wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2026 – 07:47 AM UTC

PDB ID	:	4R02 / pdb_00004r02
Title	:	yCP in complex with BSc4999 (alpha-Keto Phenylamide)
Authors	:	Voss, C.; Scholz, C.; Knorr, S.; Beck, P.; Stein, M.; Zall, A.; Kuckelkorn, U.; Kloetzel, P.-M.; Groll, M.; Hamacher, K.; Schmidt, B.
Deposited on	:	2014-07-29
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

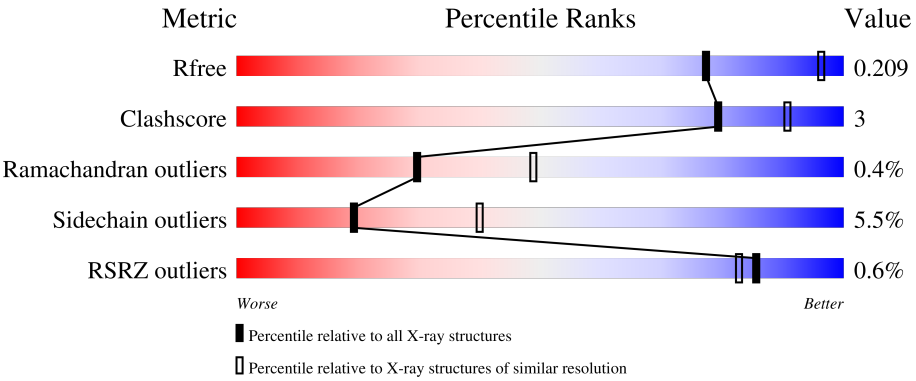
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	94%
1	O	250	92% 8%
2	B	258	83% 10% 5%
2	P	258	83% 9% 5%
3	C	254	81% 12% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	2% 84% 9% • 6%
4	D	260	79% 10% • 10%
4	R	260	78% 10% • 10%
5	E	234	89% 8% ••
5	S	234	88% 10% ••
6	F	288	% 78% • • 16%
6	T	288	2% 76% 7% • 16%
7	G	252	87% 8% • •
7	U	252	88% 6% • •
8	H	232	% 88% 9% •
8	V	232	% 89% 7% • •
9	I	205	91% 8% •
9	W	205	91% 8%
10	J	198	% 90% 7% • •
10	X	198	% 89% 8% ••
11	K	212	% 92% 6% •
11	Y	212	91% 8% •
12	L	222	92% 5% •
12	Z	222	92% 7% •
13	M	246	86% 7% • 5%
13	a	246	84% 9% • 5%
14	N	196	% 89% 9% •
14	b	196	88% 10% •

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 52173 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
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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

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

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

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

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

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	I	2	Total	Mg	0	0
			2	2		

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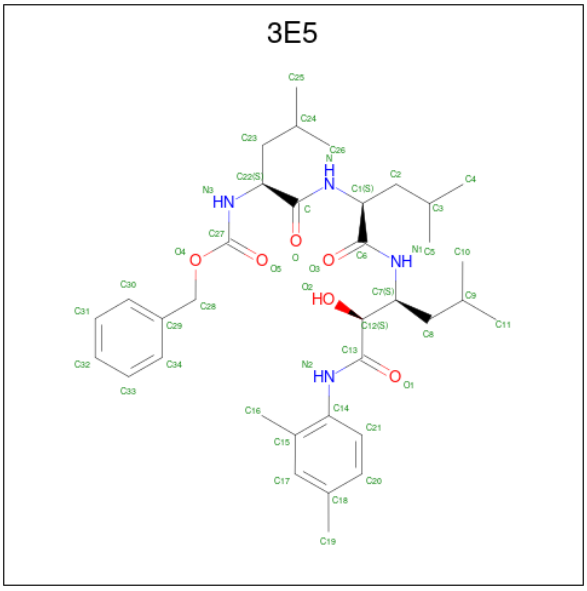
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	J	1	Total Mg 1 1	0	0
15	K	2	Total Mg 2 2	0	0
15	N	2	Total Mg 2 2	0	0
15	V	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is N-[(benzyloxy)carbonyl]-L-leucyl-N-{(2S,3S)-1-[(2,4-dimethylphenyl) amino]-2-hydroxy-5-methyl-1-oxohexan-3-yl}-L-leucinamide (CCD ID: 3E5) (formula: $C_{35}H_{52}N_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	K	1	Total C N O 45 35 4 6	0	0
16	Y	1	Total C N O 45 35 4 6	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	121	Total O 121 121	0	0
17	B	84	Total O 84 84	0	0
17	C	88	Total O 88 88	0	0
17	D	82	Total O 82 82	0	0
17	E	44	Total O 44 44	0	0
17	F	93	Total O 93 93	0	0
17	G	117	Total O 117 117	0	0
17	H	110	Total O 110 110	0	0
17	I	106	Total O 106 106	0	0
17	J	101	Total O 101 101	0	0
17	K	119	Total O 119 119	0	0
17	L	118	Total O 118 118	0	0
17	M	141	Total O 141 141	0	0
17	N	108	Total O 108 108	0	0
17	O	79	Total O 79 79	0	0
17	P	73	Total O 73 73	0	0
17	Q	61	Total O 61 61	0	0
17	R	74	Total O 74 74	0	0
17	S	38	Total O 38 38	0	0
17	T	82	Total O 82 82	0	0
17	U	109	Total O 109 109	0	0
17	V	89	Total O 89 89	0	0

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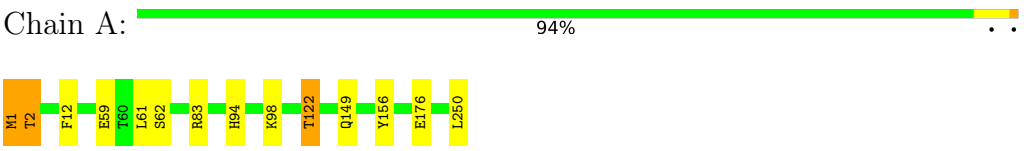
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	W	104	Total O 104 104	0	0
17	X	92	Total O 92 92	0	0
17	Y	114	Total O 114 114	0	0
17	Z	126	Total O 126 126	0	0
17	a	137	Total O 137 137	0	0
17	b	96	Total O 96 96	0	0

3 Residue-property plots (i)

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

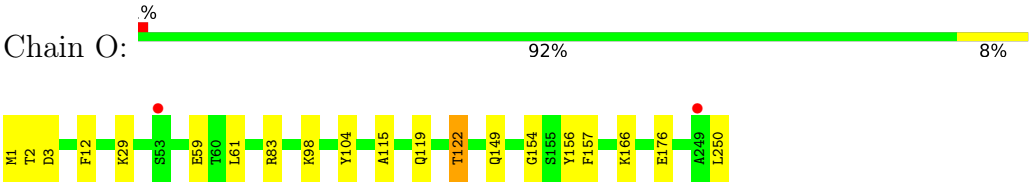
• Molecule 1: Proteasome subunit alpha type-2

Chain A:



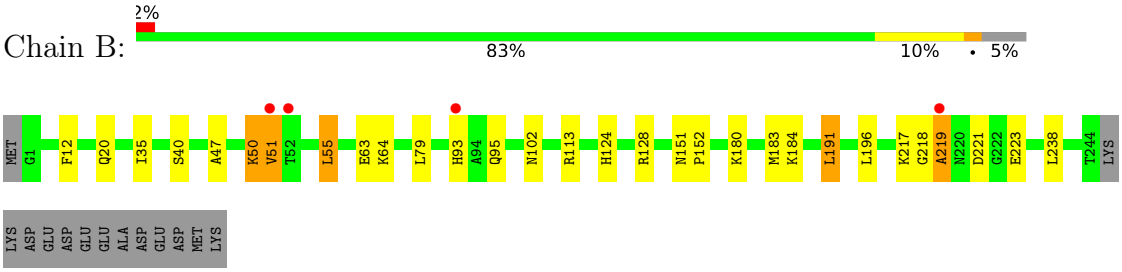
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



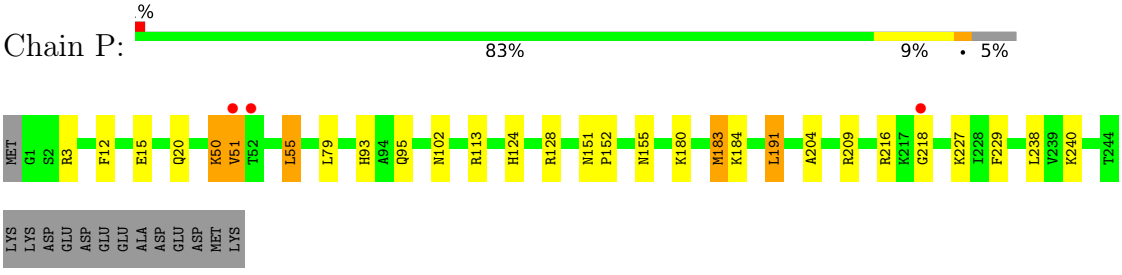
• Molecule 2: Proteasome subunit alpha type-3

Chain B:



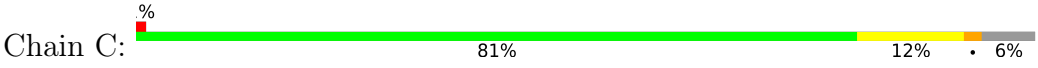
• Molecule 2: Proteasome subunit alpha type-3

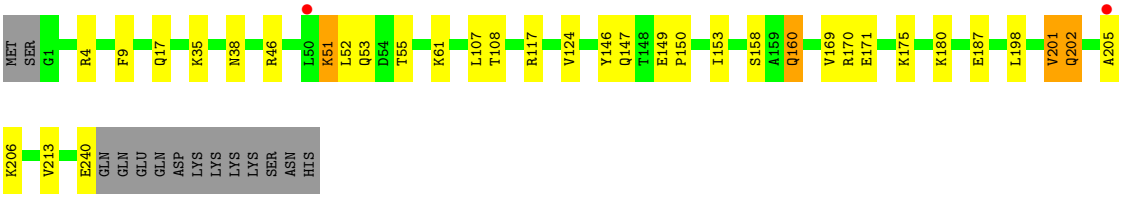
Chain P:



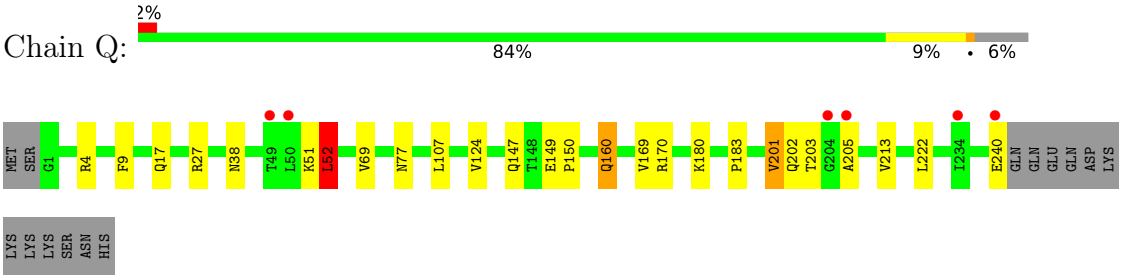
• Molecule 3: Proteasome subunit alpha type-4

Chain C:

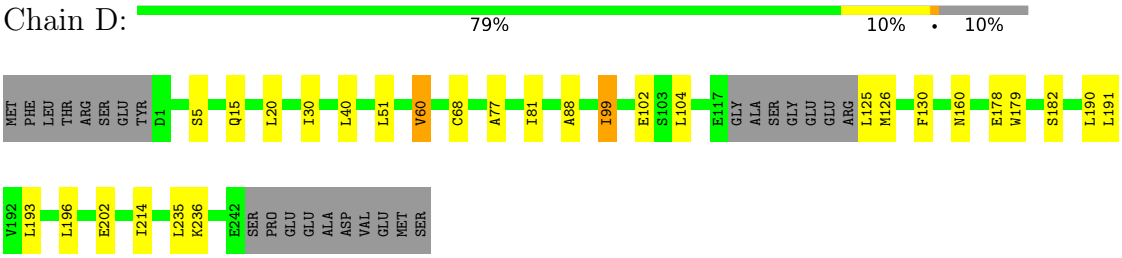




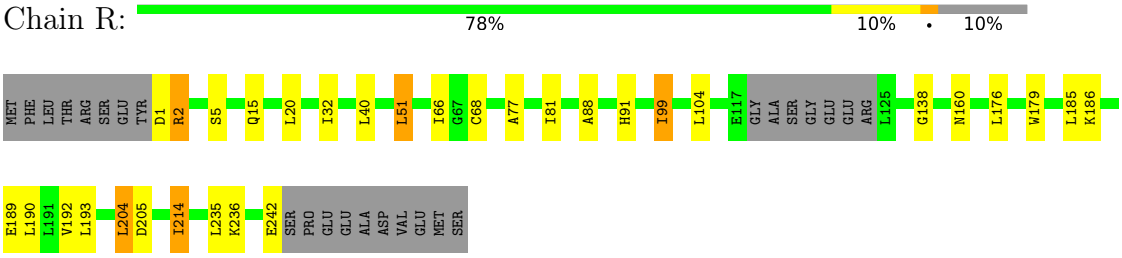
• Molecule 3: Proteasome subunit alpha type-4



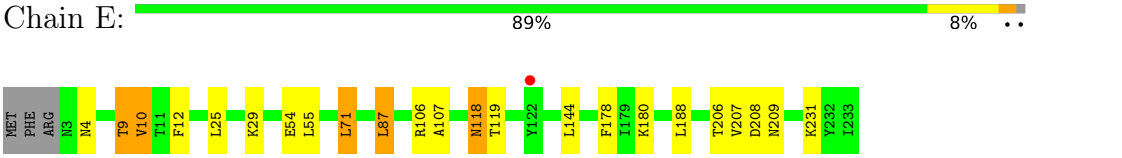
• Molecule 4: Proteasome subunit alpha type-5



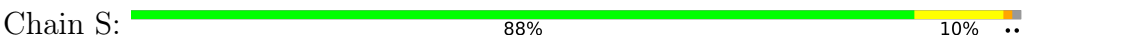
• Molecule 4: Proteasome subunit alpha type-5

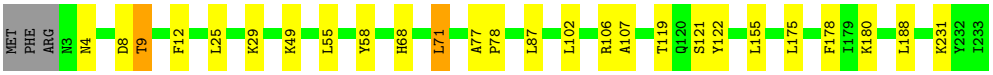


• Molecule 5: Proteasome subunit alpha type-6

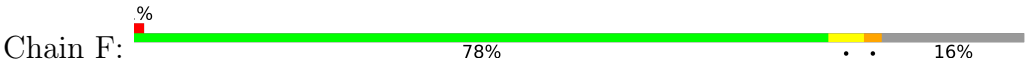


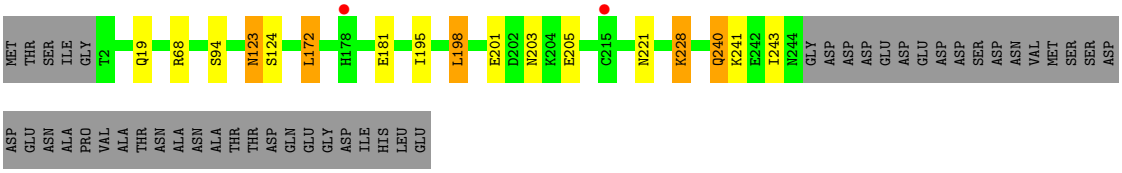
• Molecule 5: Proteasome subunit alpha type-6



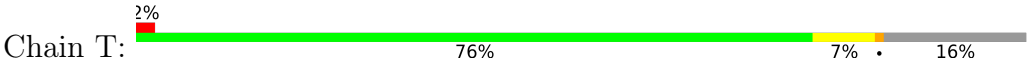


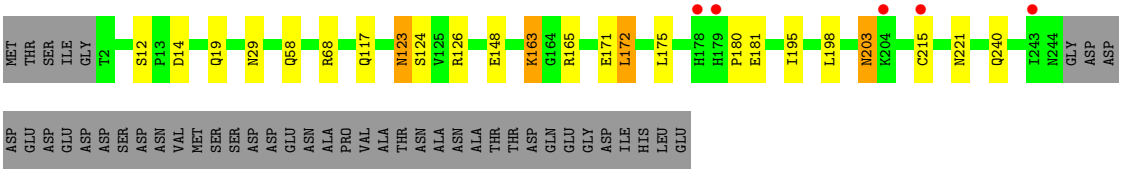
• Molecule 6: Probable proteasome subunit alpha type-7



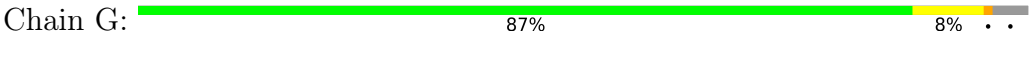


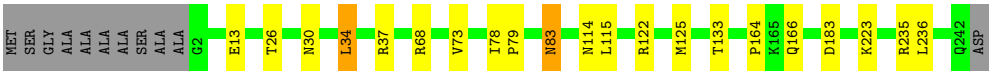
• Molecule 6: Probable proteasome subunit alpha type-7



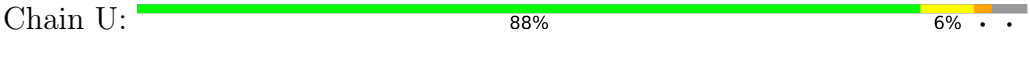


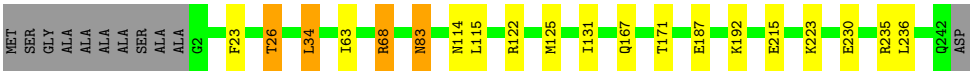
• Molecule 7: Proteasome subunit alpha type-1



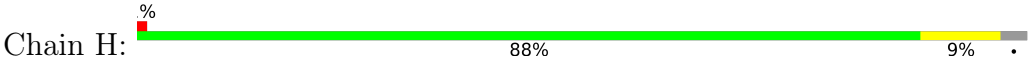


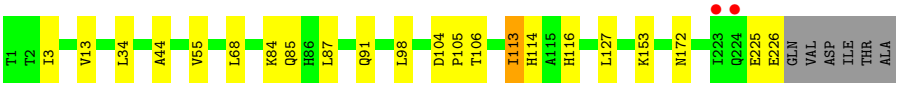
• Molecule 7: Proteasome subunit alpha type-1



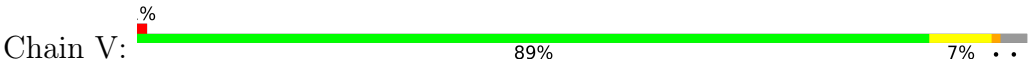


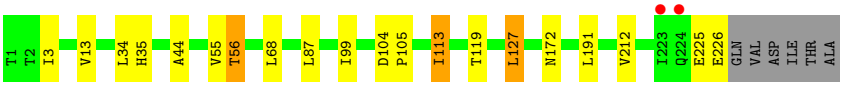
• Molecule 8: Proteasome subunit beta type-2



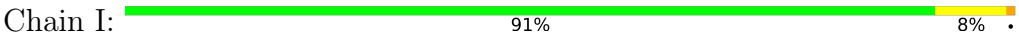


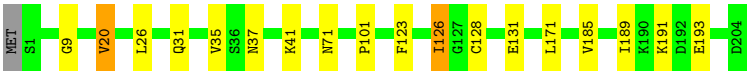
• Molecule 8: Proteasome subunit beta type-2



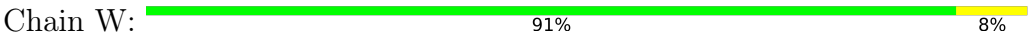


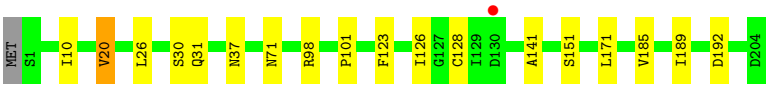
• Molecule 9: Proteasome subunit beta type-3



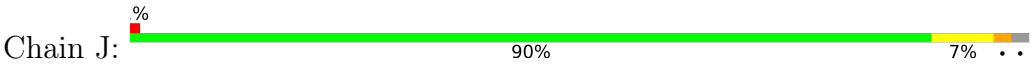


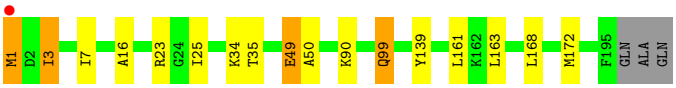
• Molecule 9: Proteasome subunit beta type-3



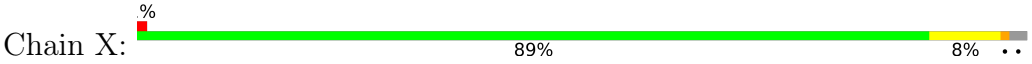


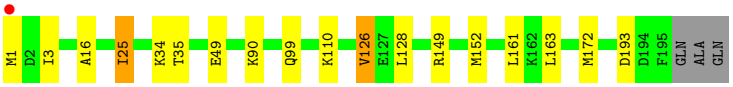
• Molecule 10: Proteasome subunit beta type-4



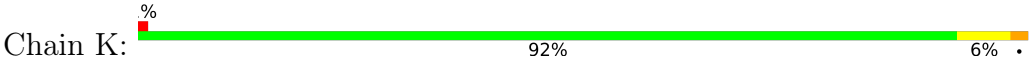


• Molecule 10: Proteasome subunit beta type-4

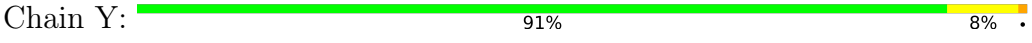




• Molecule 11: Proteasome subunit beta type-5

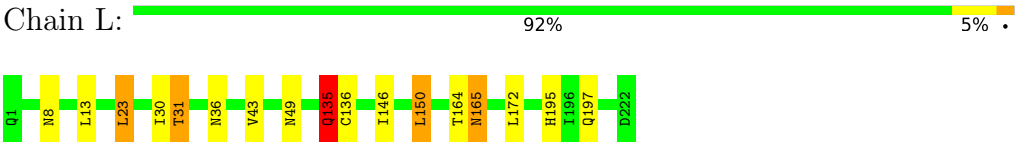


• Molecule 11: Proteasome subunit beta type-5



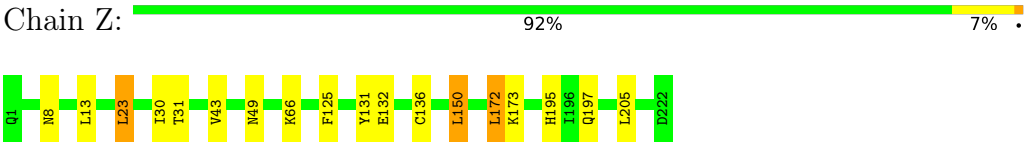
• Molecule 12: Proteasome subunit beta type-6

Chain L:



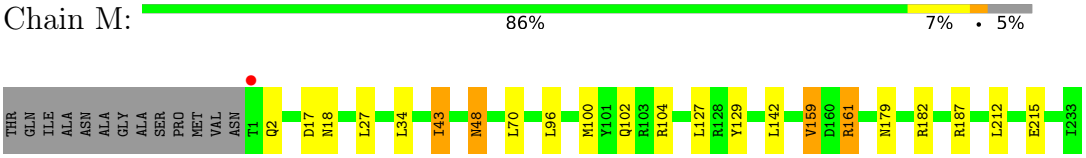
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



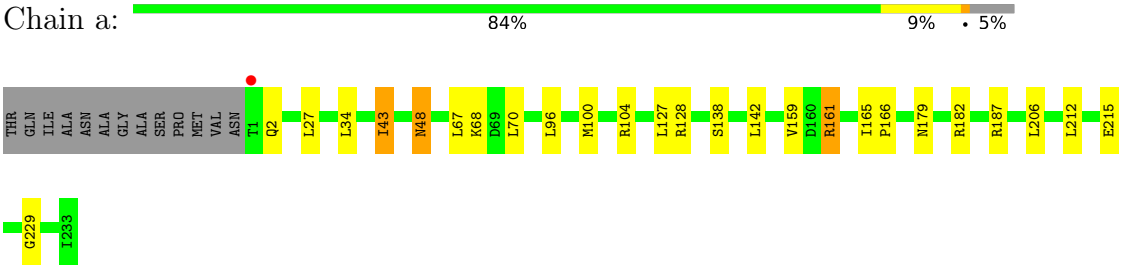
• Molecule 13: Proteasome subunit beta type-7

Chain M:



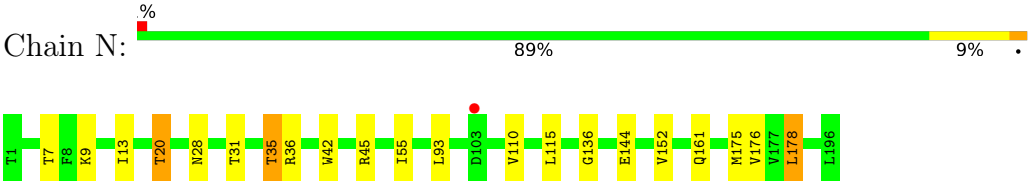
• Molecule 13: Proteasome subunit beta type-7

Chain a:



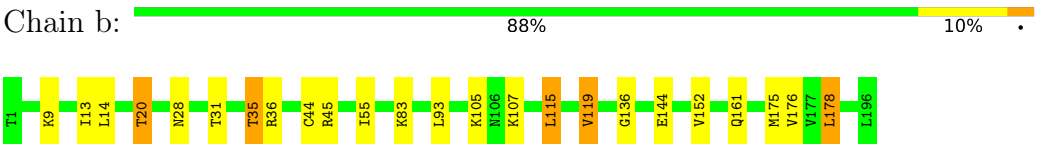
• Molecule 14: Proteasome subunit beta type-1

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	137.24Å 300.87Å 146.29Å 90.00° 113.20° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-2.50) 96.5 (15.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.207 0.172 , 0.209	Depositor DCC
R_{free} test set	18074 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.2	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	52173	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: MG, 3E5

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	0.40	0/1952	0.68	0/2642
1	O	0.41	0/1952	0.69	0/2642
2	B	0.40	0/1934	0.70	0/2618
2	P	0.40	0/1934	0.69	0/2618
3	C	0.41	0/1910	0.70	0/2586
3	Q	0.42	0/1910	0.73	1/2586 (0.0%)
4	D	0.40	0/1837	0.68	0/2475
4	R	0.40	0/1837	0.68	0/2475
5	E	0.40	0/1800	0.68	0/2433
5	S	0.40	0/1800	0.69	0/2433
6	F	0.42	0/1932	0.71	0/2609
6	T	0.42	0/1932	0.69	0/2609
7	G	0.40	0/1945	0.69	0/2634
7	U	0.38	0/1945	0.69	0/2634
8	H	0.39	0/1750	0.69	0/2373
8	V	0.39	0/1750	0.67	0/2373
9	I	0.39	0/1611	0.69	0/2174
9	W	0.39	0/1611	0.68	0/2174
10	J	0.40	0/1589	0.66	0/2142
10	X	0.40	0/1589	0.67	0/2142
11	K	0.38	0/1681	0.68	0/2274
11	Y	0.40	0/1681	0.68	0/2274
12	L	0.38	0/1795	0.68	0/2420
12	Z	0.39	0/1795	0.68	0/2420
13	M	0.40	0/1855	0.68	0/2514
13	a	0.40	0/1855	0.71	0/2514
14	N	0.38	0/1541	0.68	0/2087
14	b	0.38	0/1541	0.68	1/2087 (0.0%)
All	All	0.40	0/50264	0.69	2/67962 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	201	VAL	N-CA-C	6.57	118.41	112.17
14	b	115	LEU	N-CA-C	5.02	117.40	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	135	GLN	Peptide

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	8	0
1	O	1915	0	1929	9	0
2	B	1904	0	1904	16	0
2	P	1904	0	1904	20	0
3	C	1881	0	1895	15	0
3	Q	1881	0	1895	11	0
4	D	1813	0	1797	9	0
4	R	1813	0	1797	16	0
5	E	1773	0	1775	8	0
5	S	1773	0	1775	9	0
6	F	1892	0	1883	7	0
6	T	1892	0	1883	7	0
7	G	1907	0	1901	10	0
7	U	1907	0	1901	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1719	0	1719	8	0
8	V	1719	0	1719	11	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	8	0
10	J	1561	0	1569	10	0
10	X	1561	0	1569	8	0
11	K	1644	0	1594	9	0
11	Y	1644	0	1594	8	0
12	L	1757	0	1711	12	0
12	Z	1757	0	1711	8	0
13	M	1824	0	1832	10	0
13	a	1824	0	1832	10	0
14	N	1512	0	1481	13	0
14	b	1512	0	1481	16	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	N	2	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	K	45	0	51	1	0
16	Y	45	0	51	0	0
17	A	121	0	0	0	0
17	B	84	0	0	0	0
17	C	88	0	0	0	0
17	D	82	0	0	0	0
17	E	44	0	0	0	0
17	F	93	0	0	0	0
17	G	117	0	0	0	0
17	H	110	0	0	1	0
17	I	106	0	0	0	0
17	J	101	0	0	1	0
17	K	119	0	0	0	0
17	L	118	0	0	1	0
17	M	141	0	0	1	0
17	N	108	0	0	0	0
17	O	79	0	0	0	0
17	P	73	0	0	0	0
17	Q	61	0	0	0	0
17	R	74	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	S	38	0	0	0	0
17	T	82	0	0	0	0
17	U	109	0	0	0	0
17	V	89	0	0	1	0
17	W	104	0	0	0	0
17	X	92	0	0	0	0
17	Y	114	0	0	0	0
17	Z	126	0	0	0	0
17	a	137	0	0	0	0
17	b	96	0	0	1	0
All	All	52173	0	49230	268	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 3.

The worst 5 of 268 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)
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.54	0.89
13:a:43:ILE:HD11	13:a:67:LEU:HD12	1.62	0.80
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.81	0.80
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.71	0.73
5:E:12:PHE:H	6:F:19:GLN:HE22	1.34	0.73

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%)	241 (97%)	6 (2%)	1 (0%)	30 49
1	O	248/250 (99%)	239 (96%)	7 (3%)	2 (1%)	16 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7 13
2	P	242/258 (94%)	231 (96%)	9 (4%)	2 (1%)	16 31
3	C	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	9 18
3	Q	238/254 (94%)	232 (98%)	2 (1%)	4 (2%)	7 13
4	D	231/260 (89%)	230 (100%)	1 (0%)	0	100 100
4	R	231/260 (89%)	226 (98%)	4 (2%)	1 (0%)	30 49
5	E	229/234 (98%)	221 (96%)	7 (3%)	1 (0%)	30 49
5	S	229/234 (98%)	219 (96%)	10 (4%)	0	100 100
6	F	241/288 (84%)	235 (98%)	5 (2%)	1 (0%)	30 49
6	T	241/288 (84%)	235 (98%)	5 (2%)	1 (0%)	30 49
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100 100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100 100
8	H	224/232 (97%)	217 (97%)	7 (3%)	0	100 100
8	V	224/232 (97%)	217 (97%)	7 (3%)	0	100 100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100 100
9	W	202/205 (98%)	197 (98%)	5 (2%)	0	100 100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100 100
10	X	193/198 (98%)	186 (96%)	7 (4%)	0	100 100
11	K	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	24 43
11	Y	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	24 43
12	L	220/222 (99%)	214 (97%)	5 (2%)	1 (0%)	24 43
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100 100
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100 100
13	a	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	30 49
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%)	6108 (97%)	152 (2%)	24 (0%)	30 49

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL

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Mol	Chain	Res	Type
3	C	202	GLN
12	L	165	ASN
1	O	2	THR

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%)	203 (97%)	6 (3%)	37	65
1	O	209/209 (100%)	201 (96%)	8 (4%)	29	56
2	B	203/216 (94%)	192 (95%)	11 (5%)	20	41
2	P	203/216 (94%)	194 (96%)	9 (4%)	25	50
3	C	212/226 (94%)	194 (92%)	18 (8%)	10	22
3	Q	212/226 (94%)	199 (94%)	13 (6%)	17	35
4	D	194/215 (90%)	178 (92%)	16 (8%)	10	23
4	R	194/215 (90%)	179 (92%)	15 (8%)	12	25
5	E	190/193 (98%)	174 (92%)	16 (8%)	10	22
5	S	190/193 (98%)	177 (93%)	13 (7%)	14	31
6	F	201/239 (84%)	189 (94%)	12 (6%)	17	36
6	T	201/239 (84%)	184 (92%)	17 (8%)	10	22
7	G	206/210 (98%)	196 (95%)	10 (5%)	22	45
7	U	206/210 (98%)	196 (95%)	10 (5%)	22	45
8	H	185/190 (97%)	176 (95%)	9 (5%)	22	45
8	V	185/190 (97%)	177 (96%)	8 (4%)	26	51
9	I	172/173 (99%)	164 (95%)	8 (5%)	23	47
9	W	172/173 (99%)	165 (96%)	7 (4%)	27	53
10	J	173/175 (99%)	164 (95%)	9 (5%)	21	42
10	X	173/175 (99%)	162 (94%)	11 (6%)	16	33
11	K	169/169 (100%)	161 (95%)	8 (5%)	23	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Y	169/169 (100%)	163 (96%)	6 (4%)	31	58
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	62
12	Z	185/185 (100%)	176 (95%)	9 (5%)	22	45
13	M	199/208 (96%)	188 (94%)	11 (6%)	19	40
13	a	199/208 (96%)	188 (94%)	11 (6%)	19	40
14	N	162/162 (100%)	156 (96%)	6 (4%)	30	57
14	b	162/162 (100%)	152 (94%)	10 (6%)	16	34
All	All	5320/5540 (96%)	5027 (94%)	293 (6%)	19	40

5 of 293 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	V	13	VAL
14	b	36	ARG
8	V	191	LEU
11	Y	57	THR
8	H	153	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 171 such sidechains are listed below:

Mol	Chain	Res	Type
5	S	99	ASN
9	W	88	GLN
5	S	147	GLN
7	U	30	ASN
11	Y	143	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
16	3E5	Y	301	11	46,46,46	1.25	3 (6%)	60,62,62	1.24	5 (8%)
16	3E5	K	301	11	46,46,46	1.24	3 (6%)	60,62,62	1.17	6 (10%)

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
16	3E5	Y	301	11	-	8/49/49/49	0/2/2/2
16	3E5	K	301	11	-	8/49/49/49	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	301	3E5	O4-C27	5.52	1.46	1.35
16	Y	301	3E5	O4-C27	5.46	1.46	1.35
16	K	301	3E5	C14-C15	4.93	1.50	1.40
16	Y	301	3E5	C14-C15	4.71	1.50	1.40
16	Y	301	3E5	C14-N2	-2.62	1.36	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	301	3E5	C12-C13-N2	-3.93	111.94	115.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	301	3E5	O4-C27-N3	3.86	118.71	110.45
16	Y	301	3E5	O4-C27-O5	-3.62	117.32	124.26
16	K	301	3E5	O4-C27-N3	3.53	117.99	110.45
16	K	301	3E5	C21-C14-C15	-3.25	116.99	120.70

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	301	3E5	N3-C22-C23-C24
16	Y	301	3E5	O5-C27-O4-C28
16	Y	301	3E5	N3-C27-O4-C28
16	K	301	3E5	O5-C27-O4-C28
16	K	301	3E5	C-C22-C23-C24

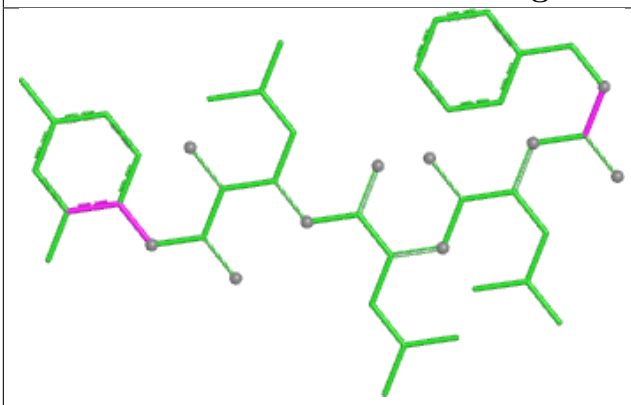
There are no ring outliers.

1 monomer is involved in 1 short contact:

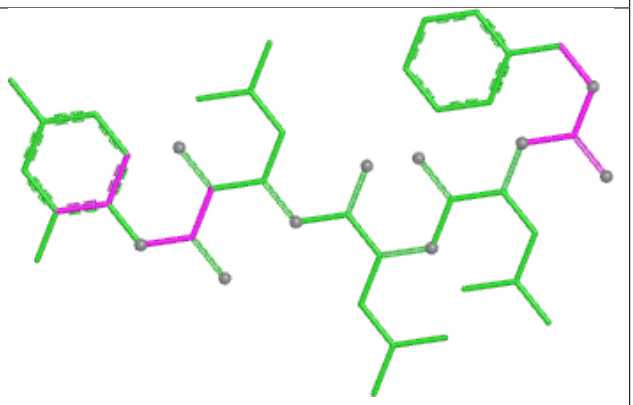
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	301	3E5	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

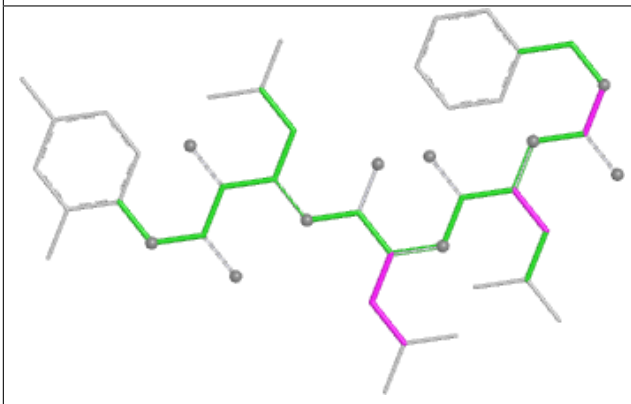
Ligand 3E5 Y 301



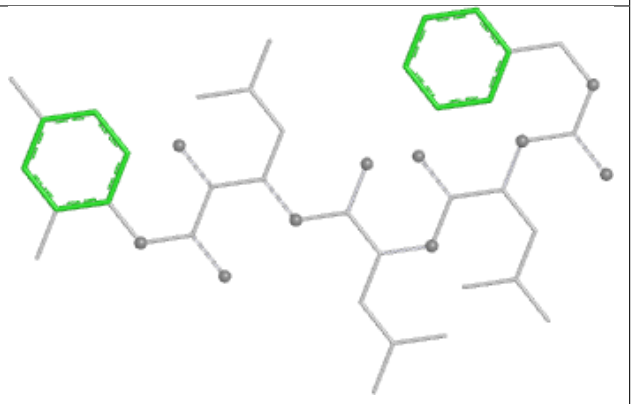
Bond lengths



Bond angles

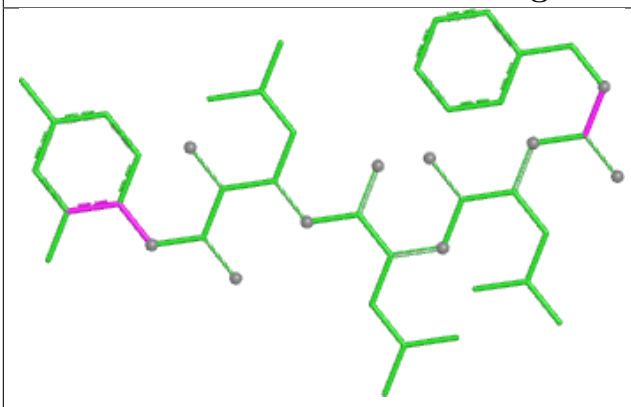


Torsions

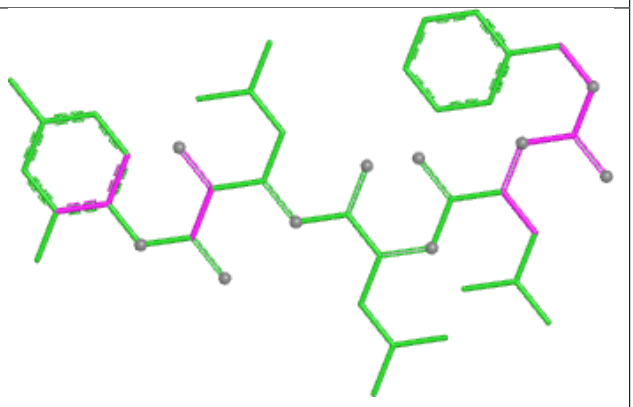


Rings

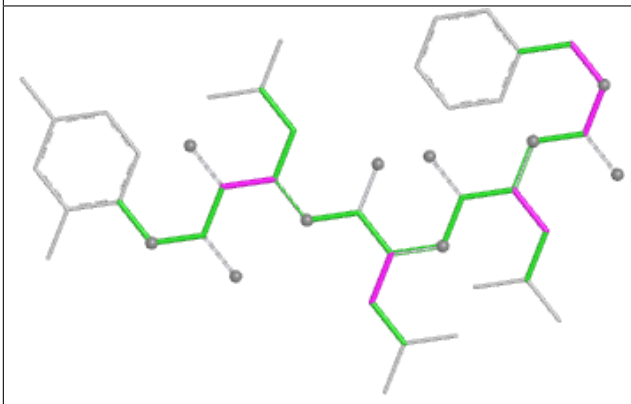
Ligand 3E5 K 301



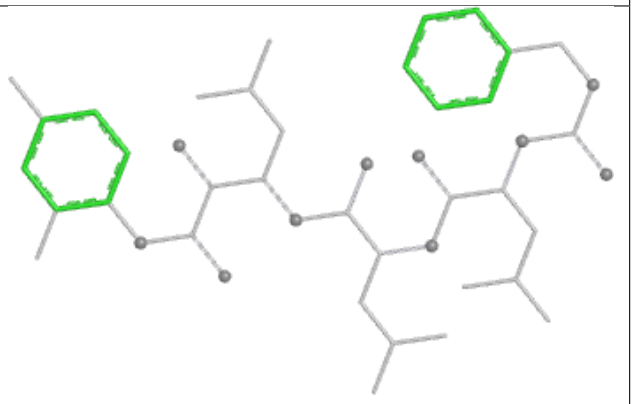
Bond lengths



Bond angles



Torsions



Rings

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%)	-0.62	0 100 100	33, 45, 74, 117	0
1	O	250/250 (100%)	-0.54	2 (0%) 82 80	36, 51, 88, 125	0
2	B	244/258 (94%)	-0.49	4 (1%) 70 67	33, 50, 90, 144	0
2	P	244/258 (94%)	-0.46	3 (1%) 76 73	37, 53, 102, 153	0
3	C	240/254 (94%)	-0.41	2 (0%) 82 80	34, 55, 115, 143	0
3	Q	240/254 (94%)	-0.26	6 (2%) 58 54	38, 64, 132, 161	0
4	D	235/260 (90%)	-0.54	0 100 100	36, 54, 82, 120	0
4	R	235/260 (90%)	-0.51	0 100 100	36, 56, 85, 136	0
5	E	231/234 (98%)	-0.46	1 (0%) 88 86	39, 57, 86, 120	0
5	S	231/234 (98%)	-0.40	0 100 100	40, 57, 87, 120	0
6	F	243/288 (84%)	-0.55	2 (0%) 82 80	33, 48, 90, 131	0
6	T	243/288 (84%)	-0.46	5 (2%) 63 59	33, 51, 93, 124	0
7	G	241/252 (95%)	-0.68	0 100 100	32, 46, 79, 122	0
7	U	241/252 (95%)	-0.65	0 100 100	33, 47, 78, 106	0
8	H	226/232 (97%)	-0.59	2 (0%) 81 78	34, 44, 73, 133	0
8	V	226/232 (97%)	-0.57	2 (0%) 81 78	34, 47, 78, 159	0
9	I	204/205 (99%)	-0.72	0 100 100	30, 45, 72, 100	0
9	W	204/205 (99%)	-0.65	1 (0%) 87 85	33, 47, 78, 106	0
10	J	195/198 (98%)	-0.63	1 (0%) 87 85	30, 45, 69, 137	0
10	X	195/198 (98%)	-0.60	1 (0%) 87 85	33, 46, 71, 125	0
11	K	212/212 (100%)	-0.56	2 (0%) 81 78	33, 46, 81, 97	0
11	Y	212/212 (100%)	-0.55	1 (0%) 87 85	33, 46, 83, 107	0
12	L	222/222 (100%)	-0.66	0 100 100	32, 46, 75, 100	0
12	Z	222/222 (100%)	-0.65	0 100 100	31, 45, 75, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.72	1 (0%)	88	86	29, 44, 63, 77	0
13	a	233/246 (94%)	-0.75	1 (0%)	88	86	29, 42, 61, 74	0
14	N	196/196 (100%)	-0.77	1 (0%)	87	85	31, 40, 66, 85	0
14	b	196/196 (100%)	-0.77	0	100	100	30, 41, 65, 94	0
All	All	6344/6614 (95%)	-0.57	38 (0%)	85	83	29, 48, 86, 161	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	7.1
10	J	1	MET	6.0
3	Q	50	LEU	5.1
6	T	178	HIS	4.2
8	H	223	ILE	3.7

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 oligosaccharides 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
16	3E5	Y	301	45/45	0.87	0.14	58,72,101,106	0
16	3E5	K	301	45/45	0.88	0.12	52,69,89,95	0
15	MG	I	302	1/1	0.89	0.30	82,82,82,82	0
15	MG	N	202	1/1	0.91	0.11	82,82,82,82	0
15	MG	K	303	1/1	0.94	0.14	49,49,49,49	0
15	MG	Z	301	1/1	0.95	0.07	54,54,54,54	0
15	MG	J	201	1/1	0.97	0.06	61,61,61,61	0

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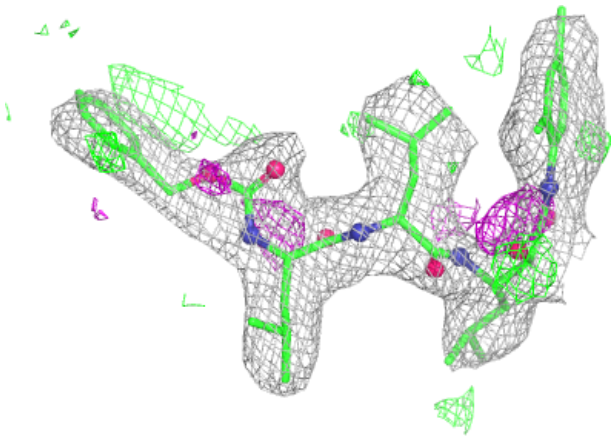
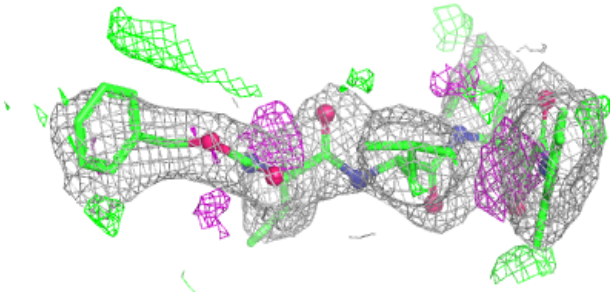
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	N	201	1/1	0.98	0.12	48,48,48,48	0
15	MG	V	301	1/1	0.98	0.11	42,42,42,42	0
15	MG	Y	302	1/1	0.98	0.10	42,42,42,42	0
15	MG	K	302	1/1	0.99	0.12	47,47,47,47	0
15	MG	G	301	1/1	0.99	0.03	40,40,40,40	0
15	MG	I	301	1/1	0.99	0.04	54,54,54,54	0

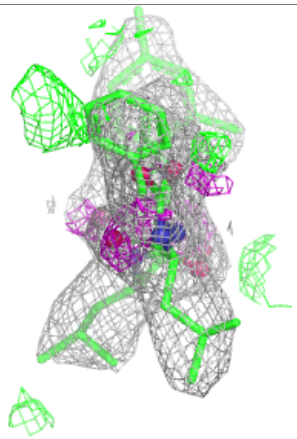
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 3E5 Y 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

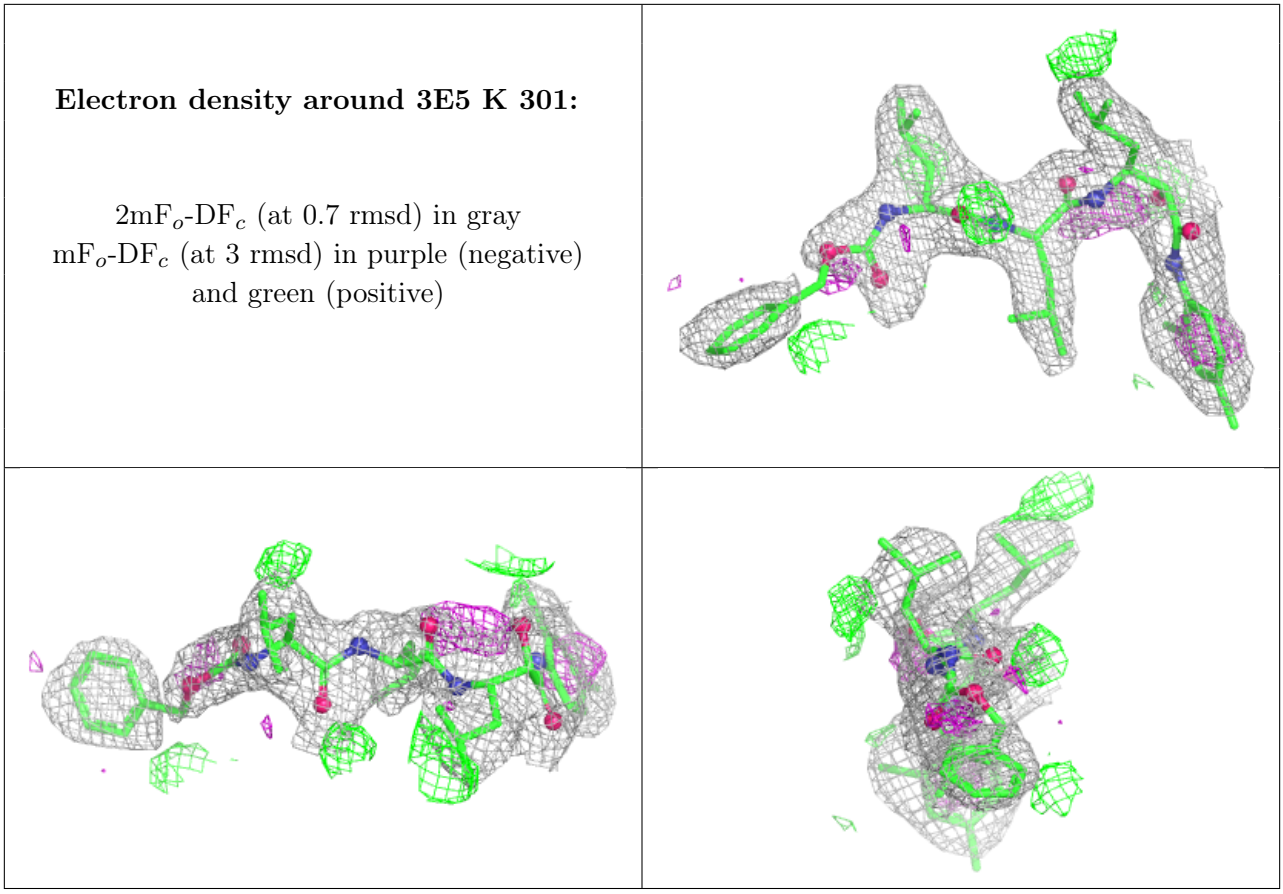






Electron density around 3E5 K 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.