Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 10:00 AM EDT

PDB ID	:	4QZZ
Title	:	yCP in complex with Omuralide
Authors	:	Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on	:	2014-07-29
Resolution	:	2.90 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:

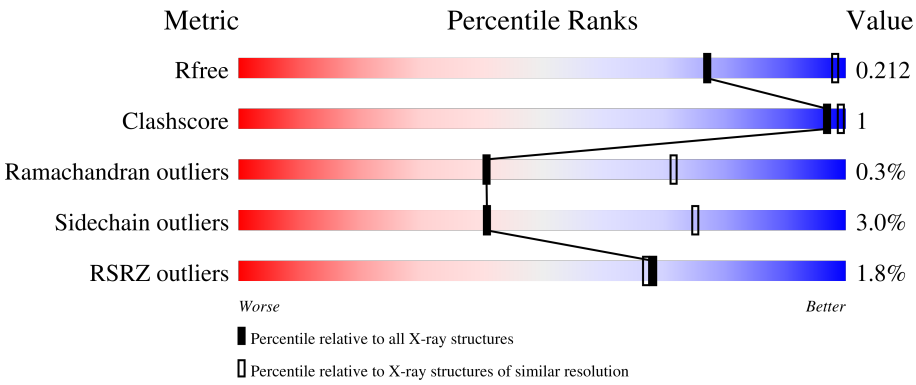
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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%, 98%, •
2	B	258	2%, 88%, 7%, 5%
2	P	258	3%, 90%, 5%, 5%
3	C	254	5%, 87%, 7%, •, 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	6% 87% 7% 6%
4	D	260	.% 87% 10%
4	R	260	2% 86% 5% 10%
5	E	234	2% 95%
5	S	234	2% 94% 5%
6	F	288	.% 82% 16%
6	T	288	2% 82% 16%
7	G	252	90% 6%
7	U	252	2% 90% 6%
8	H	232	3% 93%
8	V	232	3% 94%
9	I	205	95%
9	W	205	.% 96%
10	J	198	2% 92% 6%
10	X	198	2% 92% 6%
11	K	212	94% 6%
11	Y	212	93% 7%
12	L	222	97%
12	Z	222	98%
13	M	246	.% 92% 5%
13	a	246	92% 5%
14	N	196	.% 95%
14	b	196	.% 97%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 49796 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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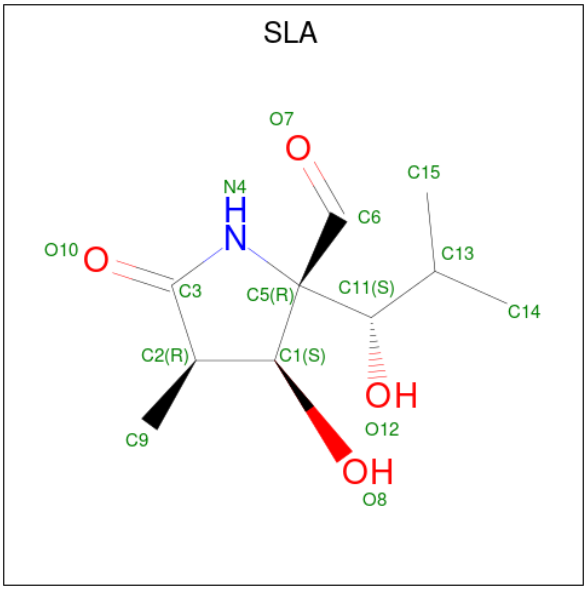
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- 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
16	N	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0
16	b	1	Total Cl 1 1	0	0

- Molecule 17 is Omuralide, open form (three-letter code: SLA) (formula: $C_{10}H_{17}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
17	H	1	15	10	1	4	0	0
17	K	1	15	10	1	4	0	0
17	N	1	15	10	1	4	0	0
17	V	1	15	10	1	4	0	0
17	Y	1	15	10	1	4	0	0
17	b	1	15	10	1	4	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	A	8	8	8	0	0
18	B	10	10	10	0	0
18	C	10	10	10	0	0
18	D	7	7	7	0	0
18	E	6	6	6	0	0
18	F	14	14	14	0	0
18	G	11	11	11	0	0
18	H	19	19	19	0	0
18	I	8	8	8	0	0
18	J	15	15	15	0	0
18	K	18	18	18	0	0
18	L	23	23	23	0	0
18	M	14	14	14	0	0
18	N	10	10	10	0	0

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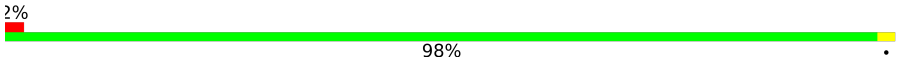
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	O	10	Total O 10 10	0	0
18	P	7	Total O 7 7	0	0
18	Q	10	Total O 10 10	0	0
18	R	7	Total O 7 7	0	0
18	S	7	Total O 7 7	0	0
18	T	18	Total O 18 18	0	0
18	U	8	Total O 8 8	0	0
18	V	9	Total O 9 9	0	0
18	W	9	Total O 9 9	0	0
18	X	18	Total O 18 18	0	0
18	Y	9	Total O 9 9	0	0
18	Z	18	Total O 18 18	0	0
18	a	19	Total O 19 19	0	0
18	b	7	Total O 7 7	0	0

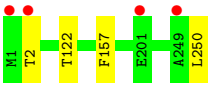
3 Residue-property plots (i)

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

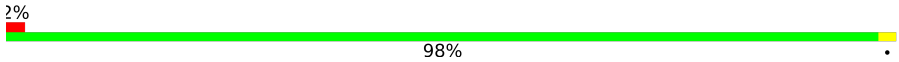
Chain A:

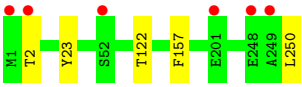




• Molecule 1: Proteasome subunit alpha type-2

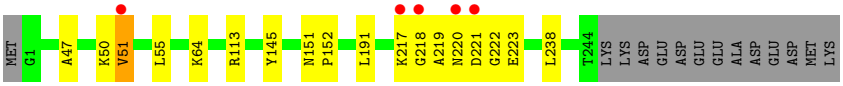
Chain O:





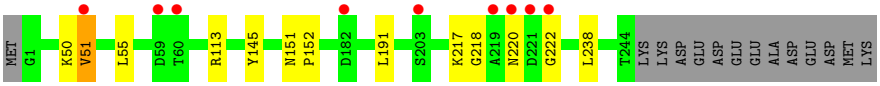
• Molecule 2: Proteasome subunit alpha type-3

Chain B:



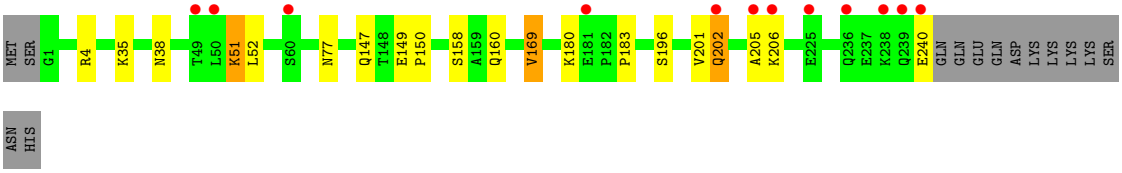
• Molecule 2: Proteasome subunit alpha type-3

Chain P:



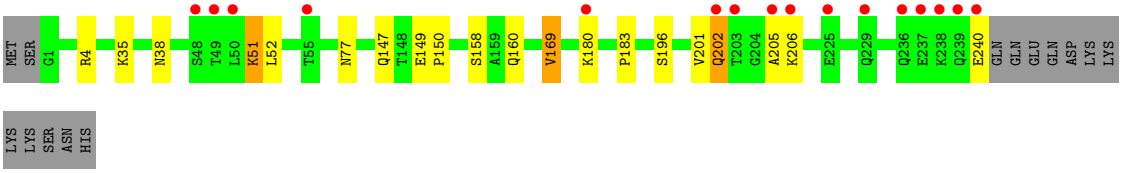
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



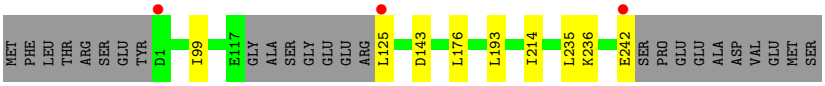
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



• Molecule 4: Proteasome subunit alpha type-5

Chain D:

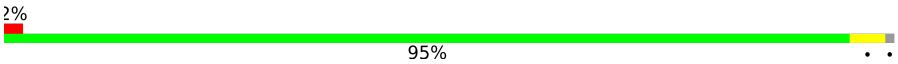


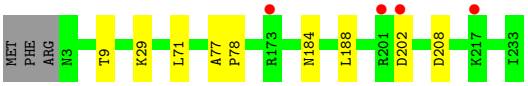
• Molecule 4: Proteasome subunit alpha type-5

Chain R:

• Molecule 5: Proteasome subunit alpha type-6

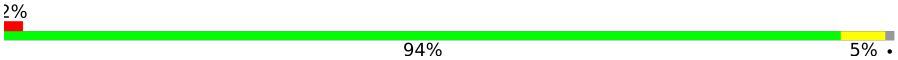
Chain E:

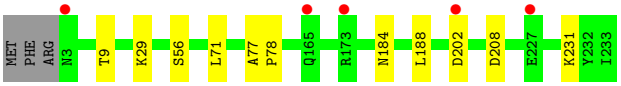




• Molecule 5: Proteasome subunit alpha type-6

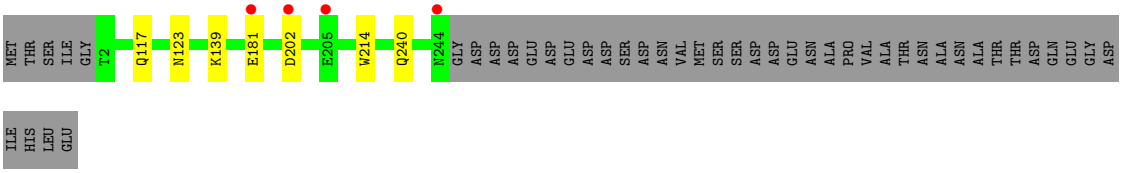
Chain S:





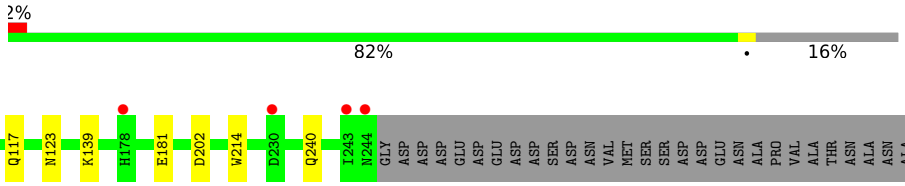
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



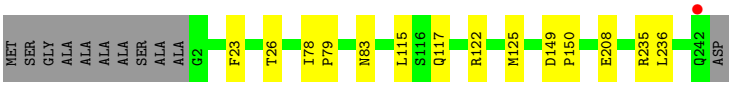
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



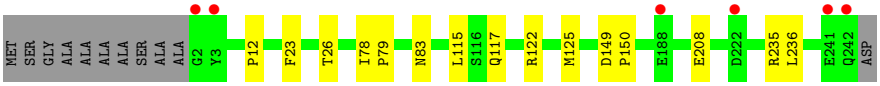
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



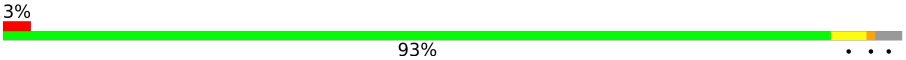
• Molecule 7: Proteasome subunit alpha type-1

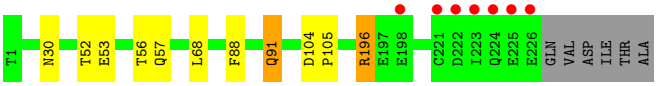
Chain U:



• Molecule 8: Proteasome subunit beta type-2

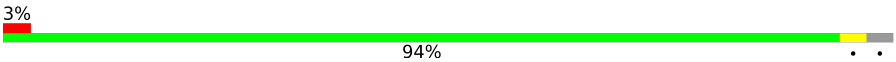
Chain H:

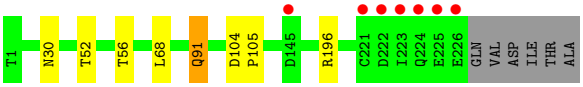




• Molecule 8: Proteasome subunit beta type-2

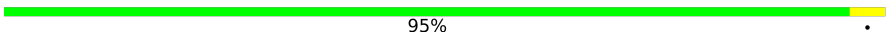
Chain V:





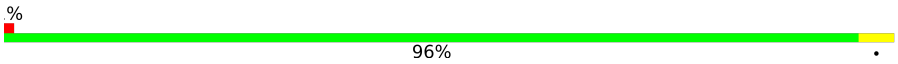
• Molecule 9: Proteasome subunit beta type-3

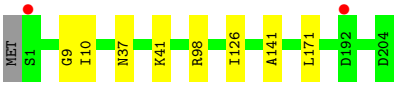
Chain I:



• Molecule 9: Proteasome subunit beta type-3

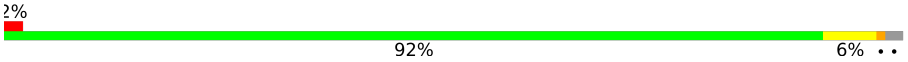
Chain W:

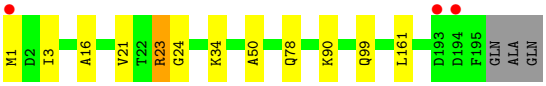




• Molecule 10: Proteasome subunit beta type-4

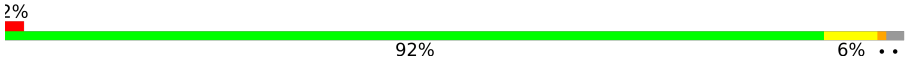
Chain J:

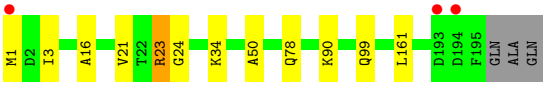




• Molecule 10: Proteasome subunit beta type-4

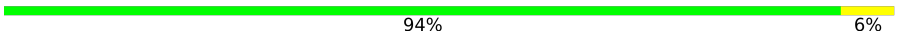
Chain X:





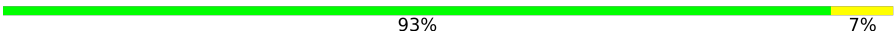
• Molecule 11: Proteasome subunit beta type-5

Chain K:



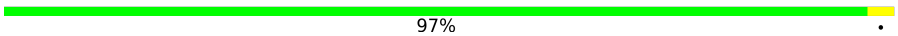
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



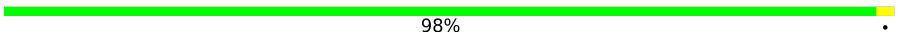
• Molecule 12: Proteasome subunit beta type-6

Chain L:



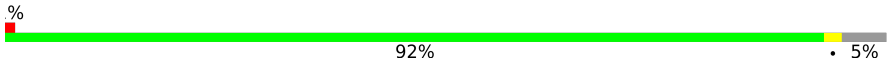
• Molecule 12: Proteasome subunit beta type-6

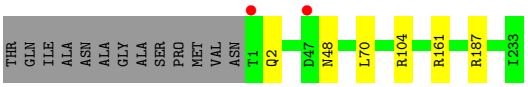
Chain Z:



• Molecule 13: Proteasome subunit beta type-7

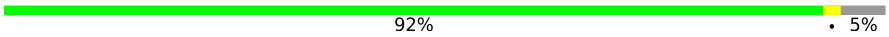
Chain M:

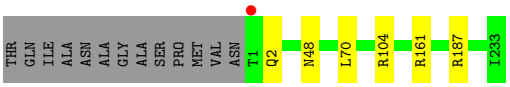




- Molecule 13: Proteasome subunit beta type-7

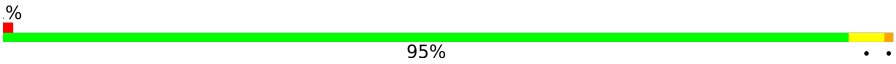
Chain a:

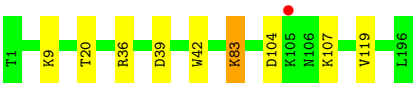




- Molecule 14: Proteasome subunit beta type-1

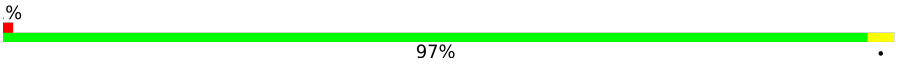
Chain N:

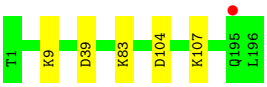




- Molecule 14: Proteasome subunit beta type-1

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	135.96Å 301.96Å 145.05Å 90.00° 113.14° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.4 (15.00-2.90) 90.5 (15.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.179 , 0.208 0.185 , 0.212	Depositor DCC
R_{free} test set	10642 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.9	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	49796	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, SLA, 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	0.27	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	0.50	0/2586
3	Q	0.27	0/1910	0.49	0/2586
4	D	0.26	0/1837	0.47	0/2475
4	R	0.26	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	0.26	0/1750	0.46	0/2373
8	V	0.26	0/1750	0.46	0/2373
9	I	0.27	0/1611	0.47	0/2174
9	W	0.27	0/1611	0.47	0/2174
10	J	0.26	0/1589	0.47	0/2142
10	X	0.26	0/1589	0.48	0/2142
11	K	0.26	0/1681	0.47	0/2274
11	Y	0.26	0/1681	0.48	0/2274
12	L	0.27	0/1795	0.46	0/2420
12	Z	0.27	0/1795	0.46	0/2420
13	M	0.27	0/1855	0.50	0/2514
13	a	0.27	0/1855	0.50	0/2514
14	N	0.26	0/1541	0.47	0/2087
14	b	0.26	0/1541	0.46	0/2087
All	All	0.27	0/50264	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	0	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	4	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	0	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	0	0
6	T	1892	0	1883	0	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1718	5	0
8	V	1719	0	1718	3	0
9	I	1581	0	1574	4	0
9	W	1581	0	1574	3	0
10	J	1561	0	1569	6	0
10	X	1561	0	1569	6	0
11	K	1644	0	1594	6	0
11	Y	1644	0	1594	6	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	1	0
13	M	1824	0	1832	0	0
13	a	1824	0	1832	0	0
14	N	1512	0	1480	4	0
14	b	1512	0	1480	0	0
15	G	1	0	0	0	0
15	J	1	0	0	0	0
15	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	1	0	0	0	0
15	V	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	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	15	0	16	2	0
17	K	15	0	16	1	0
17	N	15	0	16	1	0
17	V	15	0	16	2	0
17	Y	15	0	16	1	0
17	b	15	0	16	0	0
18	A	8	0	0	0	0
18	B	10	0	0	0	0
18	C	10	0	0	0	0
18	D	7	0	0	0	0
18	E	6	0	0	0	0
18	F	14	0	0	0	0
18	G	11	0	0	0	0
18	H	19	0	0	0	0
18	I	8	0	0	0	0
18	J	15	0	0	0	0
18	K	18	0	0	0	0
18	L	23	0	0	1	0
18	M	14	0	0	0	0
18	N	10	0	0	1	0
18	O	10	0	0	0	0
18	P	7	0	0	0	0
18	Q	10	0	0	0	0
18	R	7	0	0	0	0
18	S	7	0	0	0	0
18	T	18	0	0	0	0
18	U	8	0	0	0	0
18	V	9	0	0	0	0
18	W	9	0	0	0	0
18	X	18	0	0	0	0
18	Y	9	0	0	0	0
18	Z	18	0	0	0	0
18	a	19	0	0	0	0
18	b	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	49796	0	49220	80	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 (80) 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:X:23:ARG:NH2	10:X:50:ALA:HB2	1.95	0.82
10:J:23:ARG:NH2	10:J:50:ALA:HB2	1.95	0.80
14:N:20:THR:HG23	17:N:201:SLA:H15	1.77	0.65
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.89	0.55
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.88	0.53
7:G:23:PHE:O	7:G:26:THR:HB	2.08	0.53
7:U:23:PHE:O	7:U:26:THR:HB	2.08	0.53
8:H:88:PHE:O	8:H:91:GLN:OE1	2.26	0.53
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
17:H:301:SLA:H13	17:H:301:SLA:C6	2.42	0.50
10:J:50:ALA:O	11:K:91:LYS:NZ	2.45	0.50
10:J:23:ARG:HH22	10:J:50:ALA:HB2	1.73	0.50
10:X:23:ARG:HH22	10:X:50:ALA:HB2	1.74	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.49
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.47	0.48
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.96	0.48
17:V:301:SLA:C6	17:V:301:SLA:H13	2.42	0.48
17:K:301:SLA:C6	17:K:301:SLA:H13	2.43	0.48
17:Y:301:SLA:C6	17:Y:301:SLA:H13	2.44	0.47
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.96	0.46
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.96	0.46
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.96	0.46
3:C:201:VAL:O	3:C:202:GLN:HB3	2.15	0.46
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.47	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.16	0.46
3:C:35:LYS:HG2	3:C:158:SER:O	2.16	0.45
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.51	0.45
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.99	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.45
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.16	0.45
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.44
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.44
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.83	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.44
3:C:51:LYS:O	3:C:52:LEU:HB2	2.18	0.44
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.53	0.44
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.83	0.44
9:I:98:ARG:O	9:I:126:ILE:HD11	2.18	0.43
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.53	0.43
8:V:91:GLN:HE21	8:V:91:GLN:HB3	1.60	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
8:H:52:THR:O	8:H:56:THR:HG23	2.19	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.43
9:W:98:ARG:O	9:W:126:ILE:HD11	2.18	0.43
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.53	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.43
17:H:301:SLA:C6	17:H:301:SLA:C14	2.97	0.43
12:L:3:ASN:ND2	18:L:314:HOH:O	2.52	0.43
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.49	0.43
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.18	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
17:V:301:SLA:C6	17:V:301:SLA:C14	2.97	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.00	0.42
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.42
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.49	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.49	0.42
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.01	0.42
8:H:53:GLU:O	8:H:57:GLN:HG2	2.20	0.42
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.54	0.42
8:V:52:THR:O	8:V:56:THR:HG23	2.20	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.41
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.02	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
14:N:36:ARG:NH2	18:N:301:HOH:O	2.54	0.41
2:P:145:TYR:OH	2:P:217:LYS:N	2.53	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:LYS:C	2:B:219:ALA:H	2.25	0.40
8:H:196:ARG:NH2	9:I:150:GLU:O	2.55	0.40
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.04	0.40
2:B:221:ASP:O	2:B:223:GLU:N	2.55	0.40
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.57	0.40
2:B:145:TYR:OH	2:B:217:LYS:N	2.54	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	66
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	66
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	31
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	31
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	37
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	37
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	219 (96%)	10 (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%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	4 (2%)	1 (0%)	29	61
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
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%)	225 (97%)	6 (3%)	0	100	100
13	a	231/246 (94%)	224 (97%)	7 (3%)	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%)	6124 (98%)	142 (2%)	18 (0%)	41	71

All (18) 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
2	P	222	GLY
2	B	220	ASN
2	P	220	ASN
3	C	205	ALA
10	J	24	GLY
3	Q	205	ALA
10	X	24	GLY
3	C	183	PRO
3	Q	183	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	89
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	89
2	B	203/216 (94%)	199 (98%)	4 (2%)	55	82
2	P	203/216 (94%)	199 (98%)	4 (2%)	55	82
3	C	212/226 (94%)	202 (95%)	10 (5%)	26	59
3	Q	212/226 (94%)	202 (95%)	10 (5%)	26	59
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	60
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	60
5	E	190/193 (98%)	183 (96%)	7 (4%)	34	68
5	S	190/193 (98%)	182 (96%)	8 (4%)	30	63
6	F	201/239 (84%)	194 (96%)	7 (4%)	36	70
6	T	201/239 (84%)	194 (96%)	7 (4%)	36	70
7	G	206/210 (98%)	198 (96%)	8 (4%)	32	66
7	U	206/210 (98%)	198 (96%)	8 (4%)	32	66
8	H	185/190 (97%)	181 (98%)	4 (2%)	52	81
8	V	185/190 (97%)	181 (98%)	4 (2%)	52	81
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	91
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	91
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	76
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	76
11	K	169/169 (100%)	164 (97%)	5 (3%)	41	75
11	Y	169/169 (100%)	163 (96%)	6 (4%)	35	69
12	L	185/185 (100%)	182 (98%)	3 (2%)	62	86
12	Z	185/185 (100%)	182 (98%)	3 (2%)	62	86
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	75
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	74
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	74
All	All	5320/5540 (96%)	5162 (97%)	158 (3%)	41	75

All (158) 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
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	208	ASP
6	F	117	GLN

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Mol	Chain	Res	Type
6	F	123	ASN
6	F	139	LYS
6	F	181	GLU
6	F	202	ASP
6	F	214	TRP
6	F	240	GLN
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	30	ASN
8	H	68	LEU
8	H	91	GLN
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	107	LYS
11	K	140	LEU
12	L	23	LEU
12	L	136	CYS
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS

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Mol	Chain	Res	Type
14	N	104	ASP
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	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	208	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	181	GLU
6	T	202	ASP
6	T	214	TRP

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Mol	Chain	Res	Type
6	T	240	GLN
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	30	ASN
8	V	68	LEU
8	V	91	GLN
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	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	104	TYR
11	Y	107	LYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	136	CYS
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	104	ASP
14	b	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	58	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
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	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
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	57	GLN
8	H	66	HIS
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN

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Mol	Chain	Res	Type
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
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	120	GLN
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
8	V	91	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	70	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN

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Mol	Chain	Res	Type
13	a	194	ASN
13	a	213	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 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	SLA	V	301	8	10,15,15	4.12	2 (20%)	12,23,23	2.63	4 (33%)
17	SLA	b	201	14	10,15,15	4.19	2 (20%)	12,23,23	2.59	4 (33%)
17	SLA	K	301	11	10,15,15	4.15	1 (10%)	12,23,23	2.57	4 (33%)
17	SLA	H	301	8	10,15,15	4.07	1 (10%)	12,23,23	2.62	4 (33%)
17	SLA	N	201	14	10,15,15	4.15	2 (20%)	12,23,23	2.63	4 (33%)
17	SLA	Y	301	11	10,15,15	4.11	1 (10%)	12,23,23	2.64	4 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SLA	V	301	8	-	0/6/32/32	0/1/1/1
17	SLA	b	201	14	-	0/6/32/32	0/1/1/1
17	SLA	K	301	11	-	0/6/32/32	0/1/1/1
17	SLA	H	301	8	-	0/6/32/32	0/1/1/1
17	SLA	N	201	14	-	0/6/32/32	0/1/1/1
17	SLA	Y	301	11	-	0/6/32/32	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	301	SLA	C2-C3	-12.89	1.40	1.52
17	b	201	SLA	C2-C3	-12.78	1.40	1.52
17	Y	301	SLA	C2-C3	-12.75	1.40	1.52
17	V	301	SLA	C2-C3	-12.66	1.40	1.52
17	N	201	SLA	C2-C3	-12.63	1.40	1.52
17	H	301	SLA	C2-C3	-12.57	1.40	1.52
17	N	201	SLA	C13-C11	2.83	1.56	1.53
17	b	201	SLA	C13-C11	2.63	1.55	1.53
17	V	301	SLA	C13-C11	2.02	1.55	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	301	SLA	C5-N4-C3	-7.20	109.56	114.58
17	V	301	SLA	C5-N4-C3	-7.12	109.62	114.58
17	N	201	SLA	C5-N4-C3	-7.06	109.66	114.58
17	H	301	SLA	C5-N4-C3	-7.04	109.67	114.58
17	K	301	SLA	C5-N4-C3	-6.95	109.74	114.58
17	b	201	SLA	C5-N4-C3	-6.86	109.80	114.58
17	H	301	SLA	C9-C2-C1	-3.50	112.86	116.54
17	V	301	SLA	C9-C2-C1	-3.42	112.94	116.54
17	N	201	SLA	C9-C2-C1	-3.39	112.96	116.54
17	b	201	SLA	C9-C2-C1	-3.32	113.04	116.54
17	K	301	SLA	C9-C2-C1	-3.05	113.33	116.54
17	Y	301	SLA	C9-C2-C1	-3.05	113.33	116.54
17	b	201	SLA	O10-C3-C2	-2.88	123.89	126.17
17	N	201	SLA	O10-C3-C2	-2.73	124.00	126.17
17	Y	301	SLA	O10-C3-N4	-2.73	122.17	125.72
17	V	301	SLA	O10-C3-N4	-2.69	122.22	125.72
17	K	301	SLA	O10-C3-N4	-2.64	122.28	125.72
17	H	301	SLA	O10-C3-N4	-2.61	122.33	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	301	SLA	O10-C3-C2	-2.52	124.17	126.17
17	Y	301	SLA	O10-C3-C2	-2.46	124.22	126.17
17	b	201	SLA	O10-C3-N4	-2.43	122.56	125.72
17	N	201	SLA	O10-C3-N4	-2.42	122.58	125.72
17	H	301	SLA	O10-C3-C2	-2.12	124.49	126.17
17	V	301	SLA	O10-C3-C2	-2.10	124.51	126.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	V	301	SLA	2	0
17	K	301	SLA	1	0
17	H	301	SLA	2	0
17	N	201	SLA	1	0
17	Y	301	SLA	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.43	4 (1%)	72	71	35, 48, 88, 126	0
1	O	250/250 (100%)	-0.40	6 (2%)	59	56	37, 57, 98, 134	0
2	B	244/258 (94%)	-0.37	5 (2%)	65	63	35, 55, 99, 158	0
2	P	244/258 (94%)	-0.29	9 (3%)	41	37	38, 57, 100, 158	0
3	C	240/254 (94%)	-0.22	12 (5%)	28	25	34, 57, 120, 150	0
3	Q	240/254 (94%)	-0.04	16 (6%)	17	13	41, 69, 146, 171	0
4	D	235/260 (90%)	-0.44	3 (1%)	77	77	39, 59, 90, 129	0
4	R	235/260 (90%)	-0.30	5 (2%)	63	61	43, 64, 102, 133	0
5	E	231/234 (98%)	-0.33	4 (1%)	70	69	42, 63, 97, 135	0
5	S	231/234 (98%)	-0.24	5 (2%)	62	59	40, 66, 108, 145	0
6	F	243/288 (84%)	-0.47	4 (1%)	72	71	32, 57, 105, 131	0
6	T	243/288 (84%)	-0.39	5 (2%)	63	61	32, 62, 117, 144	0
7	G	241/252 (95%)	-0.53	1 (0%)	92	93	32, 51, 85, 130	0
7	U	241/252 (95%)	-0.45	6 (2%)	57	55	36, 53, 87, 139	0
8	H	226/232 (97%)	-0.50	7 (3%)	49	44	29, 45, 78, 143	0
8	V	226/232 (97%)	-0.44	7 (3%)	49	44	32, 48, 82, 170	0
9	I	204/205 (99%)	-0.70	1 (0%)	91	91	30, 44, 73, 100	0
9	W	204/205 (99%)	-0.65	2 (0%)	82	82	32, 48, 78, 107	0
10	J	195/198 (98%)	-0.60	3 (1%)	73	73	32, 48, 75, 109	0
10	X	195/198 (98%)	-0.56	3 (1%)	73	73	32, 50, 76, 125	0
11	K	212/212 (100%)	-0.61	0	100	100	29, 47, 76, 91	0
11	Y	212/212 (100%)	-0.58	0	100	100	34, 47, 78, 90	0
12	L	222/222 (100%)	-0.57	1 (0%)	91	91	32, 49, 89, 123	0
12	Z	222/222 (100%)	-0.53	1 (0%)	91	91	29, 49, 87, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.60	2 (0%)	84	84	29, 49, 74, 90	0
13	a	233/246 (94%)	-0.62	1 (0%)	92	93	29, 45, 67, 86	0
14	N	196/196 (100%)	-0.65	1 (0%)	91	91	29, 43, 72, 97	0
14	b	196/196 (100%)	-0.65	1 (0%)	91	91	29, 44, 73, 105	0
All	All	6344/6614 (95%)	-0.46	115 (1%)	68	67	29, 53, 96, 171	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	7.9
3	Q	50	LEU	6.8
8	V	224	GLN	6.8
2	B	221	ASP	6.0
2	P	220	ASN	5.3
3	C	206	LYS	5.1
2	P	51	VAL	5.0
10	X	1	MET	4.9
3	Q	206	LYS	4.7
3	Q	239	GLN	4.6
8	V	222	ASP	4.6
5	S	202	ASP	4.4
8	H	224	GLN	4.4
2	B	51	VAL	4.3
1	A	2	THR	4.2
2	P	59	ASP	4.1
8	V	226	GLU	4.1
3	Q	236	GLN	4.1
8	V	223	ILE	4.0
4	R	241	ALA	4.0
2	P	221	ASP	3.9
8	H	222	ASP	3.9
8	V	221	CYS	3.9
3	C	205	ALA	3.8
6	F	244	ASN	3.8
2	P	219	ALA	3.7
1	A	1	MET	3.7
2	P	222	GLY	3.7
3	C	236	GLN	3.6
8	H	226	GLU	3.6
12	L	174	TYR	3.5
3	C	240	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
5	E	202	ASP	3.5
2	B	218	GLY	3.5
3	Q	238	LYS	3.4
3	C	239	GLN	3.4
10	X	194	ASP	3.3
3	Q	240	GLU	3.3
4	R	125	LEU	3.1
12	Z	174	TYR	3.1
8	H	221	CYS	3.1
10	X	193	ASP	3.1
7	U	2	GLY	3.1
4	R	217	GLN	3.0
1	A	249	ALA	3.0
3	C	50	LEU	3.0
10	J	194	ASP	3.0
2	B	220	ASN	2.9
1	O	249	ALA	2.9
10	J	1	MET	2.9
3	C	49	THR	2.8
3	Q	202	GLN	2.8
5	E	217	LYS	2.8
8	V	225	GLU	2.8
9	W	1	SER	2.8
13	a	1	THR	2.7
6	T	244	ASN	2.6
3	Q	225	GLU	2.6
5	E	201	ARG	2.6
7	U	242	GLN	2.5
6	F	181	GLU	2.5
13	M	47	ASP	2.5
6	F	205	GLU	2.5
3	C	238	LYS	2.5
14	N	105	LYS	2.5
3	C	202	GLN	2.5
3	Q	55	THR	2.5
5	S	3	ASN	2.5
3	Q	48	SER	2.4
3	C	225	GLU	2.4
1	O	201	GLU	2.4
2	B	217	LYS	2.4
3	Q	203	THR	2.4
1	O	52	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	181	GLU	2.4
2	P	60	THR	2.4
7	G	242	GLN	2.4
13	M	1	THR	2.4
9	I	1	SER	2.4
8	H	223	ILE	2.4
3	Q	180	LYS	2.4
7	U	222	ASP	2.4
1	O	248	GLU	2.3
6	T	178	HIS	2.3
1	O	2	THR	2.3
3	Q	205	ALA	2.3
4	D	242	GLU	2.3
9	W	192	ASP	2.3
4	D	1	ASP	2.3
5	S	227	GLU	2.3
5	S	173	ARG	2.3
7	U	241	GLU	2.3
2	P	182	ASP	2.2
3	Q	229	GLN	2.2
2	P	203	SER	2.2
1	A	201	GLU	2.2
8	H	198	GLU	2.1
6	T	2	THR	2.1
4	R	1	ASP	2.1
6	T	243	ILE	2.1
8	H	225	GLU	2.1
7	U	188	GLU	2.1
8	V	145	ASP	2.1
1	O	1	MET	2.1
4	R	242	GLU	2.1
7	U	3	TYR	2.1
10	J	193	ASP	2.1
6	T	230	ASP	2.0
5	E	173	ARG	2.0
4	D	125	LEU	2.0
3	Q	237	GLU	2.0
6	F	202	ASP	2.0
3	C	60	SER	2.0
5	S	165	GLN	2.0
14	b	195	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	SLA	N	201	15/15	0.94	0.15	44,45,46,46	0
17	SLA	Y	301	15/15	0.95	0.15	37,41,43,43	0
17	SLA	b	201	15/15	0.95	0.14	44,46,46,47	0
17	SLA	K	301	15/15	0.96	0.18	41,43,44,44	0
15	MG	Z	301	1/1	0.97	0.19	46,46,46,46	0
17	SLA	V	301	15/15	0.97	0.14	40,42,45,45	0
17	SLA	H	301	15/15	0.97	0.14	38,43,45,46	0
15	MG	J	201	1/1	0.97	0.22	34,34,34,34	0
15	MG	Y	302	1/1	0.98	0.11	44,44,44,44	0
15	MG	G	301	1/1	0.98	0.05	40,40,40,40	0
16	CL	N	203	1/1	0.98	0.07	40,40,40,40	0
16	CL	b	202	1/1	0.98	0.07	41,41,41,41	0
15	MG	K	302	1/1	0.98	0.07	42,42,42,42	0
16	CL	U	301	1/1	0.99	0.20	45,45,45,45	0
15	MG	V	302	1/1	0.99	0.06	50,50,50,50	0
16	CL	G	302	1/1	0.99	0.10	38,38,38,38	0
15	MG	N	202	1/1	0.99	0.06	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.