



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:53 PM UTC

PDB ID : 5L63 / pdb_00005l63
Title : Yeast 20S proteasome with human beta5c (1-138) and human beta6 (97-111; 118-133) in complex with epoxyketone inhibitor 17
Authors : Groll, M.; Huber, E.M.
Deposited on : 2016-05-28
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) 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

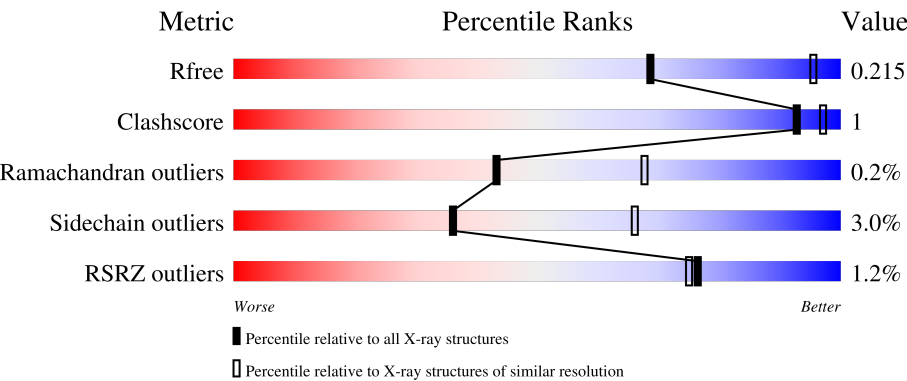
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	98% .
1	O	250	98% .
2	B	258	3% 89% 5% 5%
2	P	258	3% 89% 5% 5%
3	C	254	4% 87% 6% . 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	04C	H	301	X	-	-	-
17	04C	K	301	X	-	-	-
17	04C	V	301	X	-	-	-
17	04C	Y	301	X	-	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49924 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	1	0
			1726	1087	300	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,Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1632	1036	282	306	8			
11	Y	211	Total	C	N	O	S	0	0	0
			1632	1036	282	306	8			

- Molecule 12 is a protein called Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	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			

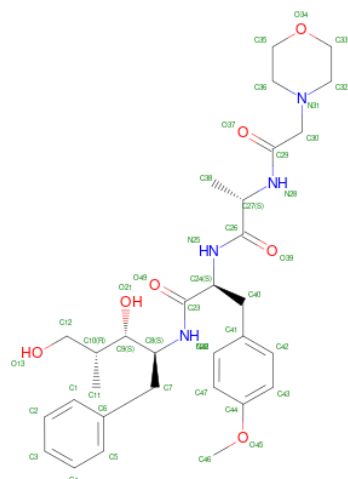
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total Mg 1 1	0	0
15	G	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	J	1	Total Mg 1 1	0	0
15	K	2	Total Mg 2 2	0	0
15	L	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	b	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

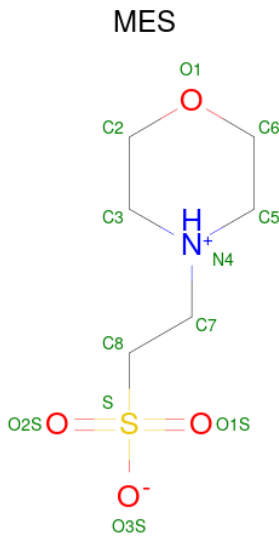
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is 1,2,4-trideoxy-4-methyl-2- {[N-(morpholin-4-ylacetyl)-L-alanyl-O-methyl-L-tyrosyl]amino}-1-phenyl-D-xylitol (CCD ID: 04C) (formula: C₃₁H₄₄N₄O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total 42	C 31	N 4	O 7	0	0
17	K	1	Total 42	C 31	N 4	O 7	0	0
17	V	1	Total 42	C 31	N 4	O 7	0	0
17	Y	1	Total 42	C 31	N 4	O 7	0	0

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	X	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	18	Total	O	0	0
			18	18		
19	B	15	Total	O	0	0
			15	15		
19	C	8	Total	O	0	0
			8	8		
19	D	9	Total	O	0	0
			9	9		
19	E	7	Total	O	0	0
			7	7		
19	F	8	Total	O	0	0
			8	8		
19	G	16	Total	O	0	0
			16	16		
19	H	11	Total	O	0	0
			11	11		
19	I	10	Total	O	0	0
			10	10		
19	J	13	Total	O	0	0
			13	13		
19	K	7	Total	O	0	0
			7	7		
19	L	14	Total	O	0	0
			14	14		
19	M	23	Total	O	0	0
			23	23		
19	N	9	Total	O	0	0
			9	9		
19	O	9	Total	O	0	0
			9	9		
19	P	11	Total	O	0	0
			11	11		

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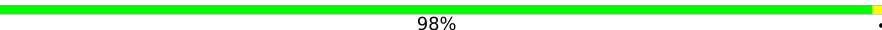
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	Q	8	Total O 8 8	0	0
19	R	10	Total O 10 10	0	0
19	S	7	Total O 7 7	0	0
19	T	13	Total O 13 13	0	0
19	U	20	Total O 20 20	0	0
19	V	16	Total O 16 16	0	0
19	W	10	Total O 10 10	0	0
19	X	12	Total O 12 12	0	0
19	Y	13	Total O 13 13	0	0
19	Z	7	Total O 7 7	0	0
19	a	19	Total O 19 19	0	0
19	b	9	Total O 9 9	0	0

3 Residue-property plots [i](#)

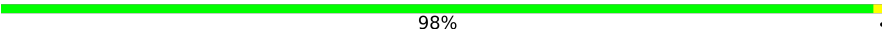
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:  98% .



- Molecule 1: Proteasome subunit alpha type-2

Chain O:  98% .



- Molecule 2: Proteasome subunit alpha type-3

Chain B:  89% 5% 5% 3%



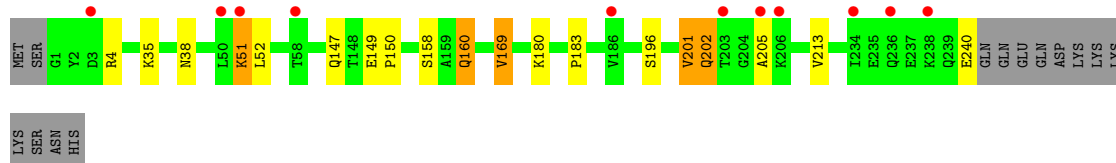
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  89% 5% 5% 3%



- Molecule 3: Proteasome subunit alpha type-4

Chain C:  87% 6% 6% 4%



[illegible]

MET	PHE	LEU	THR	ARG	SER	GLU	TYR	D1	A88	V89	I90	H91	I99	E117	GLY	ALA	SER	GLY	GLU	GLU	ARG	L125	N160	L176	W179	L193	I214	L235	K236	A241	E242	SER	PRO	GLU	GLU	ALA	ASP	VAL	GLU	MET	SER
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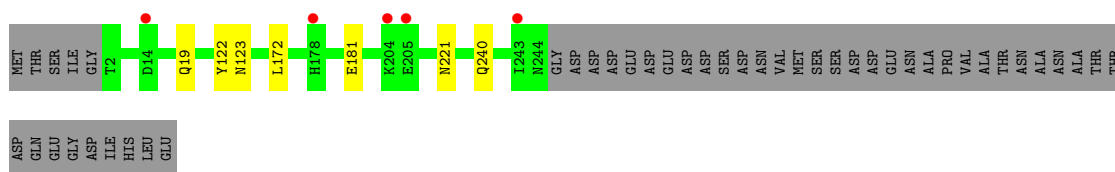
MET	PHE	LEU	THR	ARG	SER	GLU	TTR	D1	A88	V89	T90	H81	I99	A112	E117	GLY	ALA	SER	GLY	GLU	GLU	ARG	L125	M160	L176	M179	L193	I214	L235	K236	E239	A240	A241	E242	SER	PRO	GLU	GLU	ALA	ASP	VAL	GLU	MET
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Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows the amino acid sequence: MET, PHE, ARG, N3, T9, K29, L55, L71, A77, P78, L188, I233. The N3 position has the highest information content, followed by T9, K29, L55, L71, A77, P78, L188, and I233. MET and PHE have the lowest information content.

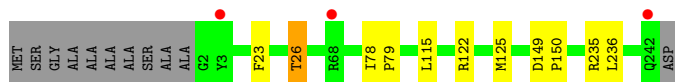
MET
PHE
ARG
N3
T9
F12
K29
L55
L71
A77 P78
L96
V97
F98
Y122
R173
L188
N209
I233

LEU	GLU	MET	THR	SER	ILE	GLY	T2	N123	L172	E181	D202	C215	N221	Q240	N243	GLY	ASP	ASP	ASP	GLU	ASP	GLU	ASP	ASP	SER	SER	ASN	VAL	MET	SER	SER	ASP	ASP	GLU	GLU	ASN	ALA	PRO	VAL	ALA	THR	ASN	ALA	ASN	ALA	THR	THR	ASP	GLN	GLU	GLY	ASP	ILE
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Chain T:



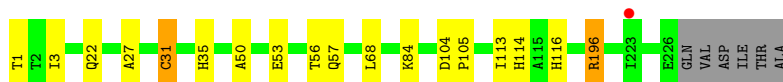
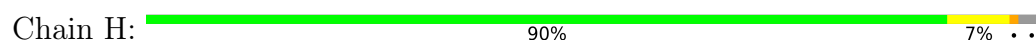
- Molecule 7: Proteasome subunit alpha type-1



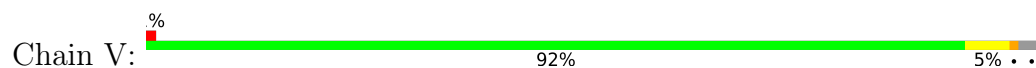
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



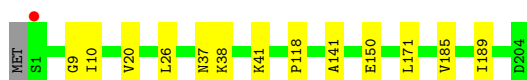
- Molecule 8: Proteasome subunit beta type-2



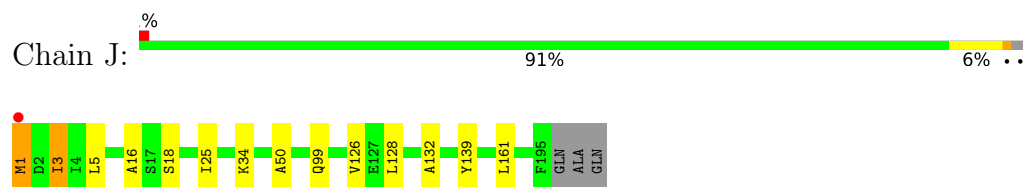
- Molecule 9: Proteasome subunit beta type-3



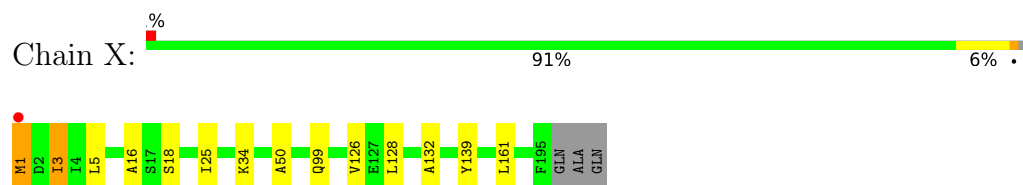
- Molecule 9: Proteasome subunit beta type-3



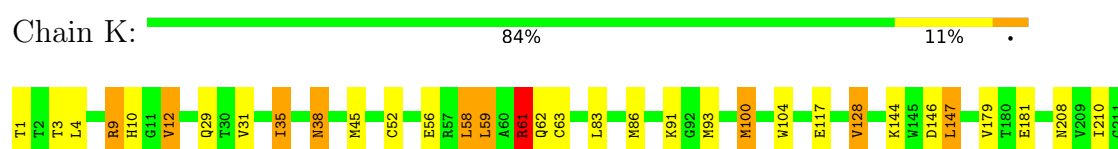
- Molecule 10: Proteasome subunit beta type-4



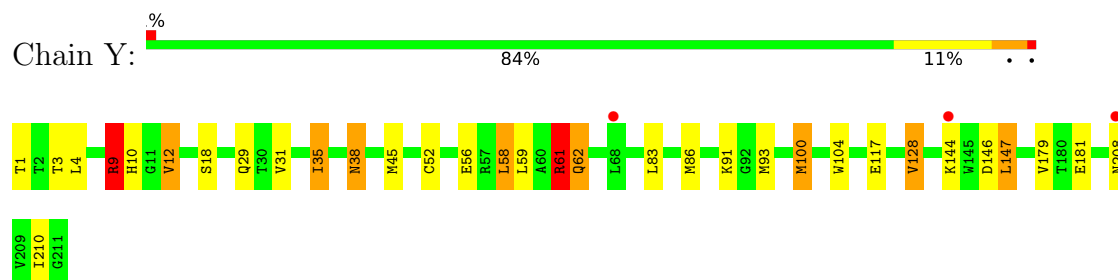
- Molecule 10: Proteasome subunit beta type-4



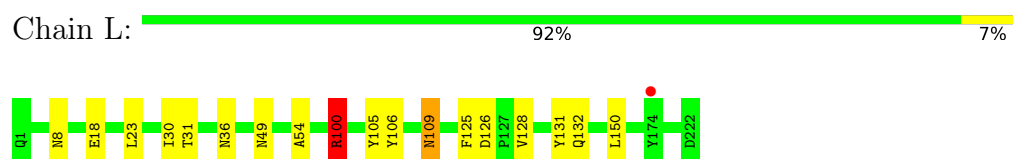
- Molecule 11: Proteasome subunit beta type-5, Proteasome subunit beta type-5



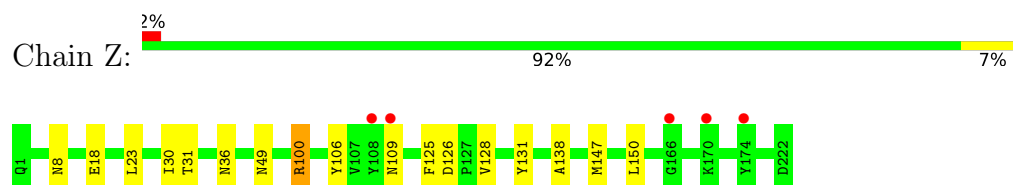
- Molecule 11: Proteasome subunit beta type-5, Proteasome subunit beta type-5



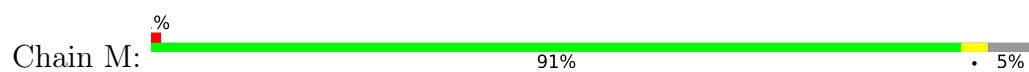
- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6



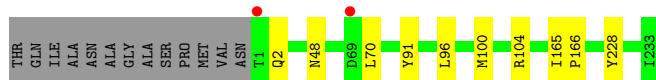
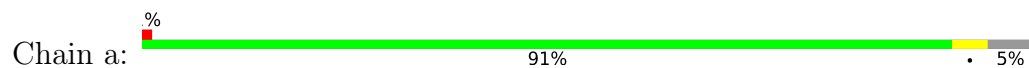
- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6



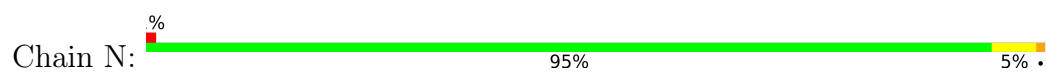
- Molecule 13: Proteasome subunit beta type-7



- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.41 Å 300.50 Å 145.72 Å 90.00° 112.82° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (15.00-2.70) 97.5 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.190 , 0.212 0.194 , 0.215	Depositor DCC
R_{free} test set	14272 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49924	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: 04C, MG, CL, MES

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	0.39	0/1952	0.68	0/2642
1	O	0.39	0/1952	0.69	0/2642
2	B	0.40	0/1934	0.67	0/2618
2	P	0.40	0/1934	0.67	0/2618
3	C	0.39	0/1910	0.69	1/2586 (0.0%)
3	Q	0.39	0/1910	0.69	1/2586 (0.0%)
4	D	0.38	0/1837	0.66	0/2475
4	R	0.38	0/1837	0.66	0/2475
5	E	0.39	0/1800	0.65	0/2433
5	S	0.39	0/1800	0.65	0/2433
6	F	0.39	0/1932	0.69	0/2609
6	T	0.39	0/1932	0.70	0/2609
7	G	0.39	0/1945	0.67	0/2634
7	U	0.39	0/1945	0.67	0/2634
8	H	0.35	0/1761	0.68	0/2388
8	V	0.35	0/1750	0.67	0/2373
9	I	0.34	0/1611	0.69	0/2174
9	W	0.34	0/1611	0.69	0/2174
10	J	0.37	0/1589	0.65	0/2142
10	X	0.37	0/1589	0.65	0/2142
11	K	0.41	0/1668	0.88	6/2253 (0.3%)
11	Y	0.40	0/1668	0.88	7/2253 (0.3%)
12	L	0.42	1/1802 (0.1%)	0.73	4/2430 (0.2%)
12	Z	0.43	1/1802 (0.1%)	0.76	4/2430 (0.2%)
13	M	0.36	0/1855	0.67	0/2514
13	a	0.36	0/1855	0.68	0/2514
14	N	0.34	0/1541	0.68	0/2087
14	b	0.34	0/1541	0.69	0/2087
All	All	0.38	2/50263 (0.0%)	0.70	23/67955 (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
12	Z	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	109	ASN	CG-ND2	-6.79	1.19	1.33
12	Z	109	ASN	CG-ND2	-6.34	1.20	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	9	ARG	NE-CZ-NH1	-11.96	109.55	121.50
11	K	9	ARG	NE-CZ-NH2	10.84	128.96	119.20
11	Y	61	ARG	NE-CZ-NH1	-10.68	110.82	121.50
12	Z	100	ARG	NE-CZ-NH2	10.61	128.75	119.20
11	Y	61	ARG	NE-CZ-NH2	10.42	128.58	119.20
11	Y	9	ARG	NE-CZ-NH2	-9.76	110.42	119.20
11	K	61	ARG	NE-CZ-NH2	-9.63	110.53	119.20
12	Z	100	ARG	NE-CZ-NH1	-9.21	112.29	121.50
11	K	9	ARG	CD-NE-CZ	7.92	135.48	124.40
11	Y	61	ARG	CD-NE-CZ	7.86	135.40	124.40
12	L	100	ARG	NE-CZ-NH2	-7.84	112.15	119.20
11	K	61	ARG	CD-NE-CZ	7.59	135.02	124.40
12	Z	100	ARG	CD-NE-CZ	7.35	134.69	124.40
12	L	100	ARG	CD-NE-CZ	7.28	134.59	124.40
11	K	61	ARG	NE-CZ-NH1	7.04	128.54	121.50
12	L	100	ARG	CG-CD-NE	-6.74	97.17	112.00
11	Y	9	ARG	CD-NE-CZ	6.64	133.69	124.40
12	L	100	ARG	NE-CZ-NH1	6.29	127.79	121.50
12	Z	100	ARG	CG-CD-NE	6.18	125.59	112.00
11	Y	9	ARG	CG-CD-NE	5.93	125.04	112.00
3	Q	201	VAL	N-CA-C	5.34	116.07	110.62
11	Y	9	ARG	NE-CZ-NH1	5.34	126.84	121.50
3	C	201	VAL	N-CA-C	5.31	116.04	110.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	100	ARG	Sidechain
12	Z	100	ARG	Sidechain

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	2	0
2	B	1904	0	1904	4	0
2	P	1904	0	1904	4	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	0	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1726	0	1723	12	0
8	V	1719	0	1716	8	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	9	0
11	K	1632	0	1591	19	0
11	Y	1632	0	1591	18	0
12	L	1764	0	1716	7	0
12	Z	1764	0	1716	5	0
13	M	1824	0	1832	3	0
13	a	1824	0	1832	4	0
14	N	1512	0	1481	5	0
14	b	1512	0	1481	4	0
15	A	1	0	0	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	1	0	0	0	0
15	b	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	42	0	42	2	0
17	K	42	0	42	1	0
17	V	42	0	42	2	0
17	Y	42	0	42	1	0
18	H	12	0	13	1	0
18	K	12	0	13	0	0
18	V	12	0	13	1	0
18	X	12	0	13	0	0
19	A	18	0	0	0	0
19	B	15	0	0	1	0
19	C	8	0	0	0	0
19	D	9	0	0	0	0
19	E	7	0	0	0	0
19	F	8	0	0	0	0
19	G	16	0	0	0	0
19	H	11	0	0	0	0
19	I	10	0	0	0	0
19	J	13	0	0	0	0
19	K	7	0	0	1	0
19	L	14	0	0	0	0
19	M	23	0	0	1	0
19	N	9	0	0	0	0
19	O	9	0	0	0	0
19	P	11	0	0	0	0
19	Q	8	0	0	0	0
19	R	10	0	0	0	0
19	S	7	0	0	0	0
19	T	13	0	0	0	0
19	U	20	0	0	0	0
19	V	16	0	0	0	0
19	W	10	0	0	0	0
19	X	12	0	0	0	0
19	Y	13	0	0	0	0
19	Z	7	0	0	0	0
19	a	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	b	9	0	0	0	0
All	All	49924	0	49353	145	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 (145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:9:ARG:HG2	11:Y:10:HIS:CD2	2.15	0.81
11:Y:35:ILE:HG13	11:Y:45:MET:CE	2.17	0.75
11:K:9:ARG:HG2	11:K:10:HIS:CD2	2.23	0.73
4:R:89:VAL:HG12	11:Y:61:ARG:HD3	1.70	0.73
11:Y:9:ARG:NH2	11:Y:146:ASP:OD1	2.27	0.67
4:D:89:VAL:HG12	11:K:61:ARG:HD2	1.76	0.67
11:K:9:ARG:NH2	11:K:146:ASP:OD1	2.29	0.65
11:Y:18:SER:O	11:Y:31:VAL:HG22	1.98	0.63
11:K:35:ILE:HG13	11:K:45:MET:CE	2.29	0.63
8:H:114[B]:HIS:HD2	8:H:116:HIS:H	1.48	0.61
11:K:208:ASN:O	9:W:38:LYS:NZ	2.35	0.60
11:K:31:VAL:HG12	12:L:132:GLN:NE2	2.19	0.58
11:K:52:CYS:O	11:K:56:GLU:HG3	2.04	0.58
11:Y:52:CYS:O	11:Y:56:GLU:HG3	2.03	0.57
10:J:25:ILE:O	10:X:139:TYR:OH	2.23	0.56
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.39	0.56
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.55
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.72	0.55
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.89	0.54
14:N:152:VAL:HA	14:N:175:MET:HE1	1.90	0.54
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.89	0.54
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.89	0.54
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.71	0.54
14:b:152:VAL:HA	14:b:175:MET:HE1	1.90	0.53
8:V:53:GLU:O	8:V:57:GLN:HG2	2.09	0.52
10:J:50:ALA:O	11:K:91:LYS:NZ	2.43	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
13:M:2:GLN:NE2	19:M:301:HOH:O	2.43	0.51
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.51
10:J:139:TYR:OH	10:X:25:ILE:O	2.29	0.51
8:H:53:GLU:O	8:H:57:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:HIS:HB3	19:B:301:HOH:O	2.11	0.50
2:P:50:LYS:O	2:P:51:VAL:C	2.54	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.50
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.50
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.42	0.50
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.42	0.49
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.45	0.49
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.93	0.49
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.95	0.49
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	1.94	0.49
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.94	0.48
17:V:301:04C:H37	18:V:302:MES:O1S	2.13	0.48
11:Y:58:LEU:HD12	11:Y:58:LEU:O	2.14	0.48
8:H:196:ARG:NH2	9:I:150:GLU:O	2.46	0.48
11:K:12:VAL:HG13	11:K:179:VAL:HB	1.94	0.48
11:K:58:LEU:O	11:K:58:LEU:HD12	2.14	0.48
8:V:31:CYS:SG	17:V:301:04C:C4	3.02	0.48
12:L:54:ALA:HB2	12:L:109:ASN:OD1	2.13	0.48
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.49	0.47
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.79	0.47
3:C:201:VAL:O	3:C:202:GLN:HB3	2.15	0.47
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.95	0.46
11:Y:1:THR:CG2	11:Y:3:THR:HG23	2.45	0.46
8:H:35:HIS:CB	8:H:56:THR:HG21	2.45	0.46
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.50	0.46
9:I:26:LEU:HD21	9:I:185:VAL:HG23	1.98	0.46
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.81	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.15	0.46
8:V:35:HIS:CB	8:V:56:THR:HG21	2.45	0.46
11:K:1:THR:CG2	11:K:3:THR:HG23	2.45	0.46
9:W:26:LEU:HD21	9:W:185:VAL:HG23	1.97	0.46
11:Y:35:ILE:HG13	11:Y:45:MET:HE3	1.96	0.46
11:K:100:MET:SD	11:K:128:VAL:CG1	3.04	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.97	0.46
11:Y:35:ILE:HG13	11:Y:45:MET:HE1	1.94	0.46
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.46
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.98	0.46
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.31	0.45
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.97	0.45
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:31:CYS:SG	17:H:301:04C:C4	3.04	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.45
17:H:301:04C:H37	18:H:302:MES:O3S	2.16	0.45
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.59	0.45
11:K:208:ASN:ND2	19:K:401:HOH:O	2.50	0.45
11:K:38:ASN:OD1	11:K:38:ASN:C	2.59	0.45
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.52	0.45
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.99	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.45
11:Y:61:ARG:HG3	11:Y:62:GLN:N	2.31	0.45
3:C:51:LYS:O	3:C:52:LEU:HB2	2.17	0.45
8:H:1:THR:CG2	8:H:3:ILE:HG23	2.47	0.44
8:H:50:ALA:HB3	9:I:126:ILE:HD12	2.00	0.44
8:V:196:ARG:NH2	9:W:150:GLU:O	2.51	0.44
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.52	0.44
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.52	0.44
11:Y:100:MET:SD	11:Y:128:VAL:CG1	3.05	0.44
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.99	0.44
8:V:1:THR:CG2	8:V:3:ILE:HG23	2.48	0.44
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.44
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.43
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.99	0.43
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.18	0.43
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.17	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.43
2:P:145:TYR:OH	2:P:217:LYS:N	2.52	0.43
17:Y:301:04C:H2	12:Z:126:ASP:HB3	2.00	0.43
8:H:22:GLN:HG3	8:H:27:ALA:HB2	2.01	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
2:P:217:LYS:C	2:P:219:ALA:H	2.27	0.43
8:V:22:GLN:HG3	8:V:27:ALA:HB2	2.00	0.43
2:B:145:TYR:OH	2:B:217:LYS:N	2.52	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.19	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.85	0.42
14:N:133:PHE:HA	14:b:132:THR:O	2.20	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.02	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.42
13:a:96:LEU:O	13:a:100:MET:HG2	2.19	0.42
11:K:59:LEU:HD22	11:K:63:CYS:SG	2.61	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.49	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.41
10:X:1:MET:HB3	10:X:34:LYS:HE3	2.03	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
5:S:12:PHE:H	6:T:19:GLN:HE22	1.68	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
4:D:89:VAL:CG1	11:K:61:ARG:HD2	2.47	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
10:J:5:LEU:HD23	10:J:132:ALA:HB2	2.03	0.41
11:K:35:ILE:HG13	11:K:45:MET:HE1	2.02	0.41
12:L:100:ARG:HD2	12:L:105:TYR:CZ	2.55	0.41
17:K:301:04C:H2	12:L:126:ASP:HB3	2.01	0.41
5:S:98:PHE:O	13:a:91:TYR:HA	2.21	0.41
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.03	0.41
10:X:5:LEU:HD23	10:X:132:ALA:HB2	2.03	0.41
8:H:84:LYS:HA	8:H:113:ILE:HD11	2.04	0.40
11:K:144:LYS:HB2	11:K:147:LEU:HD13	2.03	0.40
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.40
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.51	0.40
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.40
12:Z:138:ALA:HB3	12:Z:147:MET:HG2	2.03	0.40
10:J:1:MET:HB3	10:J:34:LYS:HE3	2.02	0.40
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.40
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.04	0.40
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.02	0.40
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	30	54
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	54
2	B	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	10	27
2	P	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	10	27
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	25
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	25
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%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	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	225/232 (97%)	220 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
11	Y	209/211 (99%)	203 (97%)	6 (3%)	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%)	221 (96%)	10 (4%)	0	100	100
13	a	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6283/6612 (95%)	6121 (97%)	148 (2%)	14 (0%)	43	68

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
3	C	205	ALA
3	Q	205	ALA
3	Q	183	PRO
3	C	183	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	50	77
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	77
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	66
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	66
3	C	212/226 (94%)	203 (96%)	9 (4%)	26	55
3	Q	212/226 (94%)	203 (96%)	9 (4%)	26	55
4	D	194/215 (90%)	187 (96%)	7 (4%)	31	60
4	R	194/215 (90%)	187 (96%)	7 (4%)	31	60
5	E	190/193 (98%)	185 (97%)	5 (3%)	40	70
5	S	190/193 (98%)	185 (97%)	5 (3%)	40	70
6	F	201/239 (84%)	196 (98%)	5 (2%)	42	71
6	T	201/239 (84%)	196 (98%)	5 (2%)	42	71
7	G	206/210 (98%)	200 (97%)	6 (3%)	37	67
7	U	206/210 (98%)	200 (97%)	6 (3%)	37	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	186/190 (98%)	183 (98%)	3 (2%)	55	80
8	V	185/190 (97%)	182 (98%)	3 (2%)	55	80
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	84
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	84
10	J	173/175 (99%)	170 (98%)	3 (2%)	53	79
10	X	173/175 (99%)	170 (98%)	3 (2%)	53	79
11	K	165/165 (100%)	148 (90%)	17 (10%)	7	18
11	Y	165/165 (100%)	147 (89%)	18 (11%)	6	16
12	L	186/186 (100%)	180 (97%)	6 (3%)	34	64
12	Z	186/186 (100%)	180 (97%)	6 (3%)	34	64
13	M	199/208 (96%)	195 (98%)	4 (2%)	48	76
13	a	199/208 (96%)	195 (98%)	4 (2%)	48	76
14	N	162/162 (100%)	159 (98%)	3 (2%)	50	77
14	b	162/162 (100%)	159 (98%)	3 (2%)	50	77
All	All	5315/5534 (96%)	5154 (97%)	161 (3%)	36	66

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU
2	B	79	LEU
2	B	102	ASN
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	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL

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Mol	Chain	Res	Type
3	C	240	GLU
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	188	LEU
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	221	ASN
6	F	240	GLN
7	G	26	THR
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	31	CYS
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	1	MET
10	J	3	ILE
10	J	99	GLN
11	K	4	LEU
11	K	12	VAL
11	K	29	GLN
11	K	35	ILE
11	K	38	ASN
11	K	58	LEU
11	K	59	LEU
11	K	61	ARG
11	K	62	GLN
11	K	83	LEU

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Mol	Chain	Res	Type
11	K	86	MET
11	K	93	MET
11	K	100	MET
11	K	117	GLU
11	K	128	VAL
11	K	147	LEU
11	K	210	ILE
12	L	18	GLU
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	128	VAL
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
14	N	9	LYS
14	N	104	ASP
14	N	178	LEU
1	O	1	MET
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
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	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	213	VAL
3	Q	240	GLU
4	R	99	ILE
4	R	176	LEU
4	R	193	LEU

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Mol	Chain	Res	Type
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	188	LEU
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	221	ASN
6	T	240	GLN
7	U	26	THR
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	31	CYS
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	1	MET
10	X	3	ILE
10	X	99	GLN
11	Y	4	LEU
11	Y	9	ARG
11	Y	12	VAL
11	Y	29	GLN
11	Y	35	ILE
11	Y	38	ASN
11	Y	58	LEU
11	Y	59	LEU
11	Y	61	ARG
11	Y	62	GLN
11	Y	83	LEU
11	Y	86	MET
11	Y	93	MET
11	Y	100	MET

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Mol	Chain	Res	Type
11	Y	117	GLU
11	Y	128	VAL
11	Y	147	LEU
11	Y	210	ILE
12	Z	18	GLU
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
12	Z	128	VAL
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
14	b	9	LYS
14	b	104	ASP
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	93	HIS
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
3	C	17	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
4	D	100	ASN
4	D	160	ASN
4	D	180	HIS
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN

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Mol	Chain	Res	Type
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	123	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	35	HIS
8	H	116	HIS
9	I	63	ASN
9	I	203	GLN
10	J	10	GLN
10	J	55	GLN
10	J	63	ASN
10	J	78	GLN
11	K	62	GLN
11	K	85	ASN
11	K	142	ASN
12	L	3	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	152	ASN
12	L	158	ASN
12	L	197	GLN
13	M	2	GLN
13	M	48	ASN
13	M	108	ASN
13	M	149	HIS
14	N	38	HIS
14	N	69	GLN
14	N	141	ASN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	220	ASN
3	Q	17	GLN
3	Q	116	GLN
3	Q	120	GLN

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Mol	Chain	Res	Type
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	180	HIS
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	123	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	172	ASN
7	U	175	ASN
8	V	30	ASN
8	V	66	HIS
8	V	189	ASN
9	W	63	ASN
9	W	203	GLN
10	X	10	GLN
10	X	55	GLN
10	X	63	ASN
11	Y	62	GLN
11	Y	85	ASN
11	Y	142	ASN
11	Y	175	ASN
11	Y	187	HIS
11	Y	207	ASN
12	Z	3	ASN
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	132	GLN

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Mol	Chain	Res	Type
12	Z	158	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	108	ASN
13	a	149	HIS
14	b	38	HIS
14	b	69	GLN
14	b	141	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 21 ligands modelled in this entry, 13 are monoatomic - leaving 8 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	04C	K	301	11	44,44,44	1.28	3 (6%)	54,58,58	1.66	11 (20%)
18	MES	H	302	-	12,12,12	2.26	1 (8%)	15,16,16	1.37	2 (13%)
18	MES	V	302	-	12,12,12	2.32	1 (8%)	15,16,16	1.21	1 (6%)
17	04C	V	301	8	44,44,44	1.43	4 (9%)	54,58,58	1.80	10 (18%)
18	MES	X	201	-	12,12,12	2.30	1 (8%)	15,16,16	1.54	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	MES	K	304	-	12,12,12	2.28	1 (8%)	15,16,16	1.40	3 (20%)
17	04C	H	301	8	44,44,44	1.45	4 (9%)	54,58,58	1.79	11 (20%)
17	04C	Y	301	11	44,44,44	1.30	3 (6%)	54,58,58	1.66	11 (20%)

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	04C	K	301	11	1/1/9/12	9/44/52/52	0/3/3/3
18	MES	H	302	-	-	6/6/14/14	0/1/1/1
18	MES	V	302	-	-	6/6/14/14	0/1/1/1
17	04C	V	301	8	1/1/9/12	19/44/52/52	0/3/3/3
18	MES	X	201	-	-	0/6/14/14	0/1/1/1
18	MES	K	304	-	-	0/6/14/14	0/1/1/1
17	04C	H	301	8	1/1/9/12	19/44/52/52	0/3/3/3
17	04C	Y	301	11	1/1/9/12	9/44/52/52	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	302	MES	C8-S	-7.79	1.66	1.77
18	X	201	MES	C8-S	-7.62	1.66	1.77
18	K	304	MES	C8-S	-7.57	1.67	1.77
18	H	302	MES	C8-S	-7.53	1.67	1.77
17	H	301	04C	C10-C9	5.34	1.62	1.53
17	V	301	04C	C10-C9	5.32	1.62	1.53
17	K	301	04C	C40-C41	-4.82	1.39	1.51
17	Y	301	04C	C10-C9	4.81	1.61	1.53
17	Y	301	04C	C40-C41	-4.65	1.40	1.51
17	H	301	04C	C40-C41	-4.46	1.40	1.51
17	K	301	04C	C10-C9	4.45	1.61	1.53
17	V	301	04C	C40-C41	-4.42	1.40	1.51
17	Y	301	04C	C7-C6	-4.10	1.41	1.51
17	H	301	04C	C7-C6	-4.10	1.41	1.51
17	K	301	04C	C7-C6	-4.08	1.41	1.51
17	V	301	04C	C7-C6	-3.93	1.42	1.51
17	H	301	04C	C12-C10	2.30	1.55	1.52
17	V	301	04C	C12-C10	2.06	1.55	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	04C	C30-N31-C32	-6.72	100.69	111.14
17	H	301	04C	C30-N31-C32	-6.60	100.88	111.14
17	Y	301	04C	C30-N31-C32	-5.62	102.41	111.14
17	K	301	04C	C30-N31-C32	-5.56	102.50	111.14
17	V	301	04C	C30-N31-C36	-4.86	103.59	111.14
17	H	301	04C	C30-N31-C36	-4.78	103.71	111.14
17	Y	301	04C	C11-C10-C12	-4.41	104.15	109.76
17	K	301	04C	C11-C10-C12	-4.40	104.16	109.76
17	V	301	04C	C32-N31-C36	3.99	117.44	108.84
17	H	301	04C	C32-N31-C36	3.94	117.33	108.84
17	Y	301	04C	C41-C40-C24	-3.68	103.56	113.36
18	H	302	MES	O2S-S-C8	3.66	112.26	106.73
17	K	301	04C	C41-C40-C24	-3.66	103.62	113.36
17	H	301	04C	C41-C40-C24	-3.30	104.58	113.36
17	V	301	04C	C41-C40-C24	-3.29	104.59	113.36
18	X	201	MES	C6-C5-N4	3.26	115.08	110.12
17	H	301	04C	C38-C27-C26	3.25	116.31	110.14
17	V	301	04C	C38-C27-C26	3.23	116.27	110.14
17	V	301	04C	C33-O34-C35	3.20	120.23	109.88
17	K	301	04C	C33-C32-N31	3.15	114.91	110.12
17	Y	301	04C	C33-C32-N31	3.04	114.74	110.12
17	H	301	04C	C33-O34-C35	3.04	119.72	109.88
17	K	301	04C	O13-C12-C10	-3.03	105.28	111.51
17	K	301	04C	O34-C33-C32	-2.95	105.42	111.77
18	V	302	MES	O3S-S-C8	2.94	111.76	106.00
18	K	304	MES	C6-C5-N4	2.91	114.55	110.12
17	Y	301	04C	C46-O45-C44	-2.90	111.29	117.50
17	Y	301	04C	O34-C33-C32	-2.87	105.59	111.77
17	Y	301	04C	O13-C12-C10	-2.86	105.63	111.51
17	V	301	04C	C29-C30-N31	-2.86	106.77	113.41
17	H	301	04C	C29-C30-N31	-2.84	106.80	113.41
17	Y	301	04C	C7-C6-C1	-2.84	115.62	120.90
17	K	301	04C	C46-O45-C44	-2.81	111.48	117.50
17	Y	301	04C	C7-C6-C5	2.77	126.06	120.90
17	K	301	04C	C7-C6-C1	-2.77	115.75	120.90
17	K	301	04C	C7-C6-C5	2.73	125.98	120.90
17	K	301	04C	C30-N31-C36	2.73	115.39	111.14
17	Y	301	04C	C30-N31-C36	2.73	115.39	111.14
17	V	301	04C	C7-C6-C5	2.63	125.79	120.90
17	V	301	04C	C7-C6-C1	-2.62	116.02	120.90
17	H	301	04C	C7-C6-C1	-2.55	116.15	120.90
17	H	301	04C	C7-C6-C5	2.54	125.64	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	04C	C46-O45-C44	-2.54	112.05	117.50
17	H	301	04C	C46-O45-C44	-2.54	112.06	117.50
17	Y	301	04C	C32-N31-C36	2.38	113.98	108.84
17	K	301	04C	C32-N31-C36	2.37	113.96	108.84
18	K	304	MES	O3S-S-C8	2.29	110.48	106.00
18	H	302	MES	O1S-S-C8	2.17	110.00	106.73
18	K	304	MES	O2S-S-C8	2.09	109.89	106.73
17	H	301	04C	C27-N28-C29	2.08	124.29	121.13
18	X	201	MES	O3S-S-C8	2.05	110.02	106.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	H	301	04C	C27
17	K	301	04C	C27
17	V	301	04C	C27
17	Y	301	04C	C27

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	04C	C11-C10-C9-C8
17	H	301	04C	C12-C10-C9-C8
17	H	301	04C	C9-C10-C12-O13
17	H	301	04C	C11-C10-C12-O13
17	K	301	04C	C29-C30-N31-C36
17	K	301	04C	C11-C10-C9-C8
17	K	301	04C	C9-C10-C12-O13
17	V	301	04C	C11-C10-C9-C8
17	V	301	04C	C12-C10-C9-C8
17	V	301	04C	C9-C10-C12-O13
17	V	301	04C	C11-C10-C12-O13
17	Y	301	04C	C29-C30-N31-C36
17	Y	301	04C	C11-C10-C9-C8
17	Y	301	04C	C9-C10-C12-O13
18	H	302	MES	C7-C8-S-O1S
18	H	302	MES	C7-C8-S-O3S
18	V	302	MES	N4-C7-C8-S
18	V	302	MES	C7-C8-S-O2S
18	V	302	MES	C7-C8-S-O3S
17	H	301	04C	C47-C44-O45-C46
17	H	301	04C	C43-C44-O45-C46

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Mol	Chain	Res	Type	Atoms
17	V	301	04C	C47-C44-O45-C46
17	V	301	04C	C43-C44-O45-C46
17	K	301	04C	C47-C44-O45-C46
17	H	301	04C	O39-C26-C27-C38
17	V	301	04C	O39-C26-C27-C38
17	Y	301	04C	C47-C44-O45-C46
17	H	301	04C	N25-C26-C27-C38
17	V	301	04C	N25-C26-C27-C38
17	K	301	04C	C43-C44-O45-C46
17	Y	301	04C	C43-C44-O45-C46
17	H	301	04C	C38-C27-N28-C29
17	V	301	04C	C38-C27-N28-C29
17	Y	301	04C	C5-C6-C7-C8
17	K	301	04C	C5-C6-C7-C8
17	H	301	04C	C5-C6-C7-C8
17	V	301	04C	C5-C6-C7-C8
17	Y	301	04C	C1-C6-C7-C8
17	K	301	04C	C1-C6-C7-C8
17	V	301	04C	C1-C6-C7-C8
17	H	301	04C	C1-C6-C7-C8
17	Y	301	04C	C11-C10-C12-O13
17	H	301	04C	C11-C10-C9-O21
17	H	301	04C	C12-C10-C9-O21
17	V	301	04C	C11-C10-C9-O21
17	V	301	04C	C12-C10-C9-O21
17	H	301	04C	N28-C29-C30-N31
17	V	301	04C	N28-C29-C30-N31
18	V	302	MES	C8-C7-N4-C5
17	H	301	04C	O37-C29-C30-N31
17	V	301	04C	O37-C29-C30-N31
17	K	301	04C	C11-C10-C12-O13
17	K	301	04C	C11-C10-C9-O21
17	Y	301	04C	C11-C10-C9-O21
18	H	302	MES	C7-C8-S-O2S
18	V	302	MES	C7-C8-S-O1S
17	H	301	04C	C6-C7-C8-N22
17	V	301	04C	C6-C7-C8-N22
18	H	302	MES	N4-C7-C8-S
18	H	302	MES	C8-C7-N4-C3
18	H	302	MES	C8-C7-N4-C5
18	V	302	MES	C8-C7-N4-C3
17	H	301	04C	C29-C30-N31-C36

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Mol	Chain	Res	Type	Atoms
17	V	301	04C	C29-C30-N31-C36
17	H	301	04C	C29-C30-N31-C32
17	V	301	04C	C29-C30-N31-C32
17	H	301	04C	C6-C7-C8-C9
17	V	301	04C	C6-C7-C8-C9

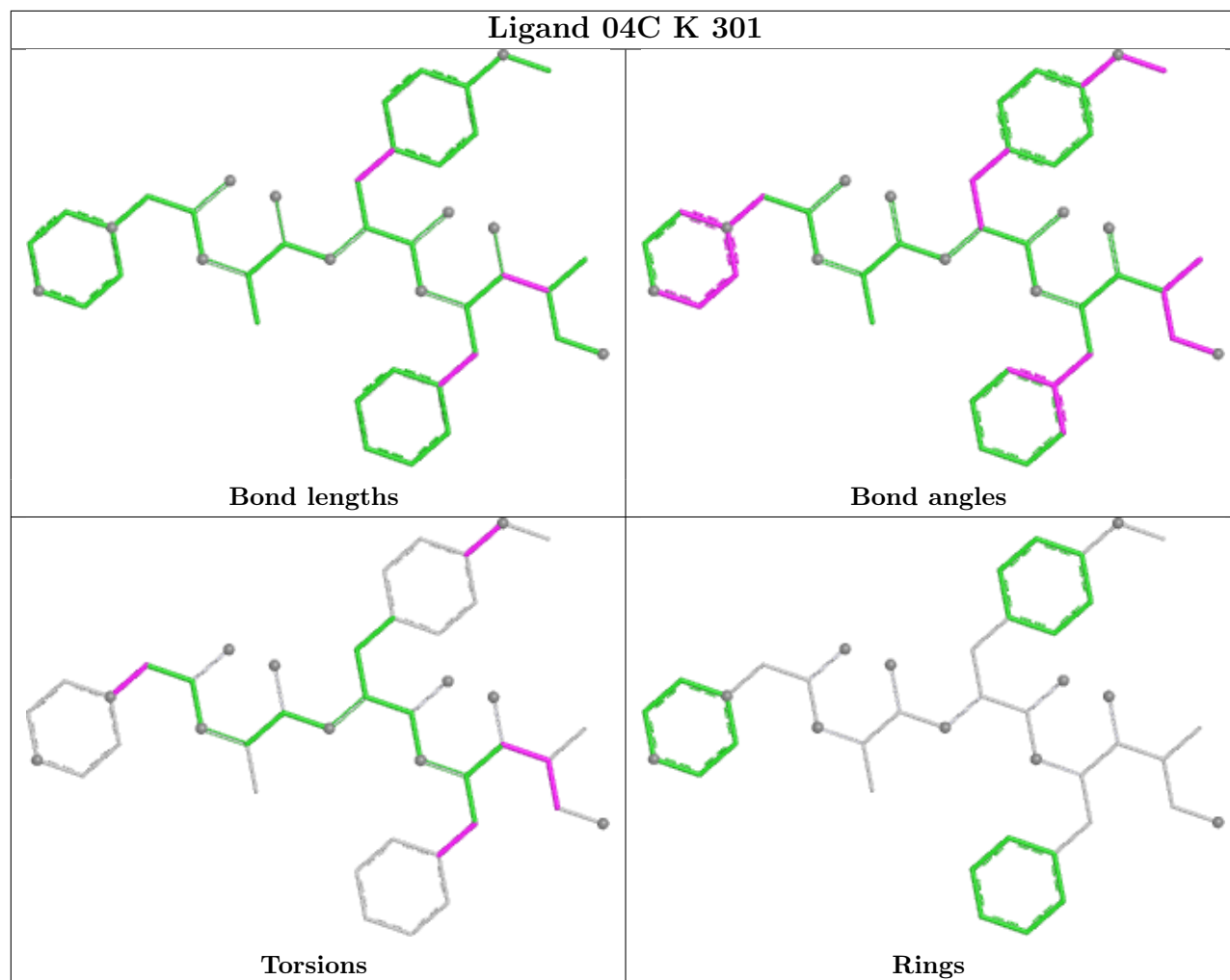
There are no ring outliers.

6 monomers are involved in 6 short contacts:

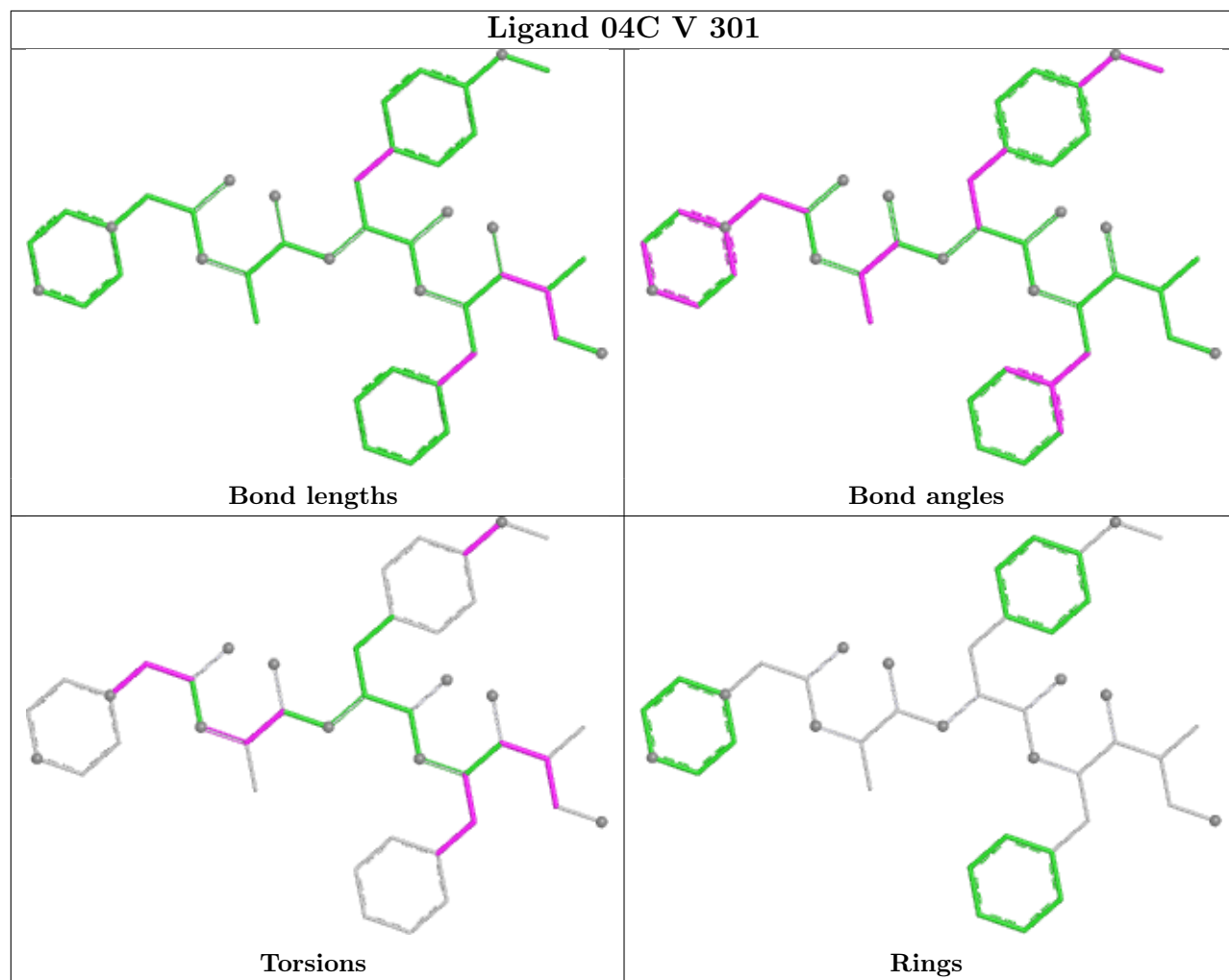
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	04C	1	0
18	H	302	MES	1	0
18	V	302	MES	1	0
17	V	301	04C	2	0
17	H	301	04C	2	0
17	Y	301	04C	1	0

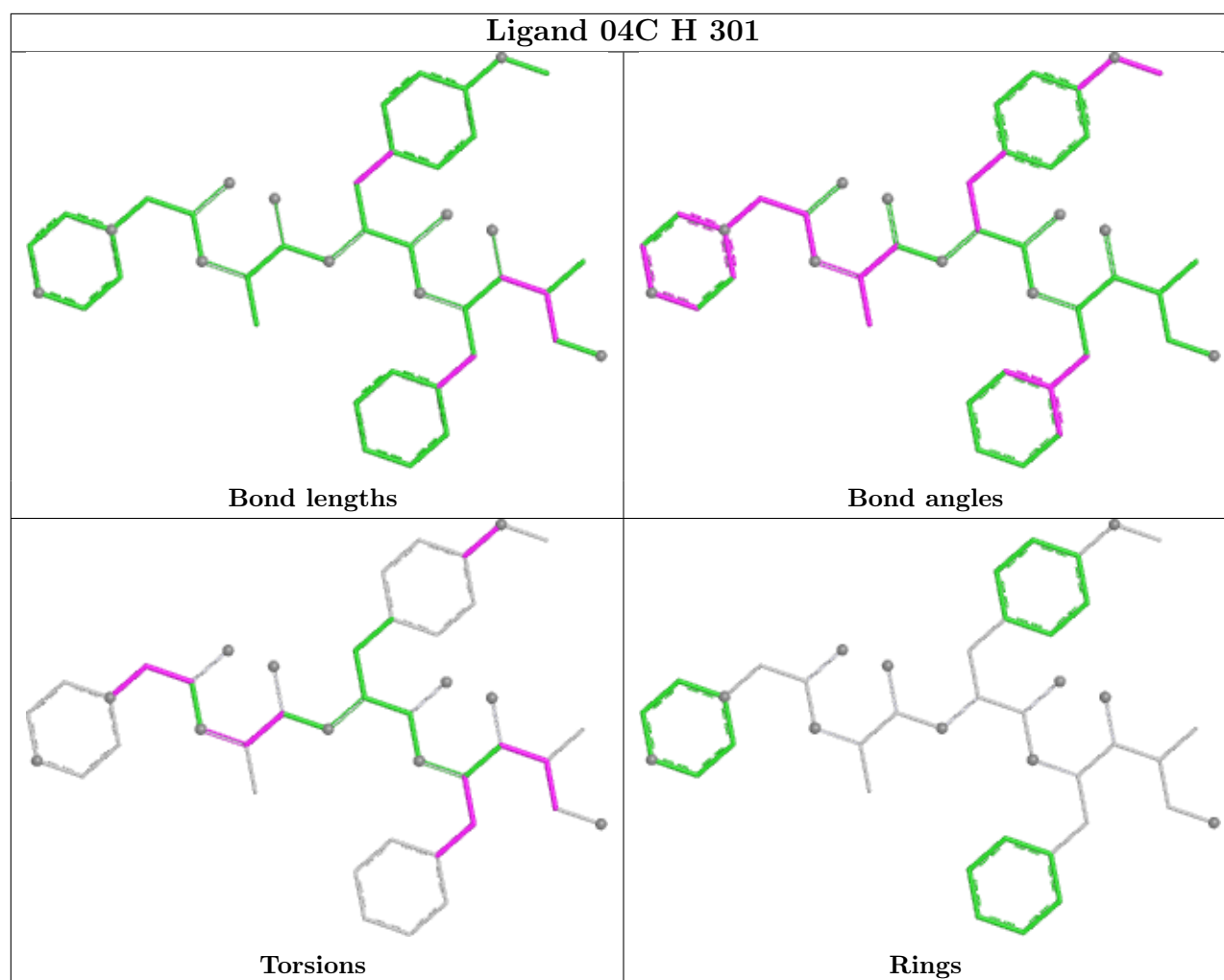
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

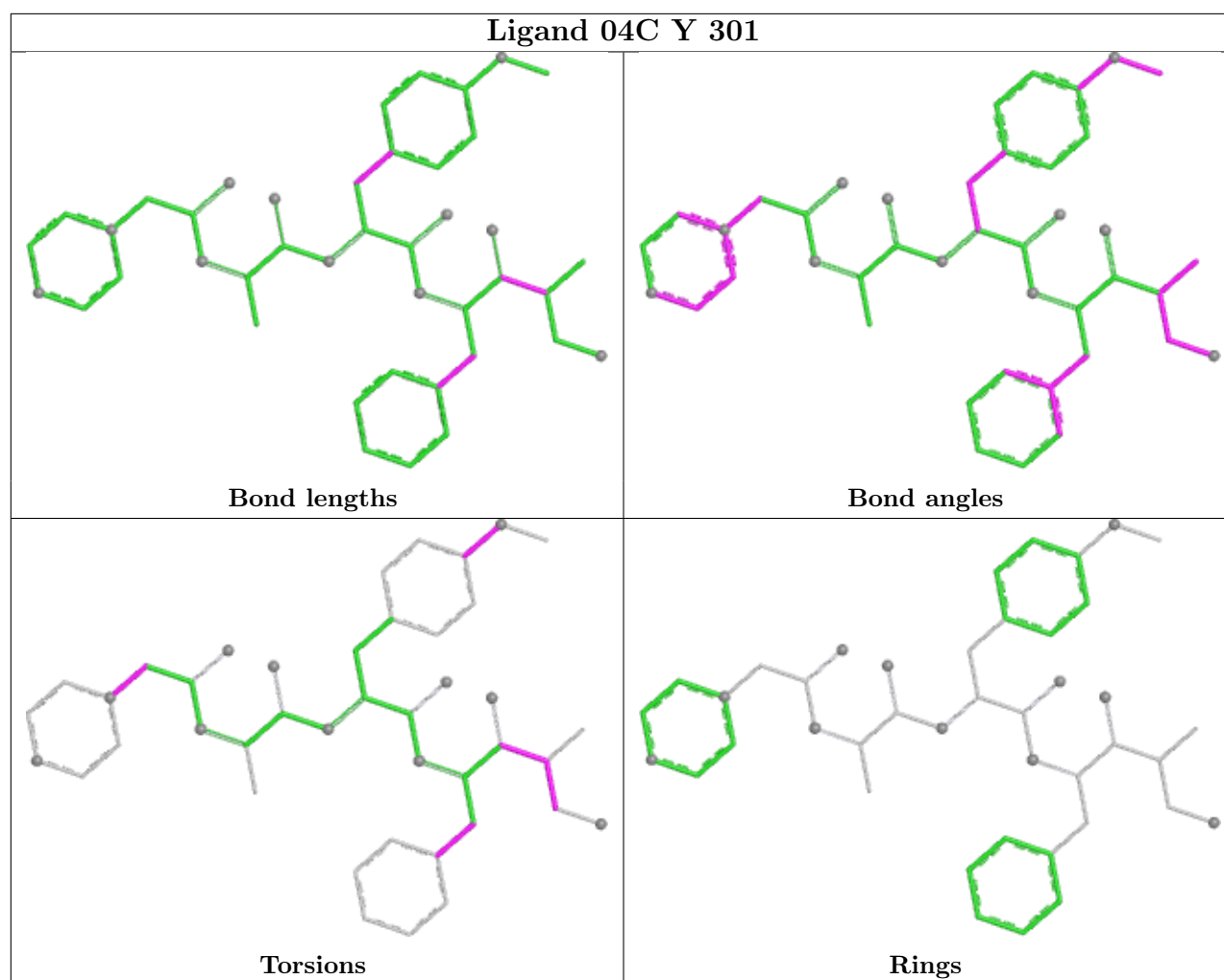
Ligand 04C K 301



Ligand 04C V 301







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, 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%)	-0.32	0 100 100	36, 54, 91, 129	0
1	O	250/250 (100%)	-0.31	1 (0%) 88 87	41, 58, 103, 140	0
2	B	244/258 (94%)	-0.13	7 (2%) 53 50	41, 60, 106, 157	0
2	P	244/258 (94%)	-0.16	7 (2%) 53 50	43, 61, 103, 156	0
3	C	240/254 (94%)	-0.02	11 (4%) 37 34	38, 67, 137, 172	0
3	Q	240/254 (94%)	0.08	8 (3%) 49 45	43, 75, 155, 199	0
4	D	235/260 (90%)	-0.27	1 (0%) 88 87	43, 62, 94, 130	0
4	R	235/260 (90%)	-0.05	5 (2%) 63 61	53, 71, 114, 141	0
5	E	231/234 (98%)	-0.17	0 100 100	44, 65, 105, 150	0
5	S	231/234 (98%)	-0.04	4 (1%) 69 67	48, 69, 113, 150	0
6	F	243/288 (84%)	-0.31	2 (0%) 82 81	38, 59, 108, 136	0
6	T	243/288 (84%)	-0.20	5 (2%) 63 61	40, 64, 120, 155	0
7	G	241/252 (95%)	-0.30	3 (1%) 76 75	38, 56, 98, 157	0
7	U	241/252 (95%)	-0.34	0 100 100	36, 55, 92, 133	0
8	H	226/232 (97%)	-0.32	1 (0%) 88 87	32, 54, 91, 145	1 (0%)
8	V	226/232 (97%)	-0.32	2 (0%) 81 80	40, 54, 88, 159	0
9	I	204/205 (99%)	-0.45	0 100 100	37, 52, 83, 106	0
9	W	204/205 (99%)	-0.48	1 (0%) 87 86	38, 54, 85, 108	0
10	J	195/198 (98%)	-0.33	1 (0%) 87 86	38, 59, 90, 132	0
10	X	195/198 (98%)	-0.31	1 (0%) 87 86	41, 61, 90, 137	0
11	K	211/211 (100%)	-0.02	0 100 100	44, 65, 97, 125	0
11	Y	211/211 (100%)	-0.02	3 (1%) 73 72	44, 65, 97, 128	0
12	L	222/222 (100%)	-0.08	1 (0%) 87 86	46, 62, 106, 135	0
12	Z	222/222 (100%)	-0.07	5 (2%) 61 58	47, 63, 106, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.36	2 (0%) 81 80	37, 56, 84, 101	0
13	a	233/246 (94%)	-0.34	2 (0%) 81 80	35, 56, 82, 99	0
14	N	196/196 (100%)	-0.45	1 (0%) 87 86	36, 50, 83, 107	0
14	b	196/196 (100%)	-0.53	0 100 100	36, 50, 81, 106	0
All	All	6342/6612 (95%)	-0.23	74 (1%) 76 75	32, 60, 105, 199	1 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	6.3
10	J	1	MET	5.6
12	Z	174	TYR	4.5
13	a	1	THR	4.3
2	P	219	ALA	3.7
3	Q	205	ALA	3.6
3	C	205	ALA	3.5
4	D	241	ALA	3.4
6	T	243	ILE	3.3
12	L	174	TYR	3.3
2	B	218	GLY	3.3
2	P	218	GLY	3.1
2	P	1	GLY	3.0
6	F	215	CYS	2.9
3	Q	50	LEU	2.9
3	Q	175	LYS	2.9
6	T	204	LYS	2.9
2	B	1	GLY	2.9
3	C	51	LYS	2.9
13	M	1	THR	2.8
2	B	51	VAL	2.8
2	B	217	LYS	2.8
3	C	50	LEU	2.8
2	P	51	VAL	2.8
7	G	3	TYR	2.7
2	P	93	HIS	2.7
2	B	222	GLY	2.6
12	Z	166	GLY	2.6
3	C	58	THR	2.6
9	W	1	SER	2.6
13	M	69	ASP	2.6
4	R	112	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
5	S	209	ASN	2.5
3	C	234	ILE	2.5
8	H	223	ILE	2.5
8	V	224	GLN	2.5
3	C	203	THR	2.5
2	P	52	THR	2.4
6	T	205	GLU	2.4
6	F	202	ASP	2.4
2	P	222	GLY	2.4
11	Y	68	LEU	2.3
3	Q	3	ASP	2.3
3	C	236	GLN	2.3
13	a	69	ASP	2.3
8	V	223	ILE	2.3
3	C	238	LYS	2.3
4	R	240	ALA	2.3
4	R	241	ALA	2.3
3	Q	238	LYS	2.3
6	T	14	ASP	2.3
2	B	220	ASN	2.2
7	G	68	ARG	2.2
7	G	242	GLN	2.2
3	C	186	VAL	2.2
12	Z	108	TYR	2.2
1	O	231	LYS	2.2
11	Y	144	LYS	2.2
3	C	3	ASP	2.2
14	N	181	ALA	2.2
5	S	122	TYR	2.2
5	S	96	LEU	2.2
3	C	206	LYS	2.1
11	Y	208	ASN	2.1
12	Z	109	ASN	2.1
12	Z	170	LYS	2.1
3	Q	204	GLY	2.1
4	R	239	GLU	2.1
3	Q	51	LYS	2.1
3	Q	240	GLU	2.1
4	R	125	LEU	2.1
5	S	173	ARG	2.0
2	B	93	HIS	2.0
6	T	178	HIS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

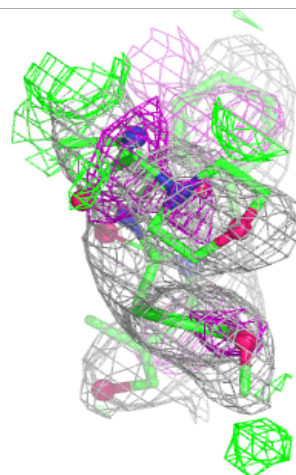
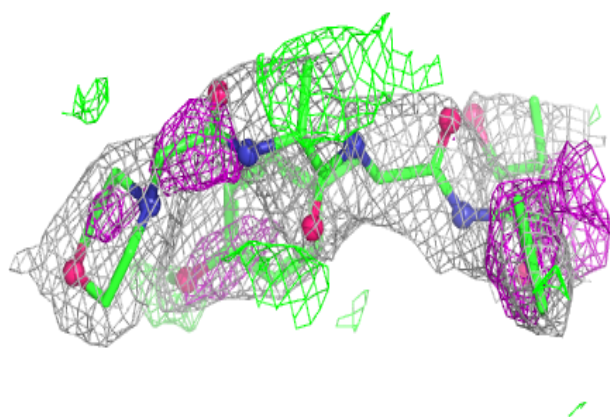
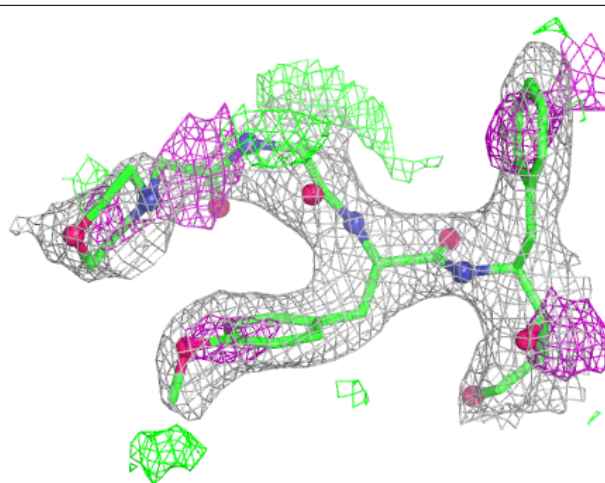
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	04C	H	301	42/42	0.83	0.14	41,57,86,88	0
17	04C	V	301	42/42	0.84	0.15	37,58,85,88	42
17	04C	Y	301	42/42	0.84	0.15	61,67,97,102	0
18	MES	K	304	12/12	0.85	0.19	53,59,77,87	12
18	MES	V	302	12/12	0.85	0.15	66,71,85,91	12
17	04C	K	301	42/42	0.86	0.14	48,67,98,100	0
18	MES	X	201	12/12	0.88	0.16	56,58,75,86	12
18	MES	H	302	12/12	0.91	0.14	68,75,86,91	12
15	MG	A	301	1/1	0.93	0.26	47,47,47,47	0
15	MG	K	303	1/1	0.93	0.06	63,63,63,63	0
15	MG	I	301	1/1	0.95	0.07	66,66,66,66	0
15	MG	G	301	1/1	0.96	0.04	54,54,54,54	0
15	MG	Z	301	1/1	0.96	0.06	72,72,72,72	0
15	MG	N	201	1/1	0.98	0.03	53,53,53,53	0
15	MG	b	201	1/1	0.98	0.06	46,46,46,46	0
16	CL	G	302	1/1	0.99	0.08	46,46,46,46	0
16	CL	U	301	1/1	0.99	0.08	47,47,47,47	0
15	MG	K	302	1/1	0.99	0.09	57,57,57,57	0
15	MG	J	201	1/1	0.99	0.07	59,59,59,59	0
15	MG	L	301	1/1	0.99	0.10	66,66,66,66	0
15	MG	I	302	1/1	1.00	0.08	58,58,58,58	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.

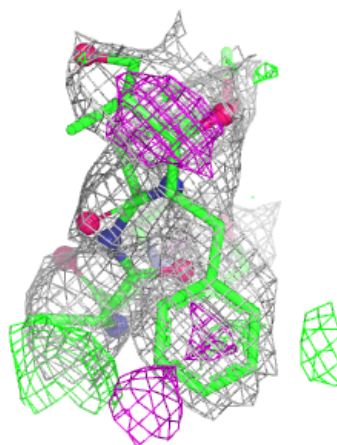
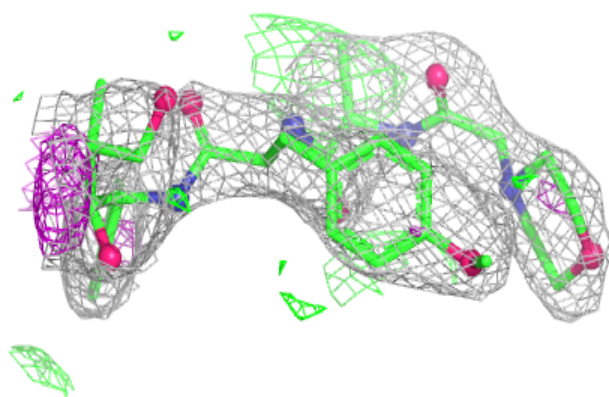
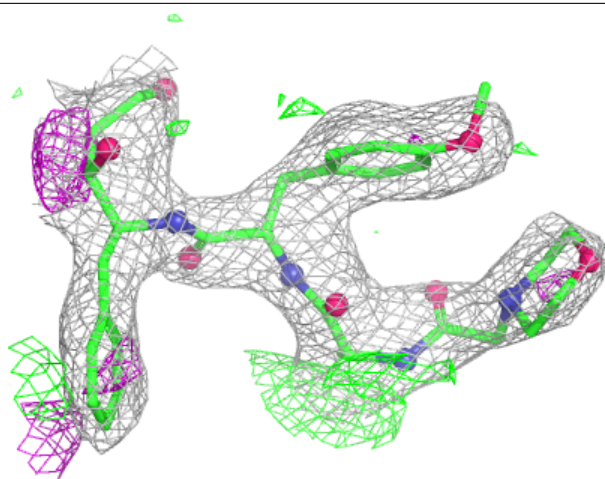
Electron density around 04C H 301:

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



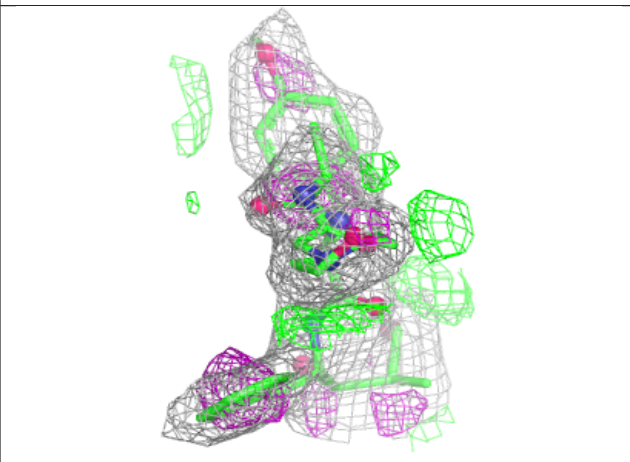
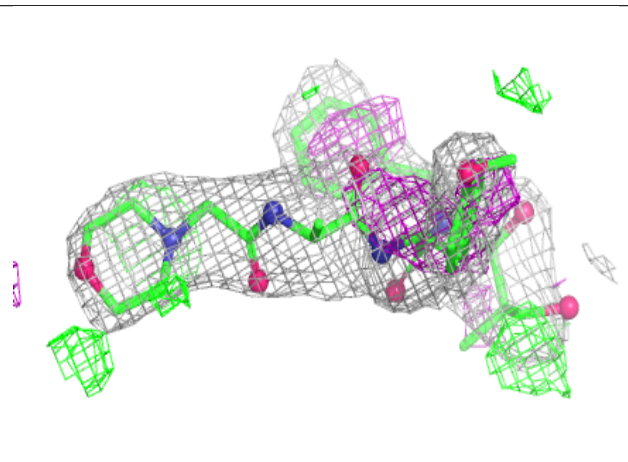
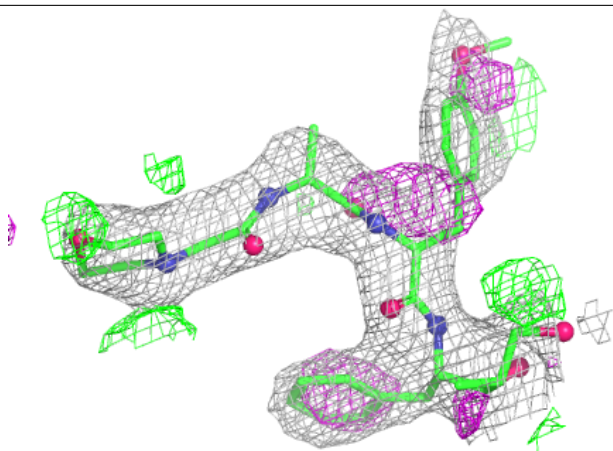
Electron density around 04C V 301:

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



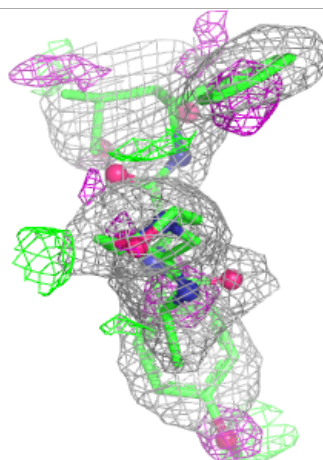
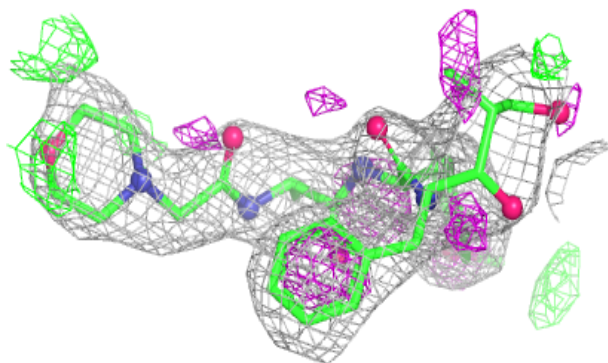
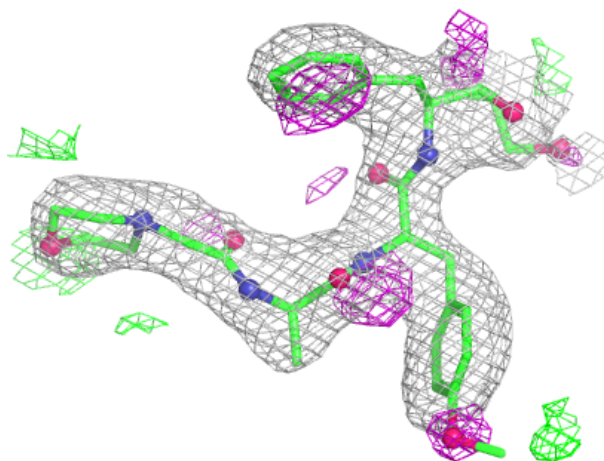
Electron density around 04C Y 301:

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



Electron density around 04C 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.