Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 01:11 pm GMT

PDB ID	:	5CGF
Title	:	Yeast 20S proteasome beta5-G48C mutant
Authors	:	Dubiella, C.; Groll, M.
Deposited on	:	2015-07-09
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

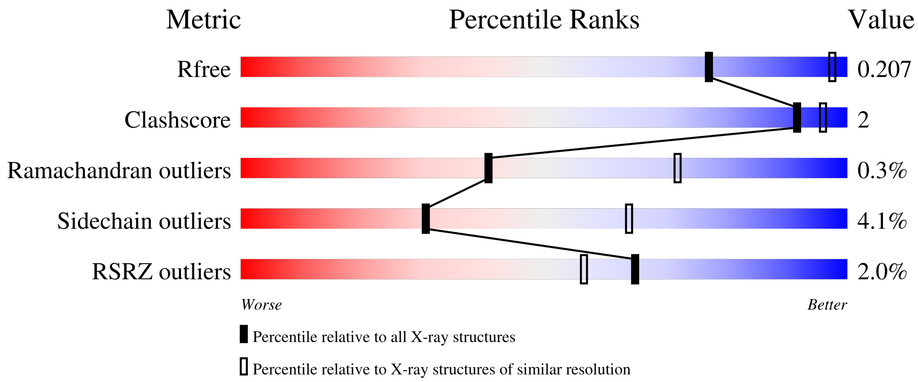
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	2% / 98% •
1	O	250	2% / 97% •
2	B	258	2% / 86% 9% 5%
2	P	258	3% / 86% 8% • 5%
3	C	254	4% / 86% 7% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	7% 86% 7% • 6%
4	D	260	% 85% 5% • 10%
4	R	260	2% 84% 5% • 10%
5	E	234	2% 90% 8% •
5	S	234	6% 89% 9% •
6	F	288	% 80% 5% 16%
6	T	288	% 80% 5% 16%
7	G	252	% 88% 8% •
7	U	252	% 89% 6% •
8	H	232	3% 89% 7% • •
8	V	232	3% 89% 7% • •
9	I	205	94% 6%
9	W	205	% 93% 6%
10	J	198	% 89% 8% • •
10	X	198	2% 90% 8% • •
11	K	212	92% 6% •
11	Y	212	92% 6% •
12	L	222	94% 5% •
12	Z	222	94% 5% •
13	M	246	88% 7% 5%
13	a	246	92% • 5%
14	N	196	% 94% 5% •
14	b	196	% 97% •

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49795 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 1915	C 1219	N 315	O 377	S 4	0	0	0
1	O	250	Total 1915	C 1219	N 315	O 377	S 4	0	0	0

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total 1904	C 1201	N 321	O 379	S 3	0	0	0
2	P	244	Total 1904	C 1201	N 321	O 379	S 3	0	0	0

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total 1881	C 1176	N 329	O 372	S 4	0	0	0
3	Q	240	Total 1881	C 1176	N 329	O 372	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total 1813	C 1136	N 304	O 366	S 7	0	0	0
4	R	235	Total 1813	C 1136	N 304	O 366	S 7	0	0	0

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total 1646	C 1046	N 280	O 312	S 8	0	0	0
11	Y	212	Total 1646	C 1046	N 280	O 312	S 8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	48	CYS	GLY	engineered mutation	UNP P30656
Y	48	CYS	GLY	engineered mutation	UNP P30656

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

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

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

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

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

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

- 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	I	2	Total Mg 2 2	0	0
15	K	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0
15	N	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

- 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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	12	Total O 12 12	0	0
17	B	12	Total O 12 12	0	0
17	C	15	Total O 15 15	0	0
17	D	7	Total O 7 7	0	0
17	E	6	Total O 6 6	0	0
17	F	13	Total O 13 13	0	0
17	G	19	Total O 19 19	0	0
17	H	19	Total O 19 19	0	0
17	I	16	Total O 16 16	0	0
17	J	13	Total O 13 13	0	0

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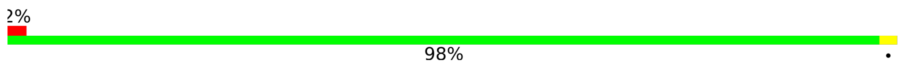
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	K	17	Total O 17 17	0	0
17	L	24	Total O 24 24	0	0
17	M	24	Total O 24 24	0	0
17	N	21	Total O 21 21	0	0
17	O	5	Total O 5 5	0	0
17	P	17	Total O 17 17	0	0
17	Q	11	Total O 11 11	0	0
17	R	10	Total O 10 10	0	0
17	S	8	Total O 8 8	0	0
17	T	9	Total O 9 9	0	0
17	U	18	Total O 18 18	0	0
17	V	16	Total O 16 16	0	0
17	W	12	Total O 12 12	0	0
17	X	13	Total O 13 13	0	0
17	Y	22	Total O 22 22	0	0
17	Z	16	Total O 16 16	0	0
17	a	21	Total O 21 21	0	0
17	b	20	Total O 20 20	0	0

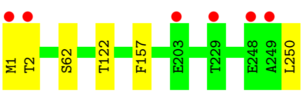
3 Residue-property plots (i)

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

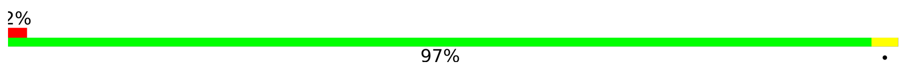
Chain A:

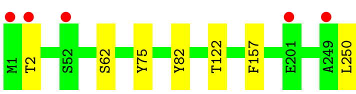




- Molecule 1: Proteasome subunit alpha type-2

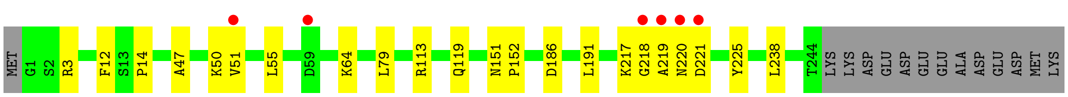
Chain O:





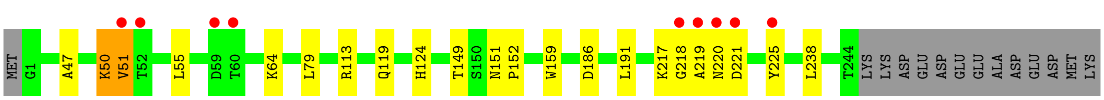
- Molecule 2: Proteasome subunit alpha type-3

Chain B:



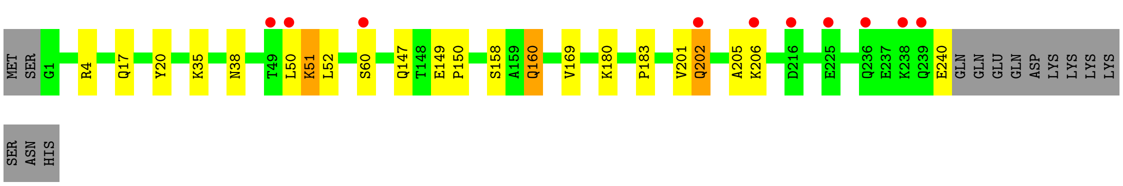
- Molecule 2: Proteasome subunit alpha type-3

Chain P:

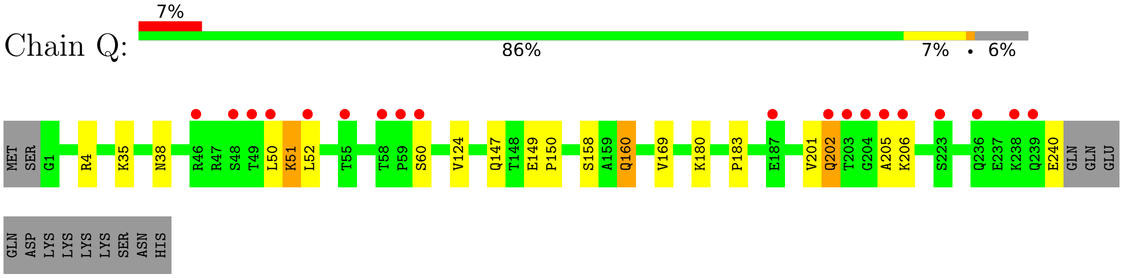


- Molecule 3: Proteasome subunit alpha type-4

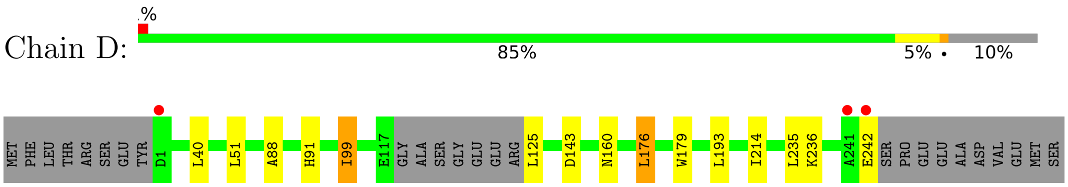
Chain C:



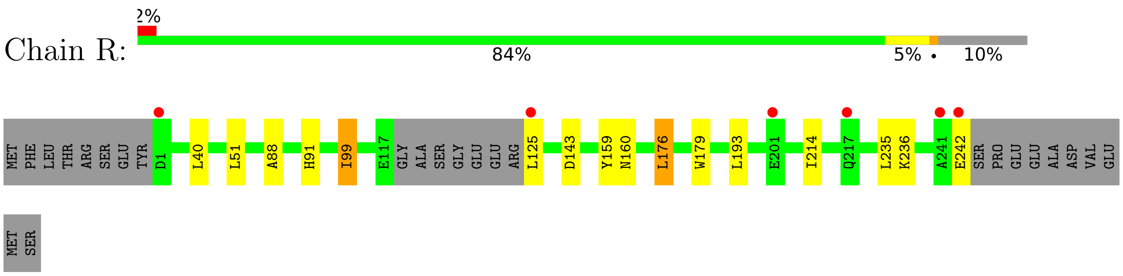
• Molecule 3: Proteasome subunit alpha type-4



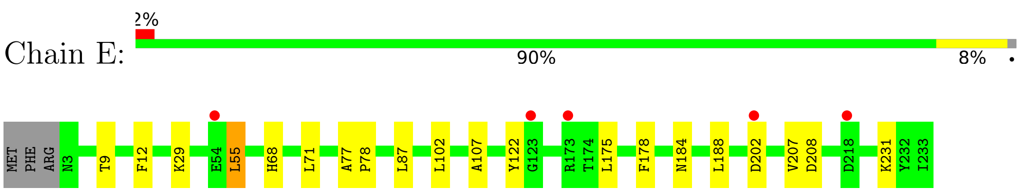
• Molecule 4: Proteasome subunit alpha type-5



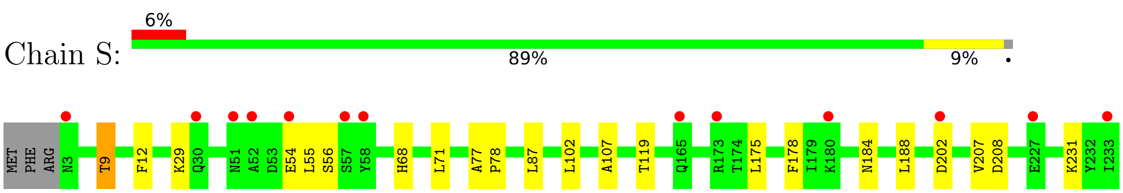
• Molecule 4: Proteasome subunit alpha type-5



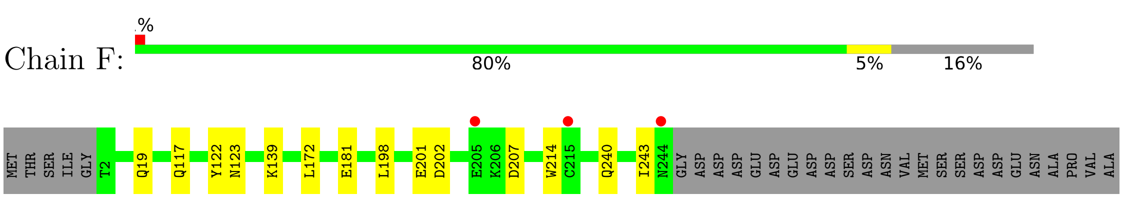
• Molecule 5: Proteasome subunit alpha type-6



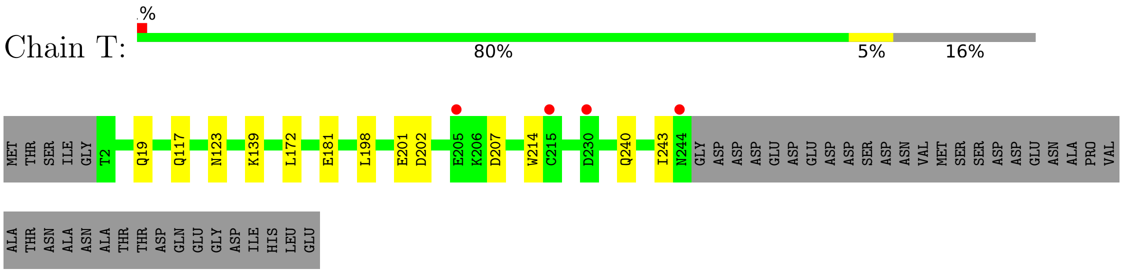
• Molecule 5: Proteasome subunit alpha type-6



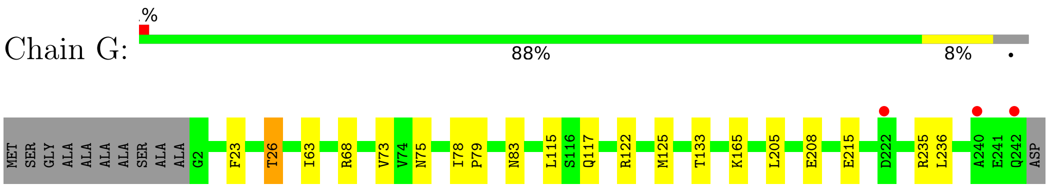
• Molecule 6: Probable proteasome subunit alpha type-7



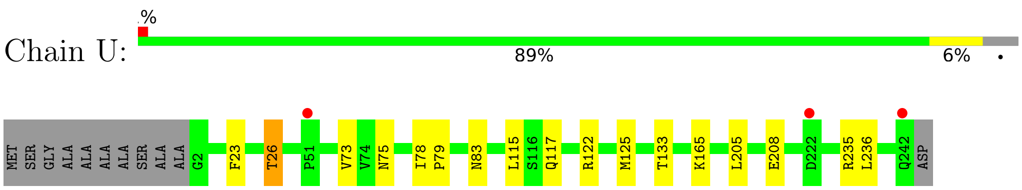
• Molecule 6: Probable proteasome subunit alpha type-7



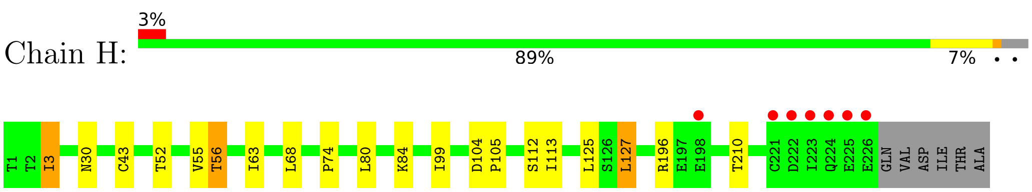
• Molecule 7: Proteasome subunit alpha type-1



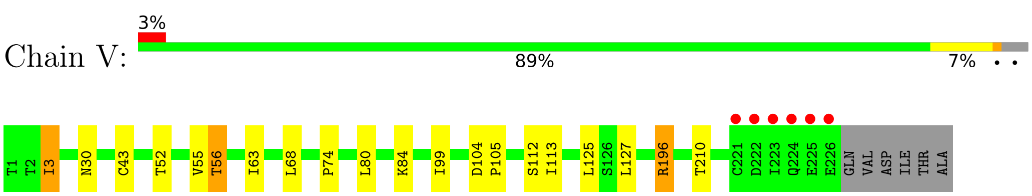
• Molecule 7: Proteasome subunit alpha type-1



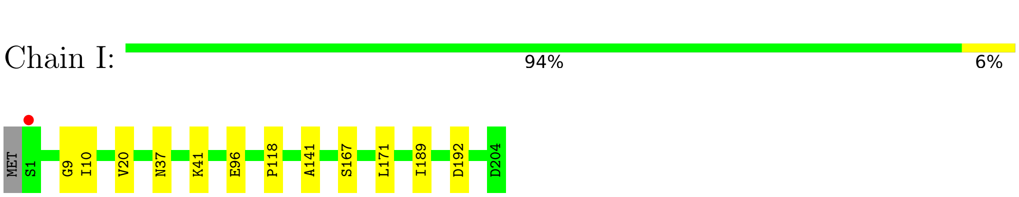
• Molecule 8: Proteasome subunit beta type-2



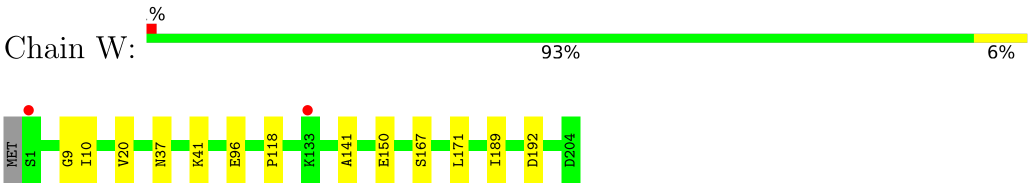
• Molecule 8: Proteasome subunit beta type-2



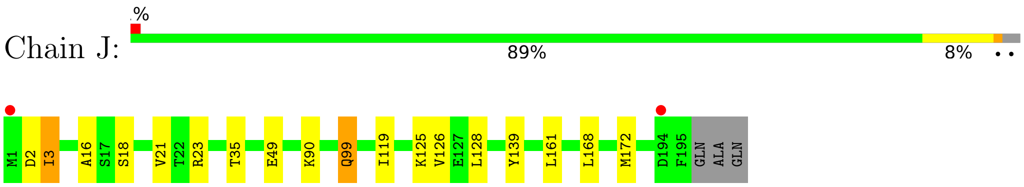
• Molecule 9: Proteasome subunit beta type-3



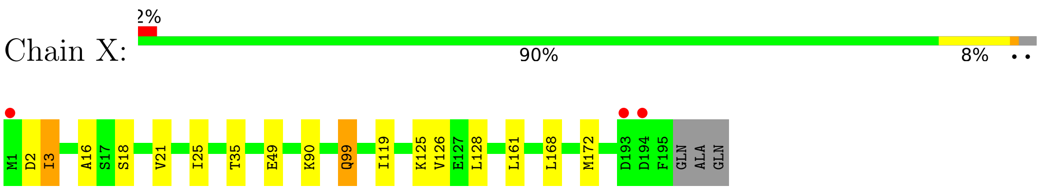
• Molecule 9: Proteasome subunit beta type-3



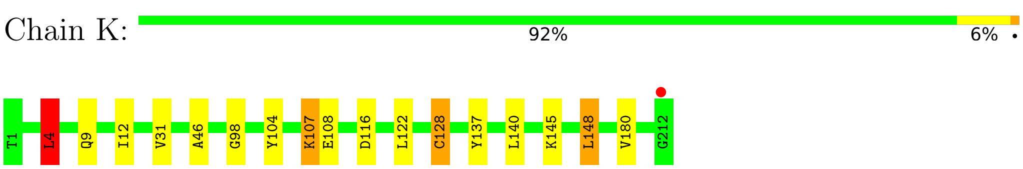
• Molecule 10: Proteasome subunit beta type-4



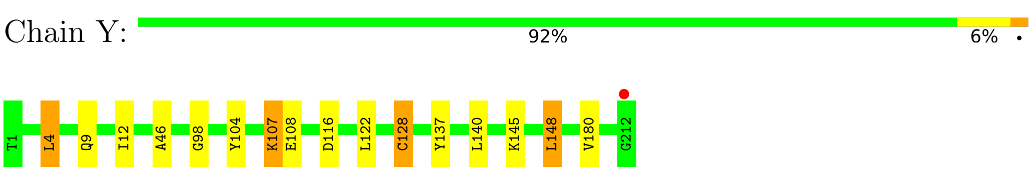
• Molecule 10: Proteasome subunit beta type-4



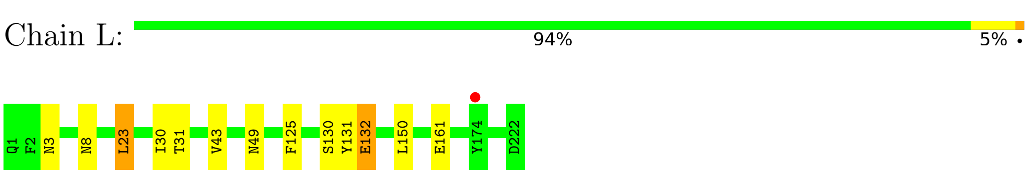
• Molecule 11: Proteasome subunit beta type-5



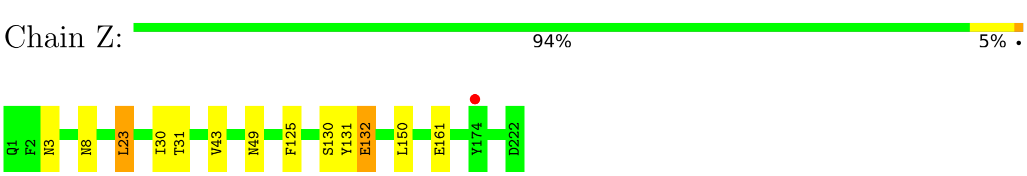
• Molecule 11: Proteasome subunit beta type-5



• Molecule 12: Proteasome subunit beta type-6

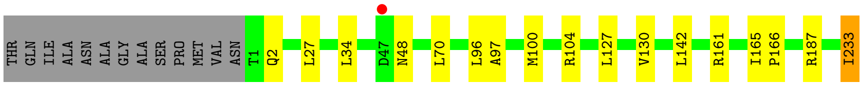


• Molecule 12: Proteasome subunit beta type-6



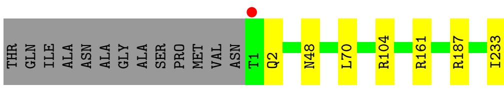
• Molecule 13: Proteasome subunit beta type-7

Chain M:



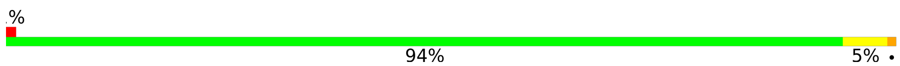
• Molecule 13: Proteasome subunit beta type-7

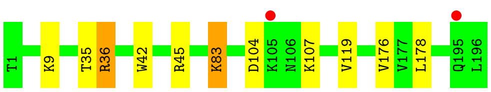
Chain a:



• Molecule 14: Proteasome subunit beta type-1

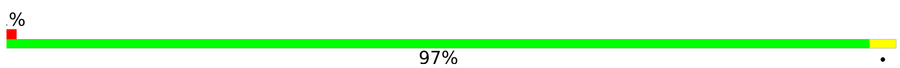
Chain N:

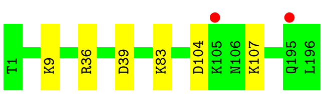




• Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.46Å 300.96Å 143.86Å 90.00° 112.88° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.80) 98.7 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.201 0.192 , 0.207	Depositor DCC
R_{free} test set	12725 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49795	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, MG

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	0.25	0/1952	0.47	0/2642
1	O	0.25	0/1952	0.47	0/2642
2	B	0.26	0/1934	0.50	0/2618
2	P	0.26	0/1934	0.50	0/2618
3	C	0.26	0/1910	0.51	0/2586
3	Q	0.26	0/1910	0.51	0/2586
4	D	0.25	0/1837	0.48	0/2475
4	R	0.25	0/1837	0.48	0/2475
5	E	0.25	0/1800	0.48	0/2433
5	S	0.25	0/1800	0.48	0/2433
6	F	0.26	0/1932	0.46	0/2609
6	T	0.25	0/1932	0.46	0/2609
7	G	0.26	0/1945	0.47	0/2634
7	U	0.26	0/1945	0.47	0/2634
8	H	0.28	0/1750	0.54	1/2373 (0.0%)
8	V	0.27	0/1750	0.52	0/2373
9	I	0.28	0/1611	0.54	0/2174
9	W	0.28	0/1611	0.54	0/2174
10	J	0.25	0/1589	0.48	0/2142
10	X	0.25	0/1589	0.48	0/2142
11	K	0.26	0/1683	0.53	1/2277 (0.0%)
11	Y	0.26	0/1683	0.53	1/2277 (0.0%)
12	L	0.30	0/1795	0.53	1/2420 (0.0%)
12	Z	0.30	0/1795	0.53	1/2420 (0.0%)
13	M	0.33	0/1855	0.54	0/2514
13	a	0.29	0/1855	0.54	0/2514
14	N	0.26	0/1541	0.51	0/2087
14	b	0.25	0/1541	0.51	0/2087
All	All	0.27	0/50268	0.50	5/67968 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Z	132	GLU	CB-CG-CD	5.32	128.55	114.20
12	L	132	GLU	CB-CG-CD	5.31	128.53	114.20
11	Y	4	LEU	CA-CB-CG	5.21	127.28	115.30
11	K	4	LEU	CA-CB-CG	5.19	127.23	115.30
8	H	127	LEU	CB-CG-CD2	-5.16	102.24	111.00

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	1	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	7	0
5	E	1773	0	1775	7	0
5	S	1773	0	1775	8	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	10	0
8	V	1719	0	1719	11	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	8	0
11	K	1646	0	1597	8	0
11	Y	1646	0	1597	6	0
12	L	1757	0	1711	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1757	0	1711	3	0
13	M	1824	0	1832	6	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	7	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	W	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
17	A	12	0	0	0	0
17	B	12	0	0	0	0
17	C	15	0	0	0	0
17	D	7	0	0	0	0
17	E	6	0	0	0	0
17	F	13	0	0	0	0
17	G	19	0	0	0	0
17	H	19	0	0	0	0
17	I	16	0	0	0	0
17	J	13	0	0	0	0
17	K	17	0	0	0	0
17	L	24	0	0	0	0
17	M	24	0	0	0	0
17	N	21	0	0	0	0
17	O	5	0	0	0	0
17	P	17	0	0	0	0
17	Q	11	0	0	0	0
17	R	10	0	0	0	0
17	S	8	0	0	0	0
17	T	9	0	0	0	0
17	U	18	0	0	0	0
17	V	16	0	0	0	0
17	W	12	0	0	0	0
17	X	13	0	0	0	0
17	Y	22	0	0	0	0
17	Z	16	0	0	0	0
17	a	21	0	0	0	0
17	b	20	0	0	0	0
All	All	49795	0	49134	140	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 (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:31:VAL:HA	12:L:132:GLU:OE1	1.87	0.73
8:V:52:THR:O	8:V:56:THR:OG1	2.11	0.68
8:H:52:THR:O	8:H:56:THR:OG1	2.12	0.67
13:M:233:ILE:OXT	13:M:233:ILE:HG13	1.98	0.62
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.46	0.62
2:B:12:PHE:H	3:C:17:GLN:HE22	1.51	0.58
8:H:43:CYS:SG	8:H:56:THR:CG2	2.92	0.58
8:V:43:CYS:SG	8:V:56:THR:CG2	2.93	0.57
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.36	0.56
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.86	0.56
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.87	0.56
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.88	0.56
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.89	0.54
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.07	0.54
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.90	0.53
14:N:35:THR:HG21	14:N:45:ARG:HE	1.72	0.53
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.90	0.53
2:P:217:LYS:C	2:P:219:ALA:H	2.12	0.53
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.74	0.53
3:C:51:LYS:O	3:C:52:LEU:HB2	2.07	0.53
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
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.74	0.52
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.92	0.52
2:B:217:LYS:C	2:B:219:ALA:H	2.12	0.52
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.92	0.52
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.92	0.51
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.93	0.51
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.93	0.50
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.47	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.13	0.49
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.93	0.49
14:N:35:THR:CG2	14:N:45:ARG:HE	2.26	0.49
7:U:23:PHE:O	7:U:26:THR:HB	2.13	0.48
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.95	0.48
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.94	0.48
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.96	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.96	0.47
3:C:35:LYS:HG2	3:C:158:SER:O	2.14	0.47
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.96	0.47
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.15	0.47
8:H:43:CYS:SG	8:H:56:THR:HG21	2.54	0.47
12:L:8:ASN:HA	12:L:30:ILE:O	2.15	0.47
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.96	0.47
4:R:176:LEU:HD11	5:S:54:GLU:HB2	1.96	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.46
5:S:12:PHE:H	6:T:19:GLN:HE22	1.62	0.46
8:V:43:CYS:SG	8:V:56:THR:HG21	2.56	0.46
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.45	0.46
8:H:3:ILE:HG13	8:H:99:ILE:HD12	1.98	0.46
2:P:149:THR:HG1	2:P:159:TRP:HE1	1.63	0.46
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.45	0.46
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.15	0.46
8:V:3:ILE:HG13	8:V:99:ILE:HD12	1.97	0.46
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.97	0.46
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.15	0.46
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.97	0.46
11:K:46:ALA:HB3	11:K:98:GLY:O	2.15	0.46
7:U:73:VAL:HG12	7:U:133:THR:HB	1.97	0.46
13:M:96:LEU:O	13:M:100:MET:HG2	2.16	0.45
7:G:73:VAL:HG12	7:G:133:THR:HB	1.97	0.45
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.17	0.45
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.51	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.52	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.45
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.99	0.45
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.99	0.45
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.99	0.45
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.99	0.45
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.52	0.45
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.99	0.44
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.99	0.44
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.47	0.44
12:L:23:LEU:HD13	12:L:43:VAL:HG13	2.00	0.44
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.53	0.44
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.53	0.43
10:J:168:LEU:O	10:J:172:MET:HB2	2.18	0.43
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.48	0.43
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.53	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.43
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.01	0.43
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.54	0.43
5:E:12:PHE:H	6:F:19:GLN:HE22	1.66	0.43
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.00	0.43
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.48	0.43
14:N:83:LYS:HG3	14:N:119:VAL:HG22	2.00	0.43
6:T:198:LEU:HD12	6:T:243:ILE:HG22	2.00	0.43
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.01	0.43
5:E:68:HIS:HE1	5:E:102:LEU:O	2.02	0.43
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.54	0.42
2:B:219:ALA:HB2	2:B:225:TYR:HB2	2.01	0.42
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.01	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.42
5:S:68:HIS:HE1	5:S:102:LEU:O	2.02	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
11:K:4:LEU:HB3	11:K:128:CYS:SG	2.60	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
8:V:84:LYS:HA	8:V:113:ILE:HD11	2.02	0.42
10:X:168:LEU:O	10:X:172:MET:HB2	2.19	0.42
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.02	0.42
8:H:84:LYS:HA	8:H:113:ILE:HD11	2.02	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.02	0.42
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.02	0.41
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.41
10:J:139:TYR:OH	10:X:25:ILE:O	2.38	0.41
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.55	0.41
10:X:49:GLU:HB2	10:X:99:GLN:HB3	2.02	0.41
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.02	0.41
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.54	0.41
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.41
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.56	0.41
10:J:49:GLU:HB2	10:J:99:GLN:HB3	2.02	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
8:V:210:THR:HG21	9:W:167:SER:HB3	2.01	0.41
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.03	0.41
2:B:217:LYS:C	2:B:219:ALA:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.03	0.41
10:J:119:ILE:HG12	10:J:125:LYS:HG3	2.02	0.41
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.03	0.41
2:P:219:ALA:HB2	2:P:225:TYR:HB2	2.01	0.41
10:X:126:VAL:HG12	10:X:128:LEU:HG	2.02	0.41
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.03	0.41
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.56	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.58	0.41
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.03	0.40
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.51	0.40
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.03	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.85	0.40
5:E:77:ALA:N	5:E:78:PRO:CD	2.85	0.40
10:J:23:ARG:HD3	10:J:23:ARG:HA	1.89	0.40
11:K:12:ILE:HB	11:K:180:VAL:HB	2.03	0.40
7:G:63:ILE:HD12	7:G:215:GLU:HG2	2.04	0.40
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.56	0.40
5:S:9:THR:HG21	5:S:119:THR:HA	2.03	0.40
10:X:119:ILE:HG12	10:X:125:LYS:HG3	2.03	0.40
8:H:210:THR:HG21	9:I:167:SER:HB3	2.04	0.40
8:V:196:ARG:HH22	9:W:150:GLU:HG3	1.87	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	66
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	66
2	B	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	29
2	P	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	36
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	36
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%)	221 (96%)	8 (4%)	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	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%)	196 (97%)	6 (3%)	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%)	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%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
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	6284/6614 (95%)	6133 (98%)	135 (2%)	16 (0%)	41	72

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP

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Mol	Chain	Res	Type
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	220	ASN
1	O	2	THR
2	P	218	GLY
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
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	85
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	85
2	B	203/216 (94%)	195 (96%)	8 (4%)	32	66
2	P	203/216 (94%)	195 (96%)	8 (4%)	32	66
3	C	212/226 (94%)	201 (95%)	11 (5%)	23	55
3	Q	212/226 (94%)	201 (95%)	11 (5%)	23	55
4	D	194/215 (90%)	183 (94%)	11 (6%)	20	50
4	R	194/215 (90%)	183 (94%)	11 (6%)	20	50
5	E	190/193 (98%)	180 (95%)	10 (5%)	22	54
5	S	190/193 (98%)	180 (95%)	10 (5%)	22	54
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	56
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	56
7	G	206/210 (98%)	196 (95%)	10 (5%)	25	57
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	57
8	H	185/190 (97%)	177 (96%)	8 (4%)	29	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	185/190 (97%)	177 (96%)	8 (4%)	29	62
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	82
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	82
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	76
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	76
11	K	170/170 (100%)	162 (95%)	8 (5%)	26	59
11	Y	170/170 (100%)	162 (95%)	8 (5%)	26	59
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	67
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29	62
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	70
13	a	199/208 (96%)	192 (96%)	7 (4%)	36	70
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	74
14	b	162/162 (100%)	156 (96%)	6 (4%)	34	68
All	All	5322/5542 (96%)	5104 (96%)	218 (4%)	30	64

All (218) 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	119	GLN
2	B	186	ASP
2	B	191	LEU
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

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	3	ILE
8	H	30	ASN
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	80	LEU
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	96	GLU
9	I	171	LEU
9	I	192	ASP
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	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	130	SER
12	L	150	LEU
12	L	161	GLU
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	233	ILE

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Mol	Chain	Res	Type
14	N	9	LYS
14	N	36	ARG
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	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	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
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU

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Mol	Chain	Res	Type
5	S	71	LEU
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	3	ILE
8	V	30	ASN
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	80	LEU
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	96	GLU
9	W	171	LEU
9	W	192	ASP
10	X	2	ASP
10	X	3	ILE
10	X	35	THR

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Mol	Chain	Res	Type
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
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	130	SER
12	Z	132	GLU
12	Z	150	LEU
12	Z	161	GLU
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	233	ILE
14	b	9	LYS
14	b	36	ARG
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN

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Mol	Chain	Res	Type
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
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	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	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

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Mol	Chain	Res	Type
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	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	146	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
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN

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Mol	Chain	Res	Type
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	22	GLN
8	V	30	ASN
8	V	66	HIS
8	V	116	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
10	X	55	GLN
10	X	146	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	190	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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 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, 95^{th} 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%)	-0.43	6 (2%)	59	49	36, 49, 84, 123	0
1	O	250/250 (100%)	-0.34	5 (2%)	65	56	41, 58, 103, 133	0
2	B	244/258 (94%)	-0.30	6 (2%)	57	47	37, 56, 98, 148	0
2	P	244/258 (94%)	-0.25	9 (3%)	41	31	41, 59, 101, 147	0
3	C	240/254 (94%)	-0.24	10 (4%)	36	26	37, 60, 122, 150	0
3	Q	240/254 (94%)	0.08	19 (7%)	12	7	45, 74, 159, 189	0
4	D	235/260 (90%)	-0.38	3 (1%)	77	72	42, 61, 95, 137	0
4	R	235/260 (90%)	-0.27	6 (2%)	56	46	44, 67, 109, 148	0
5	E	231/234 (98%)	-0.32	5 (2%)	62	52	45, 64, 102, 147	0
5	S	231/234 (98%)	-0.05	13 (5%)	24	16	47, 76, 122, 167	0
6	F	243/288 (84%)	-0.47	3 (1%)	79	73	39, 57, 110, 138	0
6	T	243/288 (84%)	-0.32	4 (1%)	72	66	43, 69, 125, 158	0
7	G	241/252 (95%)	-0.50	3 (1%)	79	73	32, 52, 85, 137	0
7	U	241/252 (95%)	-0.42	3 (1%)	79	73	40, 56, 86, 132	0
8	H	226/232 (97%)	-0.42	7 (3%)	49	39	33, 50, 82, 147	0
8	V	226/232 (97%)	-0.38	6 (2%)	54	44	38, 51, 83, 162	0
9	I	204/205 (99%)	-0.73	1 (0%)	91	88	34, 46, 70, 94	0
9	W	204/205 (99%)	-0.68	2 (0%)	82	77	35, 46, 75, 100	0
10	J	195/198 (98%)	-0.55	2 (1%)	82	77	34, 49, 74, 129	0
10	X	195/198 (98%)	-0.54	3 (1%)	73	68	34, 50, 73, 135	0
11	K	212/212 (100%)	-0.62	1 (0%)	91	88	30, 46, 67, 87	0
11	Y	212/212 (100%)	-0.60	1 (0%)	91	88	36, 49, 72, 93	0
12	L	222/222 (100%)	-0.58	1 (0%)	91	88	36, 51, 79, 114	0
12	Z	222/222 (100%)	-0.61	1 (0%)	91	88	35, 50, 82, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.68	1 (0%)	92	91	32, 49, 72, 88	0
13	a	233/246 (94%)	-0.64	1 (0%)	92	91	32, 48, 70, 86	0
14	N	196/196 (100%)	-0.70	2 (1%)	82	77	32, 43, 71, 98	0
14	b	196/196 (100%)	-0.67	2 (1%)	82	77	34, 45, 71, 104	0
All	All	6344/6614 (95%)	-0.44	126 (1%)	65	56	30, 54, 102, 189	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	9.2
2	P	219	ALA	7.7
3	Q	50	LEU	7.7
8	V	224	GLN	7.4
2	B	221	ASP	6.4
2	P	221	ASP	6.1
8	V	226	GLU	5.6
2	B	51	VAL	5.3
4	R	241	ALA	5.3
2	P	220	ASN	5.3
8	V	222	ASP	5.0
8	H	224	GLN	4.9
2	B	220	ASN	4.7
3	Q	236	GLN	4.7
5	S	202	ASP	4.7
8	H	226	GLU	4.7
1	O	2	THR	4.7
2	P	51	VAL	4.7
3	C	49	THR	4.5
8	V	223	ILE	4.5
2	B	219	ALA	4.5
7	U	242	GLN	4.5
3	C	50	LEU	4.5
8	H	222	ASP	4.4
10	J	1	MET	4.3
3	Q	206	LYS	4.3
3	C	206	LYS	4.2
3	Q	205	ALA	4.2
1	A	2	THR	4.1
1	O	1	MET	4.1
8	V	221	CYS	4.1
9	W	1	SER	4.0

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Mol	Chain	Res	Type	RSRZ
3	Q	48	SER	4.0
12	L	174	TYR	4.0
2	P	59	ASP	3.8
6	F	205	GLU	3.6
10	X	1	MET	3.6
11	Y	212	GLY	3.6
1	A	1	MET	3.5
1	O	249	ALA	3.5
1	O	52	SER	3.5
9	I	1	SER	3.5
8	H	223	ILE	3.5
10	X	194	ASP	3.5
3	Q	204	GLY	3.4
8	H	221	CYS	3.4
2	P	218	GLY	3.3
3	C	238	LYS	3.3
14	b	195	GLN	3.3
8	V	225	GLU	3.2
2	P	52	THR	3.2
14	b	105	LYS	3.1
3	Q	238	LYS	3.1
3	Q	239	GLN	3.0
1	A	249	ALA	3.0
5	S	227	GLU	3.0
12	Z	174	TYR	3.0
4	R	201	GLU	3.0
7	G	222	ASP	2.9
5	S	52	ALA	2.9
2	B	59	ASP	2.9
10	X	193	ASP	2.9
14	N	195	GLN	2.9
2	B	218	GLY	2.9
11	K	212	GLY	2.9
5	E	202	ASP	2.8
3	Q	59	PRO	2.8
5	S	173	ARG	2.8
10	J	194	ASP	2.7
3	C	216	ASP	2.7
5	S	180	LYS	2.7
6	T	244	ASN	2.7
7	U	222	ASP	2.6
7	G	242	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
9	W	133	LYS	2.6
5	E	54	GLU	2.6
3	Q	60	SER	2.5
6	F	215	CYS	2.5
4	D	241	ALA	2.5
3	Q	223	SER	2.5
3	Q	55	THR	2.4
3	C	225	GLU	2.4
5	S	51	ASN	2.4
5	S	165	GLN	2.4
1	A	248	GLU	2.4
3	Q	187	GLU	2.4
5	E	218	ASP	2.4
6	F	244	ASN	2.4
5	S	54	GLU	2.4
5	S	3	ASN	2.4
14	N	105	LYS	2.4
4	R	217	GLN	2.3
1	A	229	THR	2.3
7	G	240	ALA	2.3
4	R	242	GLU	2.3
1	A	203	GLU	2.3
3	Q	202	GLN	2.3
6	T	215	CYS	2.2
2	P	60	THR	2.2
8	H	198	GLU	2.2
5	S	57	SER	2.2
2	P	225	TYR	2.2
3	Q	203	THR	2.2
4	R	1	ASP	2.2
8	H	225	GLU	2.2
4	D	1	ASP	2.2
13	M	47	ASP	2.2
5	S	233	ILE	2.2
5	S	30	GLN	2.2
5	E	173	ARG	2.2
4	R	125	LEU	2.2
3	C	236	GLN	2.2
3	C	239	GLN	2.2
4	D	242	GLU	2.2
5	E	123	GLY	2.1
3	Q	52	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	60	SER	2.1
6	T	230	ASP	2.1
3	Q	58	THR	2.1
1	O	201	GLU	2.1
3	C	202	GLN	2.0
13	a	1	THR	2.0
7	U	51	PRO	2.0
3	Q	46	ARG	2.0
5	S	58	TYR	2.0
6	T	205	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	W	301	1/1	0.94	0.27	50,50,50,50	0
15	MG	Z	301	1/1	0.94	0.36	60,60,60,60	0
15	MG	N	201	1/1	0.95	0.12	51,51,51,51	0
15	MG	L	301	1/1	0.97	0.08	63,63,63,63	0
15	MG	G	301	1/1	0.98	0.04	47,47,47,47	0
15	MG	I	302	1/1	0.98	0.07	53,53,53,53	0
15	MG	I	301	1/1	0.99	0.19	63,63,63,63	0
15	MG	K	301	1/1	0.99	0.09	45,45,45,45	0
16	CL	G	302	1/1	0.99	0.12	37,37,37,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.