Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 03:49 AM EDT

PDB ID	:	4QV4
Title	:	yCP beta5-M45T mutant
Authors	:	Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on	:	2014-07-14
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
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:

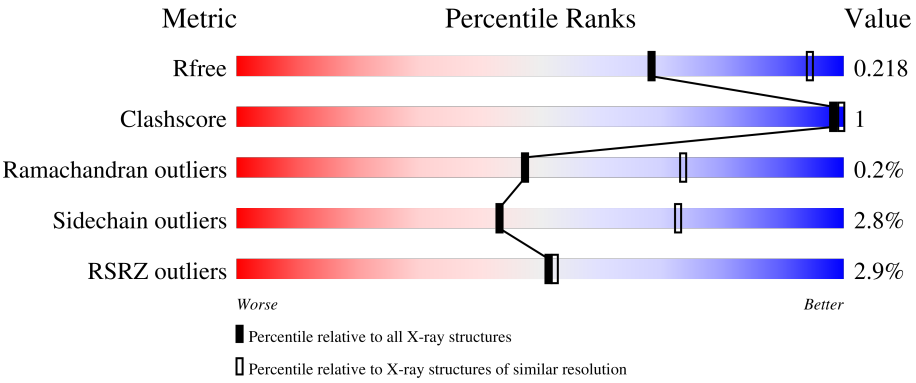
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	4% 98% ·
1	O	250	4% 98% ·
2	B	258	3% 90% 5% 5%
2	P	258	5% 90% · 5%
3	C	254	7% 87% 6% · 6%

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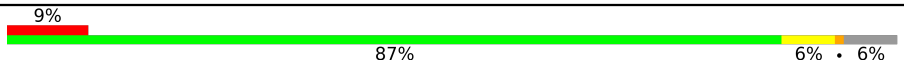
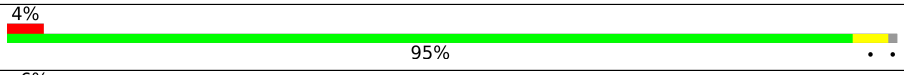
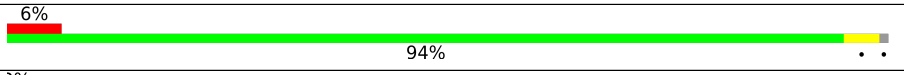
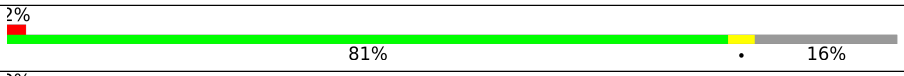
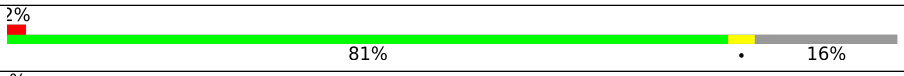
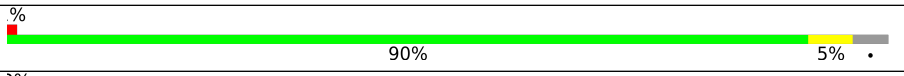
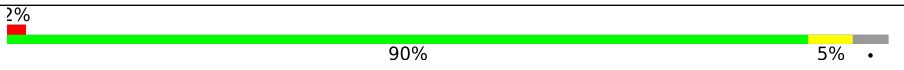
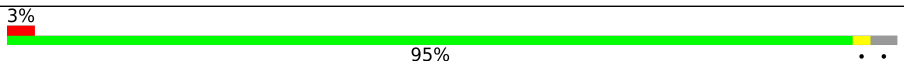
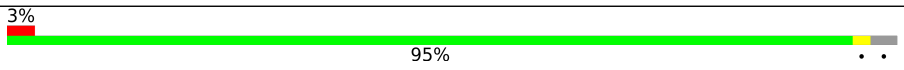
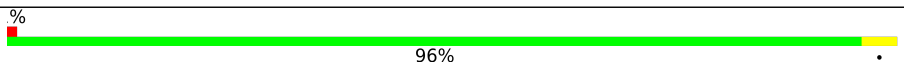
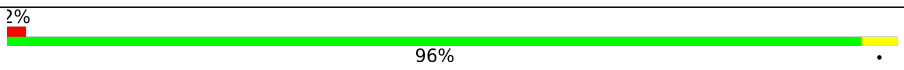
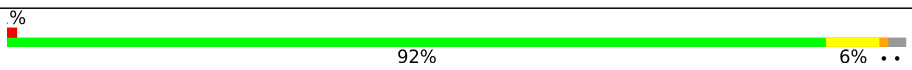
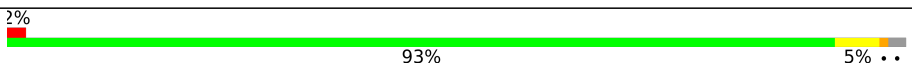
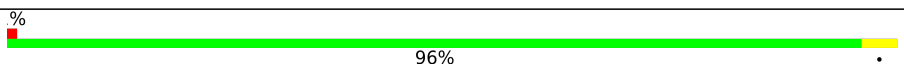
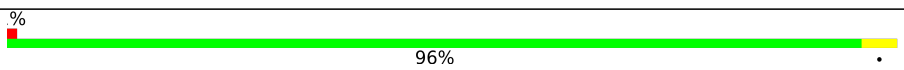
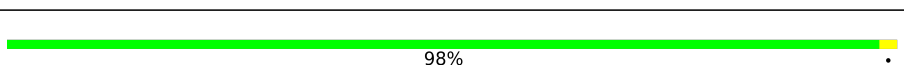
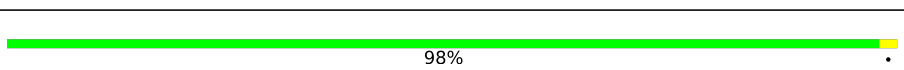
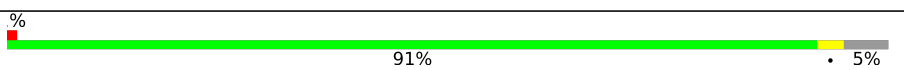
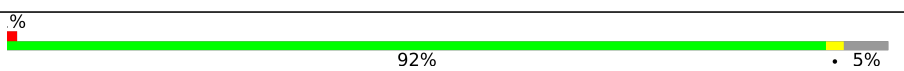
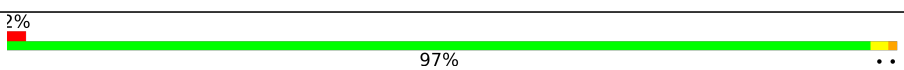
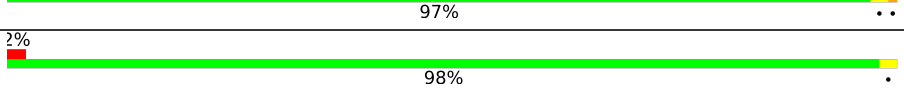
Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 49849 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1643	1044	280	313	6			
11	Y	212	Total	C	N	O	S	0	0	0
			1643	1044	280	313	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	45	THR	MET	engineered mutation	UNP P30656
Y	45	THR	MET	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	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	H	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	0	0
15	J	1	Total Mg 1 1	0	0
15	K	2	Total Mg 2 2	0	0
15	N	1	Total Mg 1 1	0	0
15	V	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	11	Total O 11 11	0	0
17	B	16	Total O 16 16	0	0
17	C	9	Total O 9 9	0	0
17	D	14	Total O 14 14	0	0
17	E	13	Total O 13 13	0	0
17	F	11	Total O 11 11	0	0
17	G	26	Total O 26 26	0	0
17	H	25	Total O 25 25	0	0

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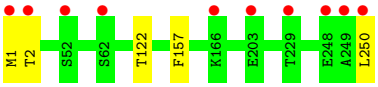
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	I	20	Total O 20 20	0	0
17	J	18	Total O 18 18	0	0
17	K	20	Total O 20 20	0	0
17	L	23	Total O 23 23	0	0
17	M	27	Total O 27 27	0	0
17	N	23	Total O 23 23	0	0
17	O	7	Total O 7 7	0	0
17	P	6	Total O 6 6	0	0
17	Q	17	Total O 17 17	0	0
17	R	8	Total O 8 8	0	0
17	S	7	Total O 7 7	0	0
17	T	18	Total O 18 18	0	0
17	U	13	Total O 13 13	0	0
17	V	11	Total O 11 11	0	0
17	W	15	Total O 15 15	0	0
17	X	18	Total O 18 18	0	0
17	Y	19	Total O 19 19	0	0
17	Z	26	Total O 26 26	0	0
17	a	28	Total O 28 28	0	0
17	b	25	Total O 25 25	0	0

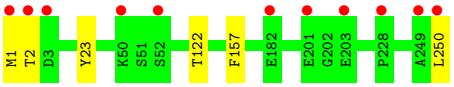
3 Residue-property plots (i)

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.

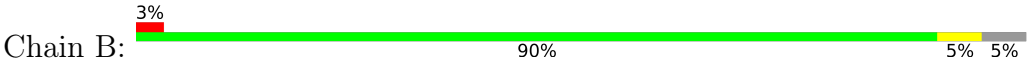
• Molecule 1: Proteasome subunit alpha type-2

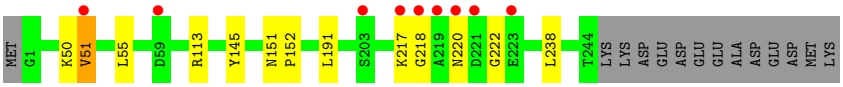


• Molecule 1: Proteasome subunit alpha type-2

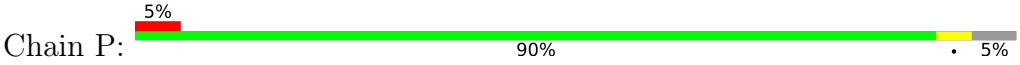


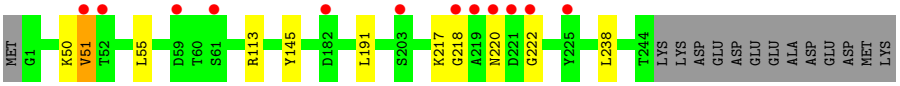
• Molecule 2: Proteasome subunit alpha type-3



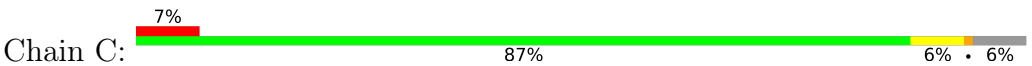


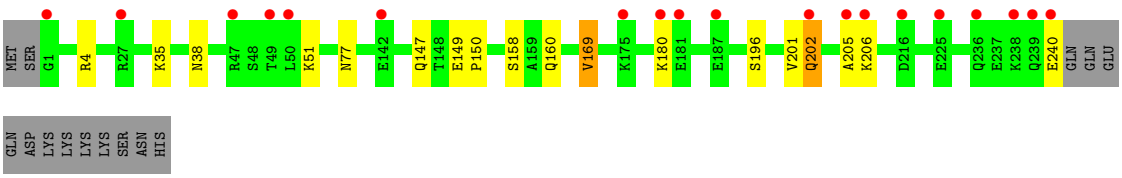
• Molecule 2: Proteasome subunit alpha type-3





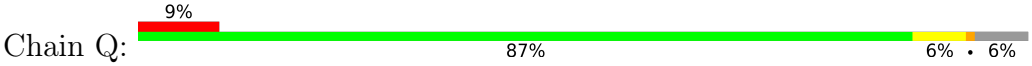
• Molecule 3: Proteasome subunit alpha type-4

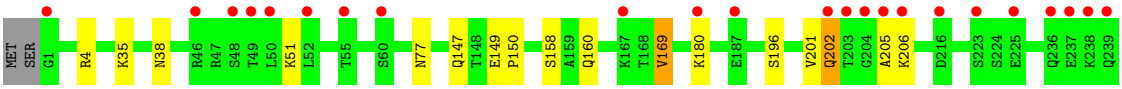


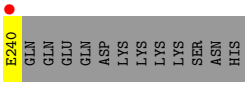


• Molecule 3: Proteasome subunit alpha type-4

Chain Q:

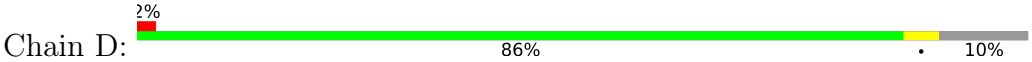






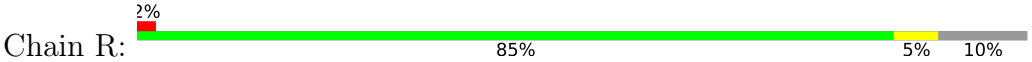
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



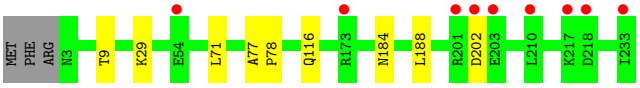
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



• Molecule 5: Proteasome subunit alpha type-6

Chain E:

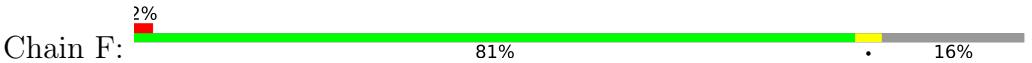


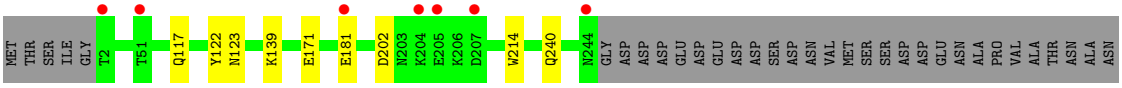
• Molecule 5: Proteasome subunit alpha type-6

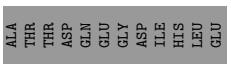
Chain S:

• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:

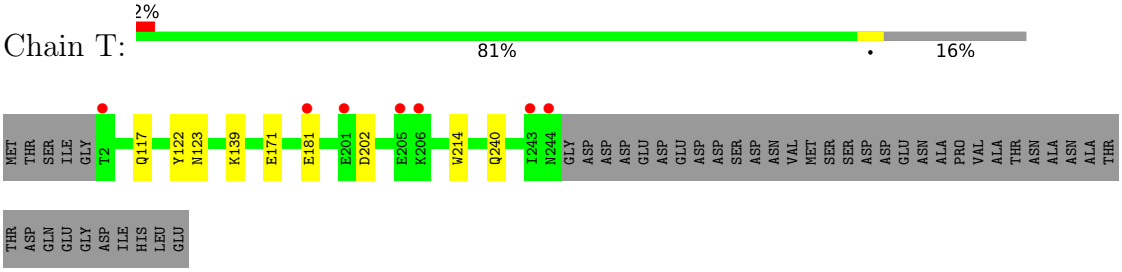






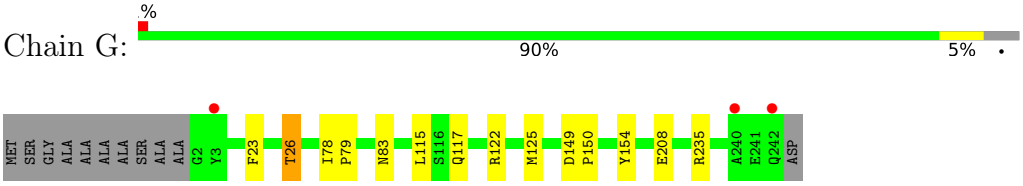
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



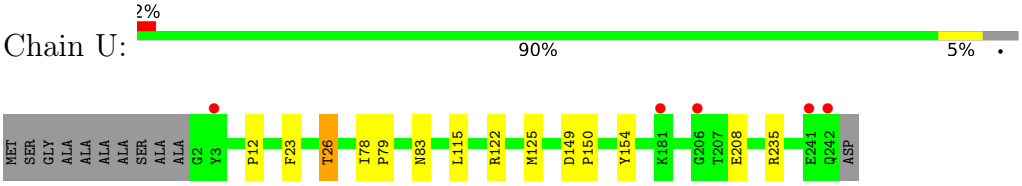
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



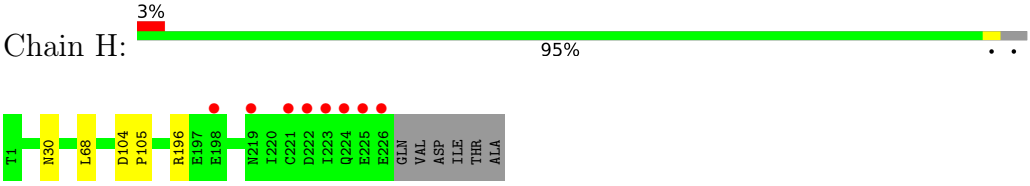
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



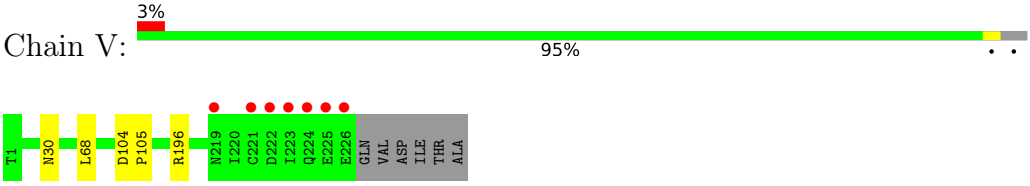
• Molecule 8: Proteasome subunit beta type-2

Chain H:



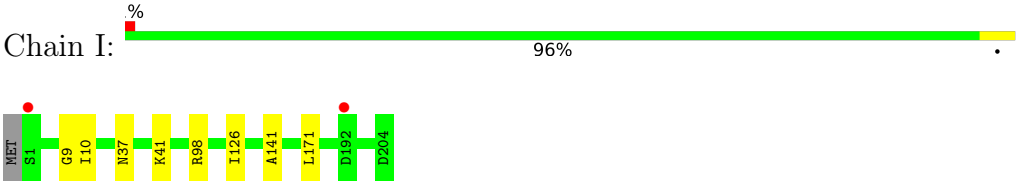
• Molecule 8: Proteasome subunit beta type-2

Chain V:



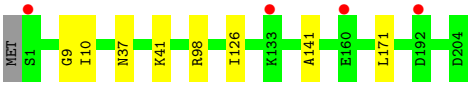
• Molecule 9: Proteasome subunit beta type-3

Chain I:



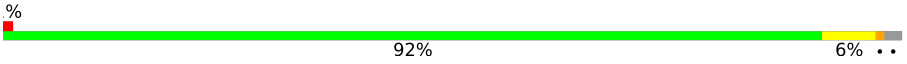
• Molecule 9: Proteasome subunit beta type-3

Chain W:



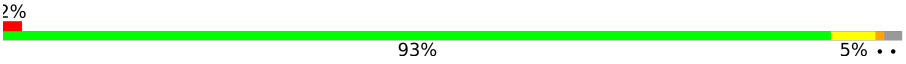
• Molecule 10: Proteasome subunit beta type-4

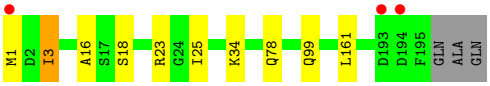
Chain J:



• Molecule 10: Proteasome subunit beta type-4

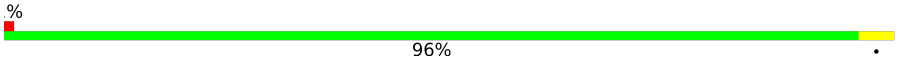
Chain X:

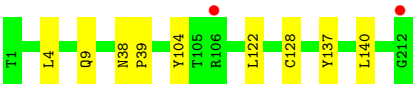




• Molecule 11: Proteasome subunit beta type-5

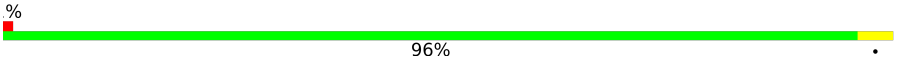
Chain K:

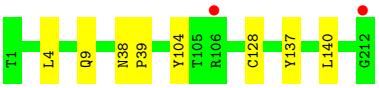




• Molecule 11: Proteasome subunit beta type-5

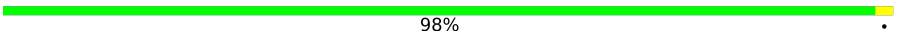
Chain Y:





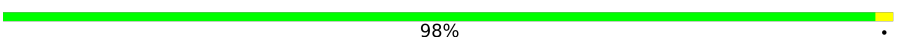
• Molecule 12: Proteasome subunit beta type-6

Chain L:



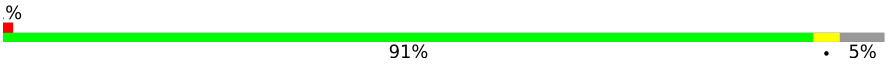
• Molecule 12: Proteasome subunit beta type-6

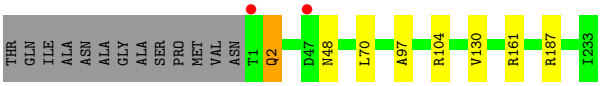
Chain Z:



• Molecule 13: Proteasome subunit beta type-7

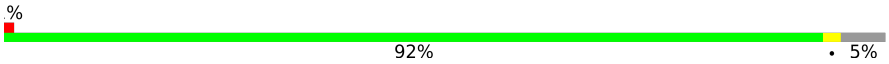
Chain M:

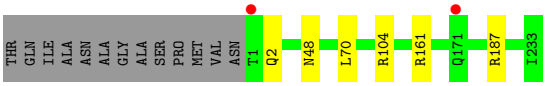




• Molecule 13: Proteasome subunit beta type-7

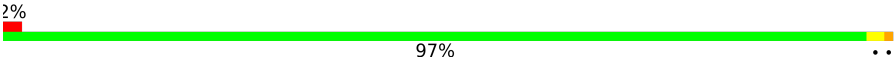
Chain a:

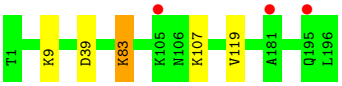




• Molecule 14: Proteasome subunit beta type-1

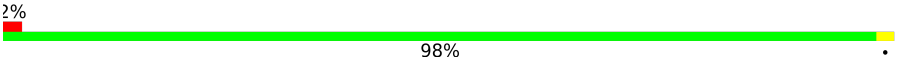
Chain N:

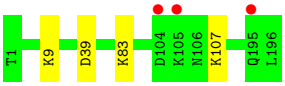




• Molecule 14: Proteasome subunit beta type-1

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	134.76Å 301.27Å 144.42Å 90.00° 112.81° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 14.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (15.00-2.70) 99.1 (14.99-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.213 0.196 , 0.218	Depositor DCC
R_{free} test set	14252 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.7	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	0.95	EDS
Total number of atoms	49849	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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

5.1 Standard geometry

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	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.48	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.27	0/1910	0.49	0/2586
3	Q	0.27	0/1910	0.49	0/2586
4	D	0.27	0/1837	0.46	0/2475
4	R	0.27	0/1837	0.46	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.27	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.25	0/1750	0.45	0/2373
8	V	0.25	0/1750	0.45	0/2373
9	I	0.27	0/1611	0.47	0/2174
9	W	0.27	0/1611	0.47	0/2174
10	J	0.30	0/1589	0.48	0/2142
10	X	0.30	0/1589	0.48	0/2142
11	K	0.26	0/1680	0.47	0/2274
11	Y	0.26	0/1680	0.47	0/2274
12	L	0.27	0/1795	0.46	0/2420
12	Z	0.27	0/1795	0.47	0/2420
13	M	0.27	0/1855	0.49	0/2514
13	a	0.27	0/1855	0.50	0/2514
14	N	0.25	0/1541	0.46	0/2087
14	b	0.25	0/1541	0.46	0/2087
All	All	0.27	0/50262	0.47	0/67962

There are no bond length outliers.

There are no bond angle outliers.

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	2	0
2	B	1904	0	1904	3	0
2	P	1904	0	1904	3	0
3	C	1881	0	1895	5	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	1	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	1	0
8	V	1719	0	1719	2	0
9	I	1581	0	1574	3	0
9	W	1581	0	1574	3	0
10	J	1561	0	1569	6	0
10	X	1561	0	1569	4	0
11	K	1643	0	1593	3	0
11	Y	1643	0	1593	2	0
12	L	1757	0	1711	1	0
12	Z	1757	0	1711	1	0
13	M	1824	0	1832	2	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	1	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	A	11	0	0	0	0
17	B	16	0	0	0	0
17	C	9	0	0	0	0
17	D	14	0	0	0	0
17	E	13	0	0	0	0
17	F	11	0	0	0	0
17	G	26	0	0	0	0
17	H	25	0	0	0	0
17	I	20	0	0	0	0
17	J	18	0	0	0	0
17	K	20	0	0	0	0
17	L	23	0	0	0	0
17	M	27	0	0	1	0
17	N	23	0	0	0	0
17	O	7	0	0	0	0
17	P	6	0	0	0	0
17	Q	17	0	0	0	0
17	R	8	0	0	0	0
17	S	7	0	0	0	0
17	T	18	0	0	0	0
17	U	13	0	0	0	0
17	V	11	0	0	0	0
17	W	15	0	0	0	0
17	X	18	0	0	0	0
17	Y	19	0	0	0	0
17	Z	26	0	0	0	0
17	a	28	0	0	0	0
17	b	25	0	0	0	0
All	All	49849	0	49126	58	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (58) 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)
10:J:22:THR:O	10:J:23:ARG:HD3	2.06	0.55
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.50
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.50
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.94	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.49
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.49
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.95	0.49
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.95	0.49
3:C:201:VAL:O	3:C:202:GLN:HB3	2.13	0.49
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.13	0.48
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.95	0.48
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.44	0.48
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.94	0.48
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.50	0.47
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.51	0.46
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.99	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.16	0.45
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.99	0.45
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.82	0.45
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.52	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.44
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.44
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.83	0.43
4:R:159:TYR:CE1	5:S:56:SER:HB3	2.54	0.43
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.01	0.43
2:P:50:LYS:O	2:P:51:VAL:C	2.57	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.53	0.43
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.49	0.42
2:P:145:TYR:OH	2:P:217:LYS:N	2.52	0.42
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.01	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
9:I:98:ARG:O	9:I:126:ILE:HD11	2.19	0.42
2:B:50:LYS:O	2:B:51:VAL:C	2.57	0.42
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.50	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.50	0.41
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.03	0.41
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:TYR:OH	2:B:217:LYS:N	2.52	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.55	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.02	0.41
13:M:2:GLN:NE2	17:M:326:HOH:O	2.53	0.41
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.93	0.41
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.51	0.40
9:W:98:ARG:O	9:W:126:ILE:HD11	2.21	0.40
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.56	0.40
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.04	0.40
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.51	0.40
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.04	0.40
10:J:139:TYR:OH	10:X:25:ILE:O	2.37	0.40
4:R:91:HIS:HB3	4:R:99:ILE:CG2	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%)	239 (96%)	8 (3%)	1 (0%)	34 60
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34 60
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9 23
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9 23
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19 43
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19 43
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (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%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6284/6614 (95%)	6122 (97%)	148 (2%)	14 (0%)	47	73

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY

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Mol	Chain	Res	Type
2	P	222	GLY
2	B	220	ASN
3	C	205	ALA
2	P	220	ASN
3	Q	205	ALA

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%)	206 (99%)	3 (1%)	67	86
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	86
2	B	203/216 (94%)	199 (98%)	4 (2%)	55	81
2	P	203/216 (94%)	199 (98%)	4 (2%)	55	81
3	C	212/226 (94%)	202 (95%)	10 (5%)	26	54
3	Q	212/226 (94%)	202 (95%)	10 (5%)	26	54
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	54
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	54
5	E	190/193 (98%)	183 (96%)	7 (4%)	34	63
5	S	190/193 (98%)	183 (96%)	7 (4%)	34	63
6	F	201/239 (84%)	193 (96%)	8 (4%)	31	60
6	T	201/239 (84%)	193 (96%)	8 (4%)	31	60
7	G	206/210 (98%)	197 (96%)	9 (4%)	28	56
7	U	206/210 (98%)	198 (96%)	8 (4%)	32	61
8	H	185/190 (97%)	182 (98%)	3 (2%)	62	85
8	V	185/190 (97%)	182 (98%)	3 (2%)	62	85
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	88
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	88
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	71
10	X	173/175 (99%)	169 (98%)	4 (2%)	50	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	169/169 (100%)	165 (98%)	4 (2%)	49 77
11	Y	169/169 (100%)	165 (98%)	4 (2%)	49 77
12	L	185/185 (100%)	183 (99%)	2 (1%)	73 90
12	Z	185/185 (100%)	183 (99%)	2 (1%)	73 90
13	M	199/208 (96%)	193 (97%)	6 (3%)	41 70
13	a	199/208 (96%)	193 (97%)	6 (3%)	41 70
14	N	162/162 (100%)	158 (98%)	4 (2%)	47 76
14	b	162/162 (100%)	158 (98%)	4 (2%)	47 76
All	All	5320/5540 (96%)	5170 (97%)	150 (3%)	43 73

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU

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Mol	Chain	Res	Type
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	171	GLU
6	F	181	GLU
6	F	202	ASP
6	F	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	154	TYR
7	G	208	GLU
7	G	235	ARG
8	H	30	ASN
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	3	ILE
10	J	23	ARG
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	104	TYR
11	K	140	LEU
12	L	23	LEU
12	L	150	LEU
13	M	2	GLN
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	107	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	117	GLN

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Mol	Chain	Res	Type
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	181	GLU
6	T	202	ASP
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	154	TYR
7	U	208	GLU
7	U	235	ARG
8	V	30	ASN
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	3	ILE
10	X	23	ARG
10	X	78	GLN
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	104	TYR
11	Y	140	LEU
12	Z	23	LEU
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
14	b	9	LYS
14	b	39	ASP
14	b	83	LYS
14	b	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) 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
3	C	147	GLN
3	C	160	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	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
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	66	HIS
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN

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Mol	Chain	Res	Type
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
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
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
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
9	W	37	ASN
10	X	55	GLN
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	48	ASN
13	a	102	GLN
13	a	179	ASN
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 (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 11 ligands modelled in this entry, 11 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

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, 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%)	-0.25	10 (4%)	38	37	38, 52, 92, 128	0
1	O	250/250 (100%)	-0.17	11 (4%)	34	33	42, 60, 108, 134	0
2	B	244/258 (94%)	-0.08	9 (3%)	41	41	39, 59, 107, 166	0
2	P	244/258 (94%)	-0.06	12 (4%)	29	28	43, 61, 105, 159	0
3	C	240/254 (94%)	-0.04	19 (7%)	12	10	39, 62, 127, 150	0
3	Q	240/254 (94%)	0.26	24 (10%)	7	5	45, 75, 162, 192	0
4	D	235/260 (90%)	-0.23	6 (2%)	56	57	44, 65, 101, 137	0
4	R	235/260 (90%)	-0.17	6 (2%)	56	57	43, 66, 108, 150	0
5	E	231/234 (98%)	-0.19	9 (3%)	39	38	42, 65, 103, 139	0
5	S	231/234 (98%)	-0.00	13 (5%)	24	23	43, 72, 117, 154	0
6	F	243/288 (84%)	-0.33	7 (2%)	51	52	38, 60, 108, 135	0
6	T	243/288 (84%)	-0.26	7 (2%)	51	52	40, 68, 123, 159	0
7	G	241/252 (95%)	-0.41	3 (1%)	79	80	35, 53, 88, 138	0
7	U	241/252 (95%)	-0.31	5 (2%)	63	65	41, 57, 90, 136	0
8	H	226/232 (97%)	-0.30	8 (3%)	44	44	33, 50, 79, 153	0
8	V	226/232 (97%)	-0.24	7 (3%)	49	49	35, 53, 84, 173	0
9	I	204/205 (99%)	-0.61	2 (0%)	82	83	33, 46, 71, 102	0
9	W	204/205 (99%)	-0.56	4 (1%)	65	67	34, 49, 76, 107	0
10	J	195/198 (98%)	-0.44	2 (1%)	82	83	34, 51, 79, 118	0
10	X	195/198 (98%)	-0.39	3 (1%)	73	76	36, 52, 77, 133	0
11	K	212/212 (100%)	-0.46	2 (0%)	84	85	32, 49, 75, 90	0
11	Y	212/212 (100%)	-0.51	2 (0%)	84	85	35, 50, 76, 94	0
12	L	222/222 (100%)	-0.51	1 (0%)	91	92	35, 52, 86, 125	0
12	Z	222/222 (100%)	-0.48	1 (0%)	91	92	30, 51, 86, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.58	2 (0%) 84 85	30, 49, 73, 93	0
13	a	233/246 (94%)	-0.51	2 (0%) 84 85	29, 49, 72, 93	0
14	N	196/196 (100%)	-0.59	3 (1%) 73 76	31, 44, 72, 101	0
14	b	196/196 (100%)	-0.54	3 (1%) 73 76	30, 45, 75, 103	0
All	All	6344/6614 (95%)	-0.31	183 (2%) 51 52	29, 55, 103, 192	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	224	GLN	9.1
3	Q	50	LEU	8.8
2	B	221	ASP	8.4
2	P	219	ALA	8.4
2	B	219	ALA	8.2
2	P	221	ASP	8.0
3	Q	49	THR	7.9
8	V	226	GLU	7.6
2	B	51	VAL	7.4
2	P	51	VAL	7.1
10	X	1	MET	7.0
2	P	220	ASN	6.7
8	V	223	ILE	6.4
8	V	222	ASP	6.0
8	H	224	GLN	5.8
5	S	202	ASP	5.8
1	A	2	THR	5.8
8	H	226	GLU	5.8
8	H	222	ASP	5.8
4	R	241	ALA	5.7
7	U	242	GLN	5.5
3	Q	205	ALA	5.4
3	Q	236	GLN	5.2
5	E	202	ASP	5.1
3	C	206	LYS	5.1
3	Q	187	GLU	4.9
8	H	221	CYS	4.8
8	H	225	GLU	4.7
10	J	1	MET	4.7
2	B	220	ASN	4.6
2	P	218	GLY	4.4
1	O	2	THR	4.3

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Mol	Chain	Res	Type	RSRZ
3	C	49	THR	4.2
3	Q	48	SER	4.1
2	P	59	ASP	4.1
6	F	181	GLU	4.1
1	A	1	MET	4.1
8	H	223	ILE	4.0
8	V	221	CYS	4.0
3	Q	238	LYS	4.0
3	C	238	LYS	4.0
12	L	174	TYR	3.9
3	C	205	ALA	3.8
3	Q	206	LYS	3.8
14	b	105	LYS	3.8
10	X	194	ASP	3.8
3	C	50	LEU	3.7
6	F	205	GLU	3.7
1	O	249	ALA	3.6
1	O	52	SER	3.6
4	R	1	ASP	3.6
1	O	1	MET	3.5
3	Q	239	GLN	3.5
3	Q	240	GLU	3.4
9	W	1	SER	3.4
14	N	105	LYS	3.3
1	A	249	ALA	3.3
11	Y	212	GLY	3.2
12	Z	174	TYR	3.2
2	B	203	SER	3.2
3	Q	55	THR	3.1
6	T	244	ASN	3.1
7	G	242	GLN	3.1
3	Q	202	GLN	3.1
9	I	1	SER	3.1
2	P	52	THR	3.0
4	D	1	ASP	3.0
3	C	225	GLU	3.0
3	C	239	GLN	3.0
6	F	244	ASN	3.0
1	A	250	LEU	3.0
3	C	180	LYS	2.9
4	D	242	GLU	2.9
4	R	217	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	O	201	GLU	2.9
6	T	181	GLU	2.9
10	X	193	ASP	2.9
3	Q	1	GLY	2.9
6	T	206	LYS	2.9
5	S	173	ARG	2.9
6	T	201	GLU	2.9
14	N	195	GLN	2.9
2	B	59	ASP	2.9
10	J	194	ASP	2.9
3	Q	204	GLY	2.8
3	Q	203	THR	2.8
3	Q	223	SER	2.8
4	D	2	ARG	2.8
4	R	125	LEU	2.8
2	P	222	GLY	2.8
1	A	203	GLU	2.8
7	G	240	ALA	2.7
13	M	47	ASP	2.7
3	C	216	ASP	2.7
7	G	3	TYR	2.7
14	b	195	GLN	2.7
6	T	2	THR	2.7
8	V	225	GLU	2.7
3	Q	225	GLU	2.7
3	Q	216	ASP	2.6
3	Q	180	LYS	2.6
9	I	192	ASP	2.6
4	R	242	GLU	2.6
1	A	248	GLU	2.6
2	P	203	SER	2.6
2	B	218	GLY	2.6
5	E	201	ARG	2.6
3	C	202	GLN	2.6
4	D	241	ALA	2.6
3	Q	237	GLU	2.5
5	S	201	ARG	2.5
5	E	233	ILE	2.5
2	P	225	TYR	2.5
7	U	241	GLU	2.5
2	B	217	LYS	2.5
5	E	217	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
14	N	181	ALA	2.5
5	S	165	GLN	2.5
3	C	27	ARG	2.5
3	Q	60	SER	2.5
5	S	210	LEU	2.5
6	F	51	THR	2.4
3	Q	52	LEU	2.4
11	Y	106	ARG	2.4
6	T	243	ILE	2.4
2	P	182	ASP	2.4
11	K	212	GLY	2.4
5	S	180	LYS	2.4
3	Q	167	LYS	2.4
3	C	1	GLY	2.4
3	C	181	GLU	2.4
1	O	250	LEU	2.4
8	V	219	ASN	2.4
13	a	1	THR	2.3
8	H	219	ASN	2.3
5	E	54	GLU	2.3
1	O	50	LYS	2.3
13	M	1	THR	2.3
9	W	133	LYS	2.3
11	K	106	ARG	2.3
1	A	229	THR	2.3
6	F	2	THR	2.3
3	C	240	GLU	2.3
5	S	54	GLU	2.3
3	C	175	LYS	2.3
5	E	173	ARG	2.2
4	R	54	ASP	2.2
5	S	233	ILE	2.2
3	C	236	GLN	2.2
5	S	56	SER	2.2
8	H	198	GLU	2.2
4	D	217	GLN	2.2
7	U	181	LYS	2.2
9	W	192	ASP	2.2
5	S	51	ASN	2.2
6	T	205	GLU	2.2
14	b	104	ASP	2.2
7	U	3	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	203	GLU	2.2
4	D	125	LEU	2.1
13	a	171	GLN	2.1
6	F	207	ASP	2.1
2	P	61	SER	2.1
7	U	206	GLY	2.1
1	O	3	ASP	2.1
3	C	47	ARG	2.1
3	C	142	GLU	2.1
1	A	52	SER	2.1
6	F	204	LYS	2.1
3	Q	46	ARG	2.1
3	C	187	GLU	2.1
5	E	203	GLU	2.1
9	W	160	GLU	2.1
1	A	166	LYS	2.1
5	S	50	ARG	2.1
5	E	218	ASP	2.1
1	O	228	PRO	2.1
5	S	30	GLN	2.1
5	S	52	ALA	2.1
1	O	182	GLU	2.1
5	E	210	LEU	2.0
1	A	62	SER	2.0
2	B	223	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 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, 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	G	301	1/1	0.89	0.12	47,47,47,47	0
15	MG	I	301	1/1	0.93	0.29	56,56,56,56	0
15	MG	N	201	1/1	0.94	0.11	58,58,58,58	0
15	MG	J	201	1/1	0.96	0.14	61,61,61,61	0
15	MG	H	301	1/1	0.96	0.10	48,48,48,48	0
15	MG	K	301	1/1	0.97	0.09	49,49,49,49	0
15	MG	K	302	1/1	0.99	0.40	48,48,48,48	0
15	MG	V	301	1/1	0.99	0.06	65,65,65,65	0
15	MG	Y	301	1/1	0.99	0.06	62,62,62,62	0
16	CL	G	302	1/1	0.99	0.05	42,42,42,42	0
16	CL	U	301	1/1	0.99	0.19	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.