ALA	4.6
2	P	221	ASP	4.6
3	Q	236	GLN	4.6
12	L	174	TYR	4.6
2	P	51	VAL	4.5
9	W	1	SER	4.4
1	A	1	MET	4.3
2	P	218	GLY	4.2
7	U	242	GLN	4.0
8	H	221	CYS	3.8
6	F	244	ASN	3.8
3	C	50	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	239	GLN	3.8
10	J	194	ASP	3.8
1	O	1	MET	3.7
5	E	202	ASP	3.7
8	V	221	CYS	3.7
2	P	219	ALA	3.7
6	T	178	HIS	3.6
4	R	1	ASP	3.6
12	Z	174	TYR	3.6
4	R	241	ALA	3.5
3	Q	240	GLU	3.5
13	a	220	ASP	3.5
2	P	59	ASP	3.5
8	H	224	GLN	3.4
8	H	226	GLU	3.4
3	C	236	GLN	3.4
1	O	250	LEU	3.4
9	W	133	LYS	3.4
1	O	2	THR	3.3
3	C	238	LYS	3.3
3	C	239	GLN	3.3
8	H	222	ASP	3.3
3	Q	205	ALA	3.3
4	R	125	LEU	3.2
6	F	205	GLU	3.2
1	A	249	ALA	3.2
5	E	122	TYR	3.2
14	b	195	GLN	3.1
3	Q	229	GLN	3.1
13	a	223	LYS	3.1
13	M	223	LYS	3.1
3	C	225	GLU	3.0
3	Q	204	GLY	3.0
7	G	222	ASP	3.0
1	A	2	THR	3.0
3	C	240	GLU	3.0
8	H	198	GLU	3.0
8	V	222	ASP	2.9
8	V	225	GLU	2.9
13	M	220	ASP	2.9
2	B	217	LYS	2.9
6	T	244	ASN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	T	243	ILE	2.9
4	R	242	GLU	2.8
5	E	233	ILE	2.8
3	C	202	GLN	2.8
13	M	47	ASP	2.7
3	Q	202	GLN	2.7
5	S	201	ARG	2.7
9	I	1	SER	2.7
5	S	180	LYS	2.7
13	a	1	THR	2.7
3	Q	187	GLU	2.6
1	O	50	LYS	2.6
7	G	68	ARG	2.6
5	E	217	LYS	2.6
6	F	202	ASP	2.6
3	C	180	LYS	2.5
5	S	227	GLU	2.5
6	T	239	ALA	2.5
9	W	192	ASP	2.5
1	O	231	LYS	2.5
14	b	105	LYS	2.5
2	P	60	THR	2.5
7	G	3	TYR	2.5
2	P	230	LYS	2.5
2	P	222	GLY	2.5
3	C	204	GLY	2.5
14	N	105	LYS	2.5
3	Q	203	THR	2.4
5	S	210	LEU	2.4
6	T	241	LYS	2.4
6	F	215	CYS	2.4
8	H	223	ILE	2.4
1	A	201	GLU	2.4
3	C	203	THR	2.4
6	F	181	GLU	2.4
6	T	204	LYS	2.3
3	Q	46	ARG	2.3
13	M	1	THR	2.3
4	R	217	GLN	2.3
2	P	50	LYS	2.3
4	D	125	LEU	2.3
1	O	249	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	59	ASP	2.2
5	S	54	GLU	2.2
11	K	147	ASP	2.2
6	F	2	THR	2.2
3	Q	238	LYS	2.2
13	a	222	ALA	2.2
8	V	223	ILE	2.2
3	Q	48	SER	2.1
10	X	193	ASP	2.1
3	C	27	ARG	2.1
3	C	175	LYS	2.1
6	T	181	GLU	2.1
7	U	2	GLY	2.1
6	F	228	LYS	2.1
7	U	222	ASP	2.1
6	T	205	GLU	2.1
4	D	177	ASN	2.1
3	Q	60	SER	2.1
5	E	123	GLY	2.1
3	Q	225	GLU	2.1
7	U	3	TYR	2.1
8	V	219	ASN	2.1
3	Q	55	THR	2.1
7	U	181	LYS	2.0
7	G	240	ALA	2.0
12	Z	173	LYS	2.0
5	E	173	ARG	2.0
3	Q	232	THR	2.0
4	D	1	ASP	2.0
2	B	220	ASN	2.0
7	U	206	GLY	2.0
1	O	201	GLU	2.0
12	L	172	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(\AA^2)	Q<0.9
15	GAU	c	4	9/9	0.92	0.16	68,72,75,76	0
15	GAU	d	4	9/9	0.95	0.13	61,66,66,72	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(\AA^2)	Q<0.9
16	MG	N	201	1/1	0.94	0.14	52,52,52,52	0
16	MG	Z	301	1/1	0.96	0.30	62,62,62,62	0
16	MG	G	301	1/1	0.97	0.05	48,48,48,48	0
16	MG	I	301	1/1	0.97	0.33	64,64,64,64	0
17	CL	G	302	1/1	0.97	0.22	30,30,30,30	0
16	MG	I	302	1/1	0.99	0.07	49,49,49,49	0
16	MG	K	301	1/1	0.99	0.04	54,54,54,54	0
16	MG	L	301	1/1	0.99	0.05	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.