



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2016 – 04:11 PM EDT

PDB ID : 5FG7
Title : Yeast 20S proteasome beta2-T1A mutant
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-12-20
Resolution : 2.70 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:

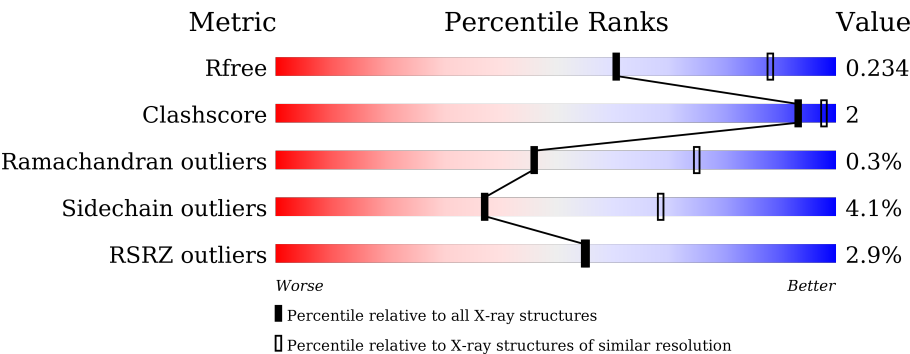
MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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>5%</div><div><div></div><div></div><div></div><div></div></div><div>98% .</div></div>
1	O	250	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>97% .</div></div>
2	B	258	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>86% 8% 5%</div></div>
2	P	258	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>86% 7% . 5%</div></div>
3	C	254	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>85% 8% . 6%</div></div>
3	Q	254	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>85% 8% . 6%</div></div>

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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	238	
8	V	238	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	W	301	-	-	-	X
15	MG	Z	301	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49981 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	228	Total	C	N	O	S	0	0	0
			1720	1082	300	331	7			
8	V	228	Total	C	N	O	S	0	0	0
			1720	1082	300	331	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	ALA	THR	engineered mutation	UNP P25043
V	1	ALA	THR	engineered mutation	UNP P25043

- 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			
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	W	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0

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

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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	17	Total O 17 17	0	0
17	B	16	Total O 16 16	0	0
17	C	22	Total O 22 22	0	0
17	D	20	Total O 20 20	0	0
17	E	16	Total O 16 16	0	0
17	F	20	Total O 20 20	0	0
17	G	35	Total O 35 35	0	0
17	H	22	Total O 22 22	0	0

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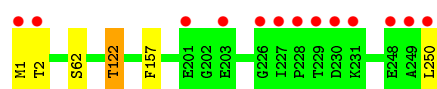
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	I	25	Total 25	O 25	0	0
17	J	18	Total 18	O 18	0	0
17	K	23	Total 23	O 23	0	0
17	L	31	Total 31	O 31	0	0
17	M	28	Total 28	O 28	0	0
17	N	25	Total 25	O 25	0	0
17	O	17	Total 17	O 17	0	0
17	P	12	Total 12	O 12	0	0
17	Q	16	Total 16	O 16	0	0
17	R	11	Total 11	O 11	0	0
17	S	9	Total 9	O 9	0	0
17	T	20	Total 20	O 20	0	0
17	U	34	Total 34	O 34	0	0
17	V	21	Total 21	O 21	0	0
17	W	21	Total 21	O 21	0	0
17	X	19	Total 19	O 19	0	0
17	Y	22	Total 22	O 22	0	0
17	Z	23	Total 23	O 23	0	0
17	a	37	Total 37	O 37	0	0
17	b	23	Total 23	O 23	0	0

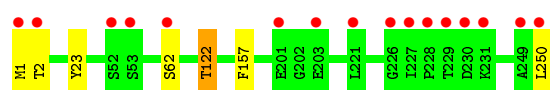
3 Residue-property plots [i](#)

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.

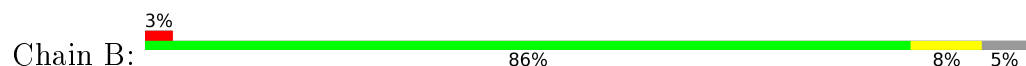
- Molecule 1: Proteasome subunit alpha type-2



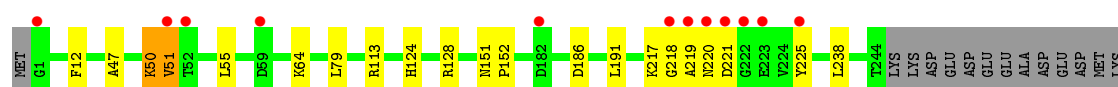
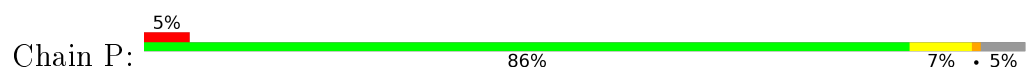
- Molecule 1: Proteasome subunit alpha type-2



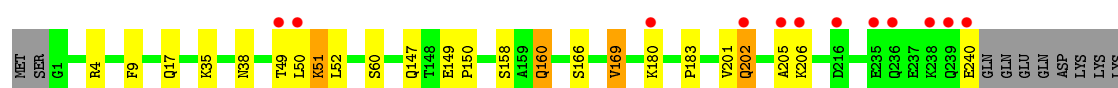
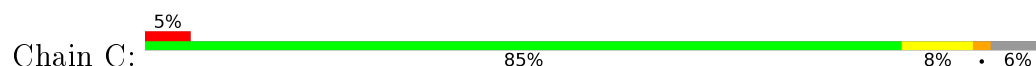
- Molecule 2: Proteasome subunit alpha type-3



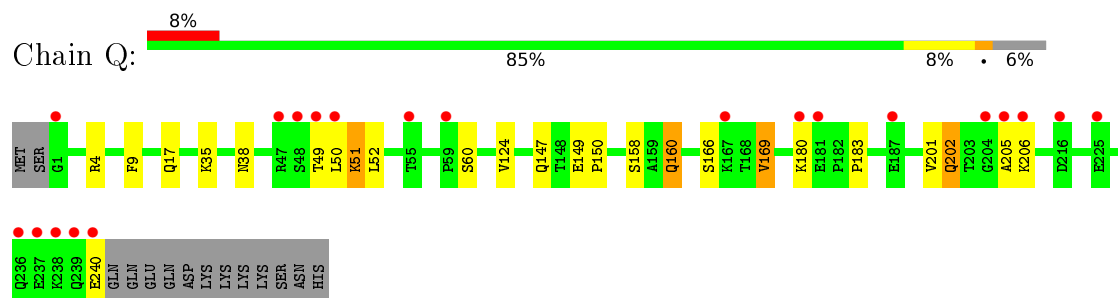
- Molecule 2: Proteasome subunit alpha type-3



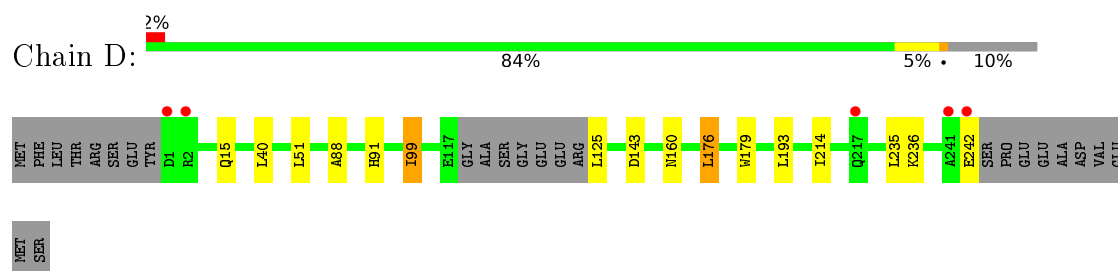
- Molecule 3: Proteasome subunit alpha type-4



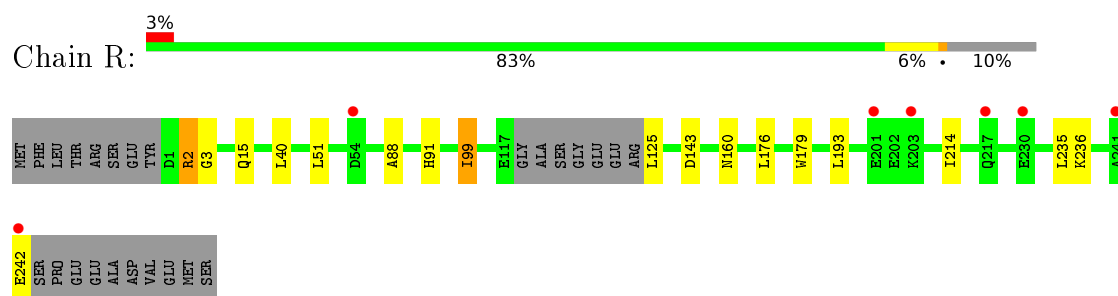
- Molecule 3: Proteasome subunit alpha type-4



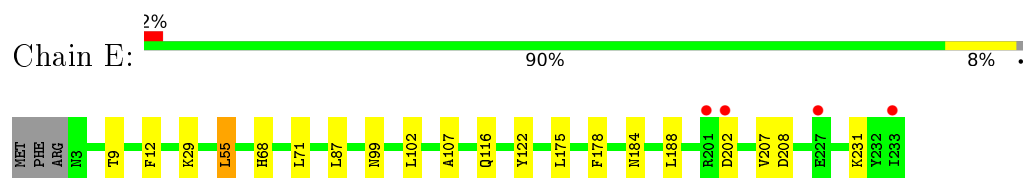
- Molecule 4: Proteasome subunit alpha type-5



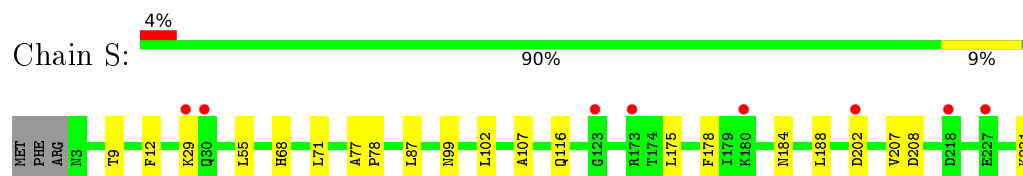
- Molecule 4: Proteasome subunit alpha type-5



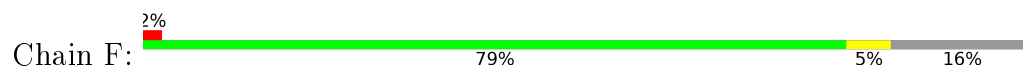
- Molecule 5: Proteasome subunit alpha type-6

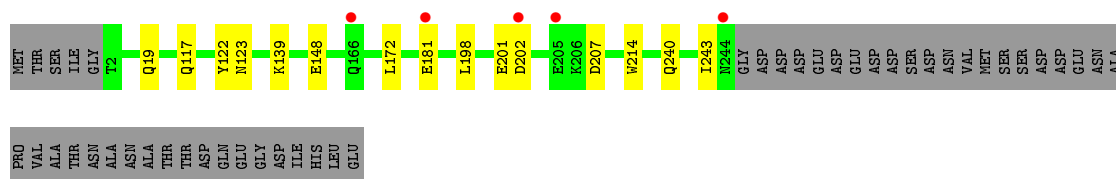


- Molecule 5: Proteasome subunit alpha type-6

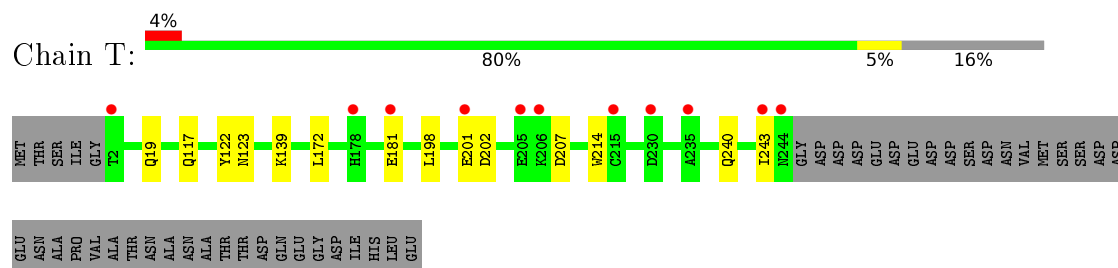


- Molecule 6: Probable proteasome subunit alpha type-7

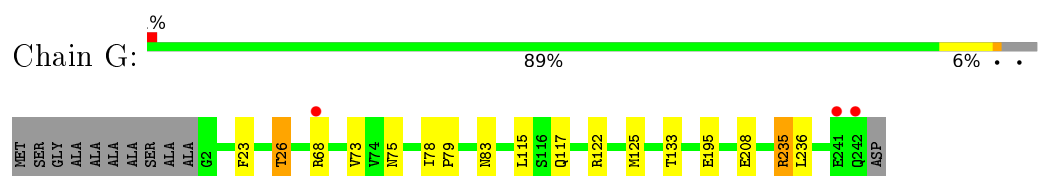




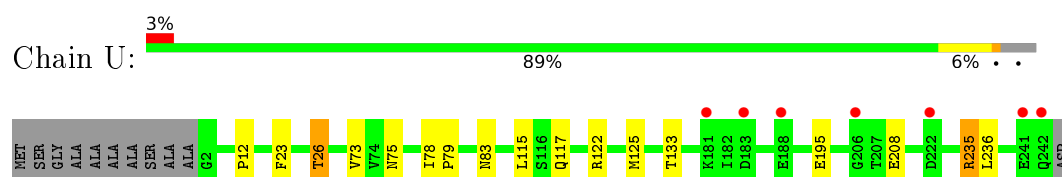
- Molecule 6: Probable proteasome subunit alpha type-7



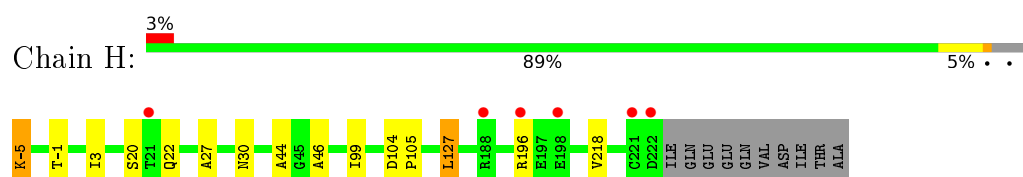
- Molecule 7: Proteasome subunit alpha type-1



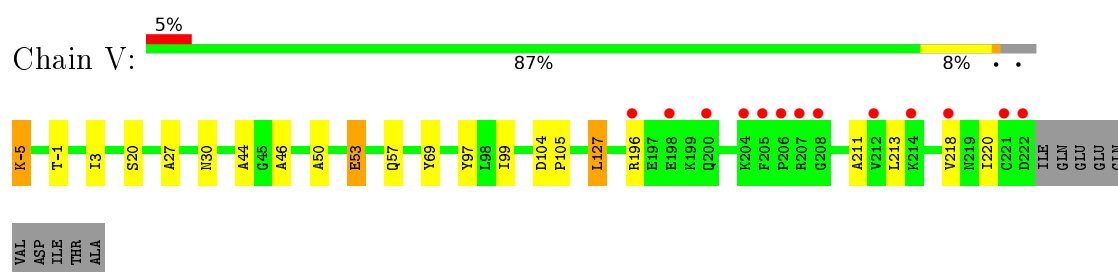
- Molecule 7: Proteasome subunit alpha type-1



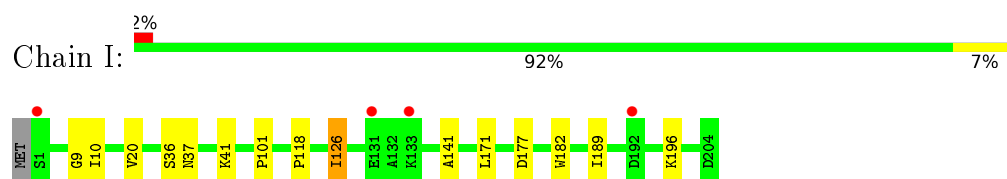
- Molecule 8: Proteasome subunit beta type-2



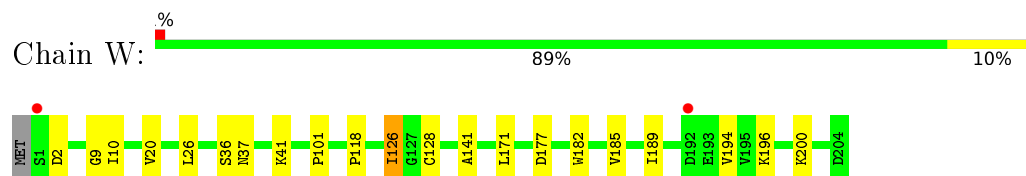
- Molecule 8: Proteasome subunit beta type-2



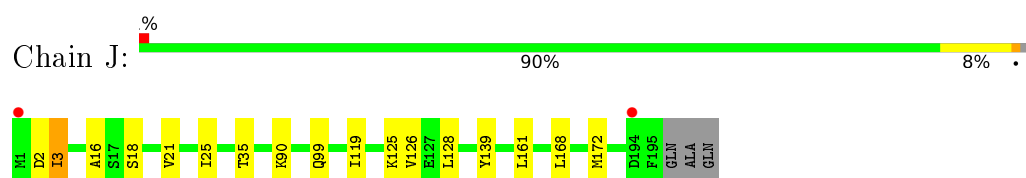
- Molecule 9: Proteasome subunit beta type-3



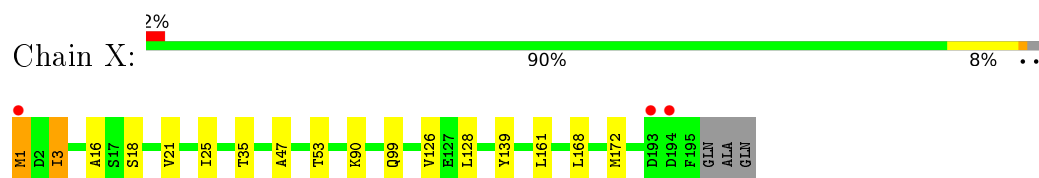
- Molecule 9: Proteasome subunit beta type-3



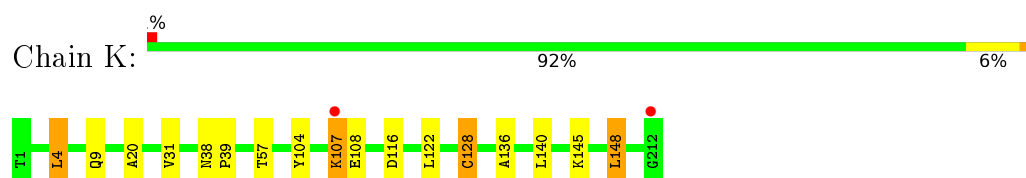
- Molecule 10: Proteasome subunit beta type-4



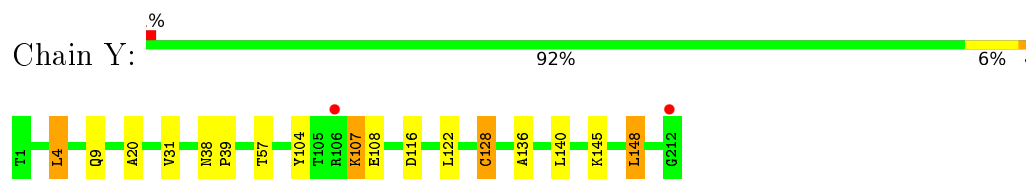
- Molecule 10: Proteasome subunit beta type-4



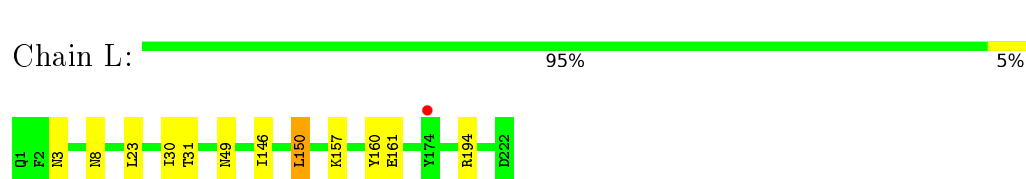
- Molecule 11: Proteasome subunit beta type-5



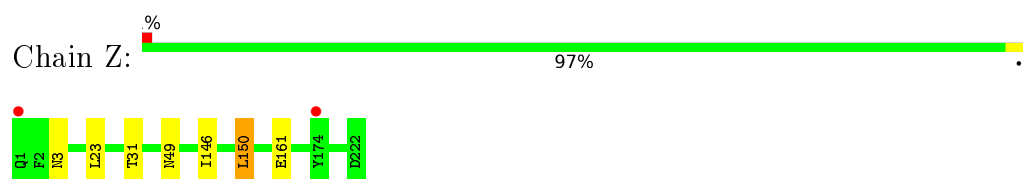
- Molecule 11: Proteasome subunit beta type-5



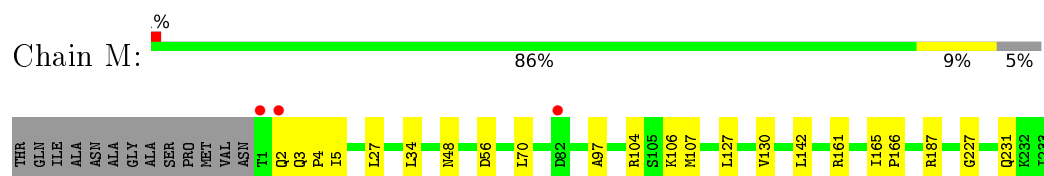
- Molecule 12: Proteasome subunit beta type-6



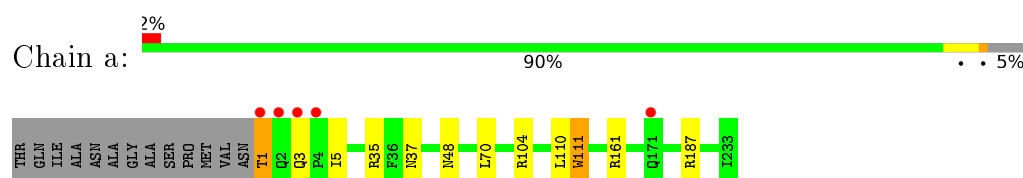
- Molecule 12: Proteasome subunit beta type-6



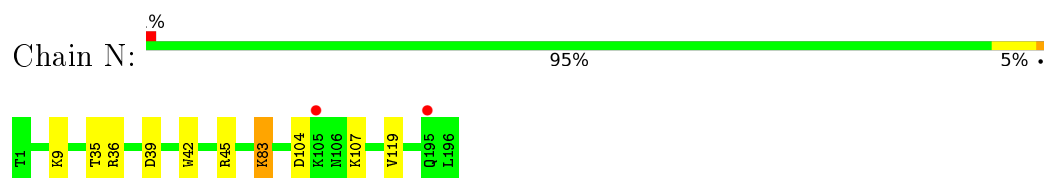
- Molecule 13: Proteasome subunit beta type-7



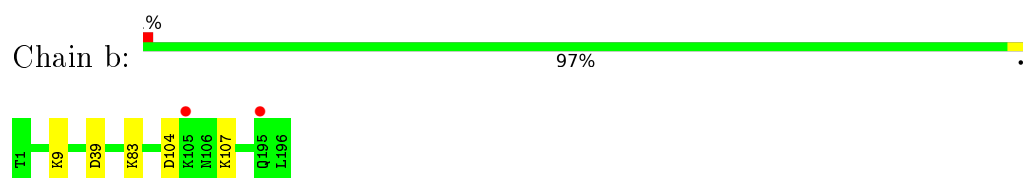
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.00Å 301.73Å 144.02Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 14.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.8 (15.00-2.70) 94.8 (14.99-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.206 , 0.231 0.211 , 0.234	Depositor DCC
R_{free} test set	13629 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 272577 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	49981	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/1952	0.47	0/2642
1	O	0.27	0/1952	0.47	0/2642
2	B	0.28	0/1934	0.50	0/2618
2	P	0.27	0/1934	0.50	0/2618
3	C	0.27	0/1910	0.51	0/2586
3	Q	0.27	0/1910	0.51	0/2586
4	D	0.27	0/1837	0.48	0/2475
4	R	0.27	0/1837	0.49	0/2475
5	E	0.27	0/1800	0.48	0/2433
5	S	0.27	0/1800	0.48	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.40	0/1751	0.49	0/2374
8	V	0.37	0/1751	0.48	0/2374
9	I	0.28	0/1611	0.48	0/2174
9	W	0.28	0/1611	0.49	0/2174
10	J	0.28	0/1589	0.49	0/2142
10	X	0.27	0/1589	0.49	0/2142
11	K	0.28	0/1681	0.49	1/2274 (0.0%)
11	Y	0.30	0/1681	0.50	1/2274 (0.0%)
12	L	0.31	0/1795	0.49	0/2420
12	Z	0.28	0/1795	0.49	0/2420
13	M	0.40	0/1855	0.54	1/2514 (0.0%)
13	a	0.66	2/1855 (0.1%)	0.73	4/2514 (0.2%)
14	N	0.26	0/1541	0.48	0/2087
14	b	0.26	0/1541	0.48	0/2087
All	All	0.31	2/50266 (0.0%)	0.50	7/67964 (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
13	a	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	111	TRP	C-N	-19.51	0.89	1.34
13	a	110	LEU	C-N	-12.91	1.04	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	110	LEU	O-C-N	-15.83	97.37	122.70
13	a	110	LEU	C-N-CA	13.24	154.80	121.70
13	a	110	LEU	CA-C-N	11.10	141.62	117.20
13	a	3	GLN	C-N-CD	5.97	140.94	128.40
13	M	3	GLN	C-N-CD	5.39	139.72	128.40
11	K	4	LEU	CA-CB-CG	5.06	126.94	115.30
11	Y	4	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	a	1	THR	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	1929	2	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1881	0	1895	9	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	5	0
8	H	1720	0	1726	14	0
8	V	1720	0	1726	27	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	16	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	12	0
11	K	1644	0	1595	6	0
11	Y	1644	0	1595	6	0
12	L	1757	0	1711	4	0
12	Z	1757	0	1711	1	0
13	M	1824	0	1832	7	0
13	a	1824	0	1830	0	0
14	N	1512	0	1481	5	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	1	0
17	A	17	0	0	0	0
17	B	16	0	0	0	0
17	C	22	0	0	0	0
17	D	20	0	0	0	0
17	E	16	0	0	0	0
17	F	20	0	0	1	0
17	G	35	0	0	0	0
17	H	22	0	0	1	0
17	I	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	J	18	0	0	0	0
17	K	23	0	0	0	0
17	L	31	0	0	0	0
17	M	28	0	0	0	0
17	N	25	0	0	0	0
17	O	17	0	0	0	0
17	P	12	0	0	0	0
17	Q	16	0	0	0	0
17	R	11	0	0	0	0
17	S	9	0	0	0	0
17	T	20	0	0	0	0
17	U	34	0	0	0	0
17	V	21	0	0	0	0
17	W	21	0	0	1	0
17	X	19	0	0	0	0
17	Y	22	0	0	0	0
17	Z	23	0	0	0	0
17	a	37	0	0	0	0
17	b	23	0	0	0	0
All	All	49981	0	49142	163	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 (163) 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:O	8:V:57:GLN:HG3	1.59	1.02
8:H:-5:LYS:HA	17:H:309:HOH:O	1.78	0.83
8:V:99:ILE:HG13	8:V:127:LEU:HD12	1.62	0.81
8:V:-5:LYS:HD2	17:W:420:HOH:O	1.83	0.78
10:X:1:MET:CE	10:X:53:THR:OG1	2.35	0.75
8:V:99:ILE:HG13	8:V:127:LEU:CD1	2.18	0.73
8:V:-5:LYS:NZ	9:W:2:ASP:OD1	2.22	0.72
8:V:3:ILE:CG2	8:V:44:ALA:HB1	2.21	0.71
8:V:3:ILE:HG21	8:V:44:ALA:HB1	1.74	0.68
8:H:46:ALA:HB3	8:H:127:LEU:HD23	1.75	0.66
10:X:1:MET:HE2	10:X:53:THR:OG1	1.95	0.66
10:X:1:MET:HE3	10:X:53:THR:OG1	1.97	0.64
8:H:46:ALA:HB3	8:H:127:LEU:CD2	2.28	0.62
8:H:-1:THR:OG1	8:H:20:SER:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:148:GLU:HG2	17:F:301:HOH:O	2.02	0.60
14:N:35:THR:HG21	14:N:45:ARG:HE	1.67	0.59
12:L:160:TYR:CD1	8:V:211:ALA:HB2	2.38	0.59
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.33	0.59
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.50	0.58
8:V:213:LEU:HG	9:W:200:LYS:HB2	1.86	0.57
5:S:12:PHE:H	6:T:19:GLN:HE22	1.53	0.57
2:B:12:PHE:H	3:C:17:GLN:HE22	1.52	0.57
2:P:217:LYS:C	2:P:219:ALA:H	2.08	0.57
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.35	0.57
2:B:217:LYS:C	2:B:219:ALA:H	2.07	0.56
8:V:213:LEU:HD21	9:W:200:LYS:HD2	1.87	0.56
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.04	0.56
8:V:3:ILE:CG2	8:V:44:ALA:CB	2.85	0.55
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.89	0.55
3:C:51:LYS:O	3:C:52:LEU:HB2	2.05	0.55
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.55
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.88	0.54
8:V:3:ILE:HG21	8:V:44:ALA:CB	2.35	0.54
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.89	0.54
13:M:4:PRO:HB3	13:M:56:ASP:HB2	1.90	0.53
10:J:25:ILE:O	10:X:139:TYR:OH	2.26	0.53
8:V:53:GLU:O	8:V:57:GLN:CG	2.47	0.53
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.74	0.53
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.91	0.53
16:U:301:CL:CL	8:V:69:TYR:OH	2.51	0.52
8:H:3:ILE:CG2	8:H:44:ALA:HB1	2.39	0.52
8:V:97:TYR:HB3	8:V:127:LEU:CD2	2.40	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.52
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.91	0.52
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.92	0.51
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.74	0.51
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.92	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.51
8:V:99:ILE:CG1	8:V:127:LEU:HD12	2.39	0.51
8:V:-1:THR:OG1	8:V:20:SER:HA	2.11	0.51
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.41	0.51
8:H:46:ALA:CB	8:H:127:LEU:HD23	2.41	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.49
5:E:12:PHE:H	6:F:19:GLN:HE22	1.61	0.49
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.49	0.48
7:U:23:PHE:O	7:U:26:THR:HB	2.14	0.48
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.96	0.48
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.96	0.48
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.96	0.47
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.96	0.47
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.96	0.47
2:B:219:ALA:HB2	2:B:225:TYR:HB2	1.96	0.47
4:R:2:ARG:O	4:R:3:GLY:C	2.53	0.47
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.97	0.47
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.97	0.47
11:K:128:CYS:SG	11:K:136:ALA:HB3	2.55	0.47
3:C:35:LYS:HG2	3:C:158:SER:O	2.15	0.47
2:P:219:ALA:HB2	2:P:225:TYR:HB2	1.96	0.47
8:V:3:ILE:HG23	8:V:44:ALA:HB1	1.96	0.47
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.96	0.47
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.51	0.46
8:V:97:TYR:HB3	8:V:127:LEU:HD22	1.96	0.46
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.45	0.46
8:H:3:ILE:CG2	8:H:44:ALA:CB	2.94	0.46
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.96	0.46
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.98	0.46
8:H:3:ILE:HG23	8:H:44:ALA:HB1	1.97	0.46
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.45	0.46
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.45	0.46
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.51	0.46
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.98	0.46
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.50	0.46
8:V:3:ILE:HD12	8:V:46:ALA:HB2	1.96	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.46
11:Y:128:CYS:SG	11:Y:136:ALA:HB3	2.56	0.46
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.98	0.46
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.98	0.45
14:N:35:THR:CG2	14:N:45:ARG:HE	2.30	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.99	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.99	0.45
13:M:106:LYS:O	13:M:107:MET:HB2	2.16	0.45
10:J:168:LEU:O	10:J:172:MET:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.16	0.45
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.99	0.45
10:J:139:TYR:OH	10:X:25:ILE:O	2.35	0.45
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.65	0.45
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.99	0.45
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.65	0.44
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.98	0.44
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.98	0.44
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.98	0.44
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.47	0.44
10:X:1:MET:HG3	10:X:47:ALA:HA	1.99	0.44
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.00	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.48	0.44
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.52	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.43
8:V:213:LEU:HD21	9:W:200:LYS:CD	2.48	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.53	0.43
7:G:73:VAL:HG12	7:G:133:THR:HB	1.99	0.43
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.00	0.43
7:U:73:VAL:HG12	7:U:133:THR:HB	2.00	0.43
5:E:68:HIS:HE1	5:E:102:LEU:O	2.02	0.43
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.01	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.42
10:X:168:LEU:O	10:X:172:MET:HB2	2.19	0.42
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.01	0.42
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.00	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.01	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.01	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.02	0.42
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.02	0.42
10:X:126:VAL:HG12	10:X:128:LEU:HG	2.02	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.02	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.41
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.50	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.02	0.41
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:195:GLU:HG3	7:G:235:ARG:HG3	2.02	0.41
8:V:220:ILE:HG21	9:W:194:VAL:HG21	2.02	0.41
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.86	0.41
7:U:195:GLU:HG3	7:U:235:ARG:HG3	2.02	0.41
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.21	0.41
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.41
13:M:227:GLY:HA3	13:M:231:GLN:HB3	2.03	0.41
8:V:213:LEU:HD11	9:W:200:LYS:HA	2.02	0.41
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.02	0.41
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.02	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.03	0.41
10:J:119:ILE:HG12	10:J:125:LYS:HG3	2.03	0.41
3:C:9:PHE:H	4:D:15:GLN:HE22	1.68	0.41
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.85	0.41
12:L:194:ARG:NH1	8:V:27:ALA:O	2.54	0.41
8:H:3:ILE:HG21	8:H:44:ALA:CB	2.51	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.40
8:H:3:ILE:HG21	8:H:44:ALA:HB1	2.03	0.40
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.01	0.40
3:Q:166:SER:HA	3:Q:169:VAL:HG13	2.03	0.40
5:S:68:HIS:HE1	5:S:102:LEU:O	2.03	0.40
3:C:166:SER:HA	3:C:169:VAL:HG13	2.02	0.40
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.40
2:B:217:LYS:C	2:B:219:ALA:N	2.74	0.40
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	69
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	39	69
2	B	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	11	29
2	P	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	11	29
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	15	37
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	15	37
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	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	226/238 (95%)	221 (98%)	5 (2%)	0	100	100
8	V	226/238 (95%)	220 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
13	a	231/246 (94%)	223 (96%)	6 (3%)	2 (1%)	21	49
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6288/6626 (95%)	6143 (98%)	127 (2%)	18 (0%)	46	75

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
1	O	2	THR
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
13	a	111	TRP
2	B	220	ASN
2	P	220	ASN
2	B	218	GLY
3	C	205	ALA
2	P	218	GLY
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO
13	a	5	ILE

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%)	205 (98%)	4 (2%)	65	88
1	O	209/209 (100%)	205 (98%)	4 (2%)	65	88
2	B	203/216 (94%)	196 (97%)	7 (3%)	44	75
2	P	203/216 (94%)	196 (97%)	7 (3%)	44	75
3	C	212/226 (94%)	200 (94%)	12 (6%)	25	53
3	Q	212/226 (94%)	200 (94%)	12 (6%)	25	53
4	D	194/215 (90%)	183 (94%)	11 (6%)	25	53
4	R	194/215 (90%)	182 (94%)	12 (6%)	23	49
5	E	190/193 (98%)	178 (94%)	12 (6%)	22	48
5	S	190/193 (98%)	178 (94%)	12 (6%)	22	48
6	F	201/239 (84%)	191 (95%)	10 (5%)	30	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	201/239 (84%)	191 (95%)	10 (5%)	30	60
7	G	206/210 (98%)	196 (95%)	10 (5%)	31	61
7	U	206/210 (98%)	196 (95%)	10 (5%)	31	61
8	H	184/193 (95%)	180 (98%)	4 (2%)	60	86
8	V	184/193 (95%)	179 (97%)	5 (3%)	52	82
9	I	172/173 (99%)	168 (98%)	4 (2%)	58	85
9	W	172/173 (99%)	168 (98%)	4 (2%)	58	85
10	J	173/175 (99%)	168 (97%)	5 (3%)	50	80
10	X	173/175 (99%)	168 (97%)	5 (3%)	50	80
11	K	169/169 (100%)	160 (95%)	9 (5%)	28	57
11	Y	169/169 (100%)	160 (95%)	9 (5%)	28	57
12	L	185/185 (100%)	178 (96%)	7 (4%)	40	71
12	Z	185/185 (100%)	179 (97%)	6 (3%)	46	77
13	M	199/208 (96%)	192 (96%)	7 (4%)	43	74
13	a	199/208 (96%)	191 (96%)	8 (4%)	38	69
14	N	162/162 (100%)	157 (97%)	5 (3%)	47	78
14	b	162/162 (100%)	157 (97%)	5 (3%)	47	78
All	All	5318/5546 (96%)	5102 (96%)	216 (4%)	37	69

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	55	LEU
2	B	79	LEU
2	B	113	ARG
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR

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Mol	Chain	Res	Type
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	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	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
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
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	240	GLN

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Mol	Chain	Res	Type
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	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	-5	LYS
8	H	30	ASN
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP
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	57	THR
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
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	150	LEU
12	L	157	LYS
12	L	161	GLU
13	M	2	GLN
13	M	5	ILE
13	M	48	ASN

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Mol	Chain	Res	Type
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	62	SER
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
2	P	113	ARG
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR
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	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	2	ARG
4	R	40	LEU
4	R	51	LEU
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

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Mol	Chain	Res	Type
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	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	-5	LYS
8	V	30	ASN
8	V	53	GLU
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU

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Mol	Chain	Res	Type
9	W	182	TRP
10	X	1	MET
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	57	THR
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
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	150	LEU
12	Z	161	GLU
13	a	1	THR
13	a	35	ARG
13	a	37	ASN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) 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

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Mol	Chain	Res	Type
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	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	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	66	HIS
8	H	116	HIS
9	I	37	ASN
9	I	203	GLN
10	J	55	GLN
10	J	146	HIS

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Mol	Chain	Res	Type
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	158	ASN
12	L	159	GLN
12	L	165	ASN
13	M	3	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
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	146	GLN
4	R	210	GLN
4	R	225	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	151	ASN
5	S	184	ASN
6	T	19	GLN

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Mol	Chain	Res	Type
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	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	116	HIS
9	W	37	ASN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
12	Z	159	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	a	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	110:LEU	C	111:TRP	N	1.04
1	a	111:TRP	C	112:ASN	N	0.89

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%)	-0.19	13 (5%)	31 30	33, 46, 82, 120	0
1	O	250/250 (100%)	-0.06	16 (6%)	23 21	39, 55, 98, 128	0
2	B	244/258 (94%)	-0.14	8 (3%)	50 50	35, 53, 92, 143	0
2	P	244/258 (94%)	-0.10	12 (4%)	33 32	41, 56, 95, 140	0
3	C	240/254 (94%)	-0.10	12 (5%)	32 31	35, 57, 111, 140	0
3	Q	240/254 (94%)	0.18	21 (8%)	12 10	38, 66, 145, 171	0
4	D	235/260 (90%)	-0.31	5 (2%)	67 68	36, 56, 86, 127	0
4	R	235/260 (90%)	-0.18	7 (2%)	54 54	37, 59, 99, 131	0
5	E	231/234 (98%)	-0.20	4 (1%)	73 74	35, 56, 91, 133	0
5	S	231/234 (98%)	-0.11	9 (3%)	43 43	43, 66, 101, 145	0
6	F	243/288 (84%)	-0.35	5 (2%)	67 68	35, 52, 101, 127	0
6	T	243/288 (84%)	-0.23	11 (4%)	37 36	36, 61, 108, 135	0
7	G	241/252 (95%)	-0.40	3 (1%)	81 81	30, 48, 78, 130	0
7	U	241/252 (95%)	-0.29	7 (2%)	55 55	38, 52, 81, 124	0
8	H	228/238 (95%)	0.02	6 (2%)	59 59	33, 49, 90, 121	0
8	V	228/238 (95%)	0.15	13 (5%)	27 26	34, 55, 100, 139	0
9	I	204/205 (99%)	-0.54	4 (1%)	68 69	31, 42, 69, 93	0
9	W	204/205 (99%)	-0.53	2 (0%)	84 85	32, 44, 70, 94	0
10	J	195/198 (98%)	-0.44	2 (1%)	84 85	33, 46, 72, 128	0
10	X	195/198 (98%)	-0.27	3 (1%)	76 76	35, 49, 73, 134	0
11	K	212/212 (100%)	-0.42	2 (0%)	85 86	27, 44, 63, 85	0
11	Y	212/212 (100%)	-0.46	2 (0%)	85 86	33, 47, 69, 91	0
12	L	222/222 (100%)	-0.39	1 (0%)	91 93	31, 45, 74, 111	0
12	Z	222/222 (100%)	-0.42	2 (0%)	85 86	33, 46, 76, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.52	3 (1%)	79 79	31, 46, 67, 83	0
13	a	233/246 (94%)	-0.38	5 (2%)	67 68	24, 45, 65, 84	0
14	N	196/196 (100%)	-0.49	2 (1%)	84 85	30, 41, 69, 94	0
14	b	196/196 (100%)	-0.45	2 (1%)	84 85	32, 43, 70, 100	0
All	All	6348/6626 (95%)	-0.26	182 (2%)	55 55	24, 51, 93, 171	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	220	ASN	7.5
3	Q	50	LEU	7.3
2	B	51	VAL	6.9
2	B	219	ALA	6.7
12	L	174	TYR	6.4
2	B	221	ASP	5.9
1	O	231	LYS	5.7
8	V	222	ASP	5.7
2	P	220	ASN	5.7
2	P	51	VAL	5.6
3	Q	49	THR	5.4
13	a	2	GLN	5.3
2	P	221	ASP	5.3
3	Q	236	GLN	5.2
1	A	231	LYS	5.2
13	a	1	THR	5.2
5	S	202	ASP	5.0
8	H	222	ASP	4.9
3	Q	240	GLU	4.8
4	R	241	ALA	4.7
1	A	2	THR	4.6
13	M	1	THR	4.6
5	E	202	ASP	4.5
3	C	206	LYS	4.5
1	A	229	THR	4.5
2	P	219	ALA	4.4
3	C	49	THR	4.4
1	O	249	ALA	4.3
1	O	2	THR	4.2
3	C	205	ALA	4.2
10	X	194	ASP	4.2
1	O	1	MET	4.1

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Mol	Chain	Res	Type	RSRZ
2	P	59	ASP	4.0
1	O	229	THR	4.0
5	S	173	ARG	4.0
1	A	1	MET	4.0
3	Q	206	LYS	3.9
9	W	1	SER	3.9
8	V	204	LYS	3.9
3	Q	205	ALA	3.9
12	Z	174	TYR	3.7
3	Q	225	GLU	3.7
1	O	52	SER	3.6
7	U	242	GLN	3.6
14	b	195	GLN	3.6
3	C	239	GLN	3.5
1	A	226	GLY	3.5
8	V	207	ARG	3.5
8	H	221	CYS	3.5
1	O	228	PRO	3.5
1	O	201	GLU	3.5
3	Q	237	GLU	3.5
14	b	105	LYS	3.5
1	A	250	LEU	3.5
2	P	225	TYR	3.4
3	C	240	GLU	3.4
8	H	198	GLU	3.4
8	V	221	CYS	3.3
3	Q	238	LYS	3.3
3	C	238	LYS	3.3
3	Q	180	LYS	3.3
6	F	181	GLU	3.3
10	J	194	ASP	3.3
2	P	222	GLY	3.2
3	C	235	GLU	3.2
14	N	195	GLN	3.2
4	D	242	GLU	3.2
1	O	53	SER	3.2
3	C	180	LYS	3.1
2	B	218	GLY	3.1
10	X	1	MET	3.1
3	Q	48	SER	3.1
6	T	244	ASN	3.1
1	O	227	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	236	GLN	3.1
13	a	3	GLN	3.1
1	O	250	LEU	3.1
2	P	218	GLY	3.0
9	I	133	LYS	3.0
1	A	203	GLU	3.0
1	A	249	ALA	3.0
1	A	230	ASP	2.9
3	Q	187	GLU	2.9
6	T	178	HIS	2.9
4	D	1	ASP	2.9
5	S	227	GLU	2.9
5	E	233	ILE	2.8
8	V	205	PHE	2.8
9	I	1	SER	2.8
6	T	243	ILE	2.8
13	M	2	GLN	2.8
8	V	206	PRO	2.8
4	R	203	LYS	2.8
8	V	198	GLU	2.8
6	T	2	THR	2.8
1	O	226	GLY	2.8
3	C	50	LEU	2.8
3	Q	204	GLY	2.8
5	S	233	ILE	2.8
14	N	105	LYS	2.8
1	O	62	SER	2.7
8	V	212	VAL	2.7
6	F	202	ASP	2.7
1	A	201	GLU	2.7
1	O	230	ASP	2.7
13	M	82	ASP	2.7
4	D	217	GLN	2.6
4	R	217	GLN	2.6
1	A	228	PRO	2.6
1	A	248	GLU	2.6
7	U	188	GLU	2.6
4	R	201	GLU	2.6
4	D	241	ALA	2.6
6	T	205	GLU	2.6
7	U	183	ASP	2.5
8	V	196	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
3	Q	239	GLN	2.5
7	G	242	GLN	2.5
5	E	201	ARG	2.5
6	T	206	LYS	2.5
1	O	203	GLU	2.5
2	B	217	LYS	2.5
4	R	54	ASP	2.5
3	C	216	ASP	2.5
10	X	193	ASP	2.5
8	V	208	GLY	2.4
2	P	52	THR	2.4
11	Y	106	ARG	2.4
9	I	131	GLU	2.4
1	A	227	ILE	2.4
3	Q	181	GLU	2.4
10	J	1	MET	2.4
6	T	215	CYS	2.4
8	V	218	VAL	2.3
3	Q	47	ARG	2.3
12	Z	1	GLN	2.3
5	S	180	LYS	2.3
7	U	181	LYS	2.3
5	E	227	GLU	2.3
3	Q	55	THR	2.3
7	G	68	ARG	2.3
1	O	221	LEU	2.3
6	F	244	ASN	2.3
11	Y	212	GLY	2.2
8	H	196	ARG	2.2
9	W	192	ASP	2.2
11	K	212	GLY	2.2
6	T	181	GLU	2.2
3	Q	59	PRO	2.2
3	Q	1	GLY	2.2
2	P	182	ASP	2.2
7	U	222	ASP	2.2
4	R	242	GLU	2.2
13	a	171	GLN	2.2
2	B	59	ASP	2.2
7	U	241	GLU	2.2
2	P	1	GLY	2.2
9	I	192	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
6	F	166	GLN	2.2
3	Q	216	ASP	2.2
5	S	218	ASP	2.2
6	F	205	GLU	2.1
6	T	201	GLU	2.1
6	T	230	ASP	2.1
13	a	4	PRO	2.1
7	U	206	GLY	2.1
8	V	200	GLN	2.1
11	K	107	LYS	2.1
5	S	30	GLN	2.1
8	H	21	THR	2.1
4	D	2	ARG	2.1
8	H	188	ARG	2.1
5	S	123	GLY	2.1
2	P	223	GLU	2.1
3	Q	167	LYS	2.1
5	S	29	LYS	2.1
4	R	230	GLU	2.1
3	C	202	GLN	2.0
8	V	214	LYS	2.0
6	T	235	ALA	2.0
2	B	50	LYS	2.0
7	G	241	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
15	MG	W	301	1/1	0.96	0.28	8.52	70,70,70,70	0
15	MG	Z	301	1/1	0.97	0.24	2.20	56,56,56,56	0
15	MG	I	301	1/1	0.97	0.16	0.72	54,54,54,54	0
15	MG	G	301	1/1	0.90	0.09	-1.20	44,44,44,44	0
15	MG	Y	301	1/1	0.98	0.08	-1.78	47,47,47,47	0
15	MG	K	301	1/1	0.98	0.07	-2.33	45,45,45,45	0
15	MG	N	201	1/1	0.99	0.04	-3.16	44,44,44,44	0
15	MG	V	301	1/1	0.99	0.04	-3.90	46,46,46,46	0
16	CL	G	302	1/1	0.99	0.10	-	30,30,30,30	0
16	CL	U	301	1/1	0.96	0.24	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.