



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 06:42 PM UTC

PDB ID : 4QZ7 / pdb_00004qz7
Title : yCP beta5-A50V mutant in complex with the epoxyketone inhibitor ONX 0914
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2014-07-27
Resolution : 2.80 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 ⓘ 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

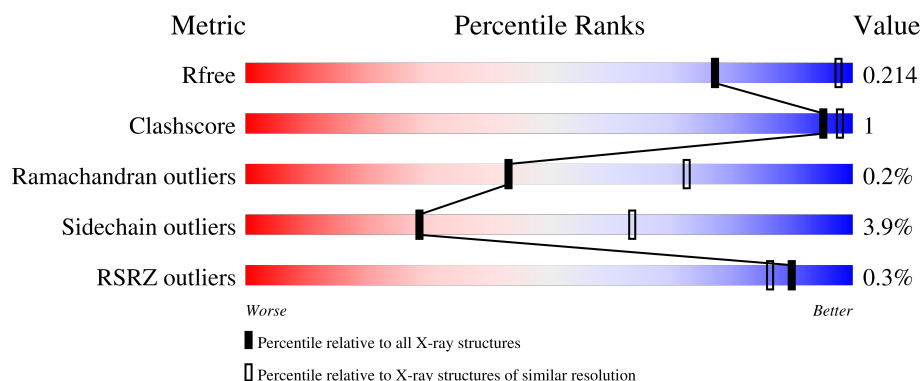
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



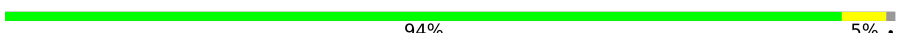
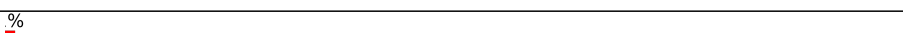
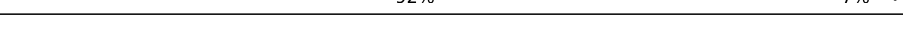
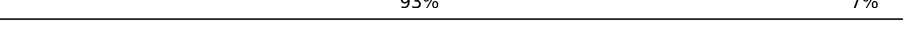
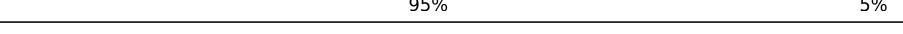
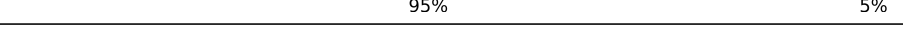
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	% 89% 5% • 5%
2	P	258	89% 5% • 5%
3	C	254	88% 5% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 89% . . 6%
4	D	260	 84% 6% 10%
4	R	260	 84% 6% 10%
5	E	234	 94% 5% .
5	S	234	 92% 6% .
6	F	288	 80% . 16%
6	T	288	 80% . 16%
7	G	252	 89% 6% .
7	U	252	 90% 6% .
8	H	232	 91% . .
8	V	232	 91% . .
9	I	205	 95% .
9	W	205	 96% .
10	J	198	 % 92% 6% . .
10	X	198	 % 92% 7% .
11	K	212	 91% 8% .
11	Y	212	 93% 7%
12	L	222	 95% 5%
12	Z	222	 95% 5%
13	M	246	 88% 7% 6%
13	a	246	 88% 7% 5%
14	N	196	 91% 8% .
14	b	196	 % 91% 8% .

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49808 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	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	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
			1646	1047	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1646	1047	280	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	50	VAL	ALA	engineered mutation	UNP P30656
Y	50	VAL	ALA	engineered mutation	UNP P30656

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	232	Total	C	N	O	S	0	0	0
			1815	1148	311	349	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			

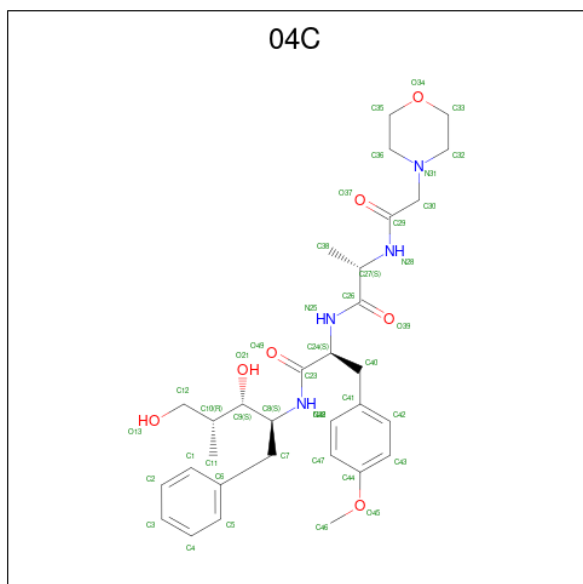
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

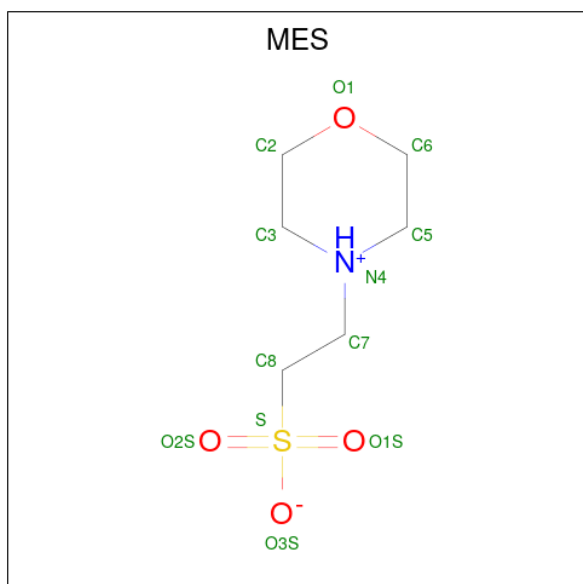
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- 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	C	N	O	0	0
			42	31	4	7		
17	K	1	Total	C	N	O	0	0
			42	31	4	7		
17	N	1	Total	C	N	O	0	0
			42	31	4	7		
17	V	1	Total	C	N	O	0	0
			42	31	4	7		
17	Y	1	Total	C	N	O	0	0
			42	31	4	7		
17	b	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	B	8	Total 8	O 8	0	0
19	C	10	Total 10	O 10	0	0
19	D	3	Total 3	O 3	0	0
19	E	3	Total 3	O 3	0	0
19	F	8	Total 8	O 8	0	0
19	G	10	Total 10	O 10	0	0
19	H	10	Total 10	O 10	0	0
19	I	6	Total 6	O 6	0	0
19	J	10	Total 10	O 10	0	0
19	K	9	Total 9	O 9	0	0
19	L	11	Total 11	O 11	0	0
19	M	9	Total 9	O 9	0	0
19	N	6	Total 6	O 6	0	0
19	O	3	Total 3	O 3	0	0
19	P	8	Total 8	O 8	0	0
19	Q	6	Total 6	O 6	0	0
19	R	5	Total 5	O 5	0	0
19	S	6	Total 6	O 6	0	0
19	T	9	Total 9	O 9	0	0
19	U	10	Total 10	O 10	0	0
19	V	10	Total 10	O 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	W	5	Total 5	O 5	0	0
19	X	12	Total 12	O 12	0	0
19	Y	14	Total 14	O 14	0	0
19	Z	16	Total 16	O 16	0	0
19	a	11	Total 11	O 11	0	0
19	b	8	Total 8	O 8	0	0

3 Residue-property plots [i](#)

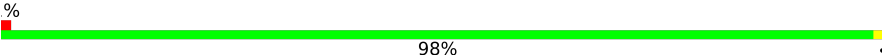
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



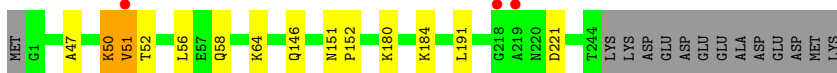
- Molecule 1: Proteasome subunit alpha type-2

Chain O:  98%



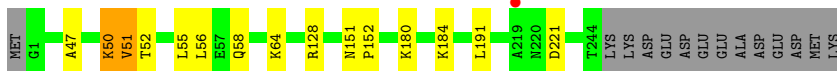
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  89% 5% 5%



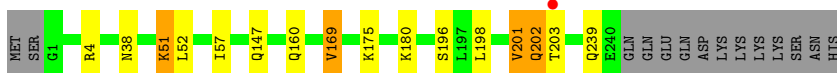
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  89% 5% 5%



- Molecule 3: Proteasome subunit alpha type-4

Chain C:  88% 5% 6%



- Molecule 3: Proteasome subunit alpha type-4

Met	Ser	G1	R4	N38	L50	K51	L52	Q147	Q160	V169	K175	K180	S196	L197	L198	V201	Q202	T203	Q239	G240	G241	G242	G243	G244	G245	G246	G247	G248	G249	G250	G251	G252	G253	G254	G255	G256	G257	G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	G270	G271	G272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	G300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674
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- [illegible]

-
- The following table lists all amino acid labels shown in the figure:
- | Amino Acid |
|------------|
| MET |
| PHE |
| THR |
| ARG |
| SER |
| GLU |
| Tyr |
| D1 |
| L20 |
| L40 |
| L51 |
| I99 |
| L104 |
| L113 |
| E117 |
| ALA |
| SER |
| GLY |
| VAL |
| ARG |
| L128 |
| N160 |
| L176 |
| W179 |
| L190 |
| L193 |
| K197 |
| I214 |
| D224 |
| L235 |
| K236 |
| E242 |
| SER |
| PRO |
| GLU |
| ALA |
| ASP |
| VAL |
| Cys |

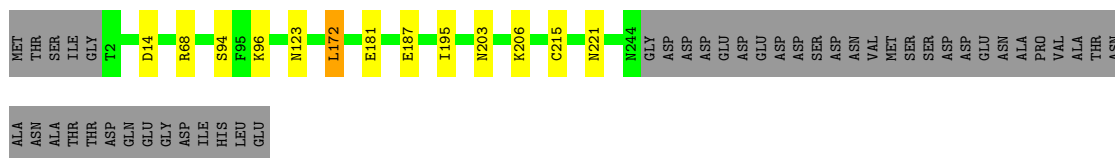
-
- | Amino Acid | Percentage (%) |
|------------|----------------|
| MET | ~10 |
| PHE | ~10 |
| ARG | ~10 |
| N3 | ~10 |
| T9 | ~10 |
| L25 | ~10 |
| K29 | ~10 |
| L55 | ~10 |
| L71 | ~10 |
| L87 | ~10 |
| A107 | ~10 |
| T174 | ~10 |
| L175 | ~10 |
| F178 | ~10 |
| L188 | ~10 |
| T219 | ~10 |
| I233 | ~10 |

- | | | | | | | | | | | | | | | | | |
|-----|-----|----|----|-----|-----|-----|-----|------------|-----|------|------|--------------|------|------|------|------|
| MTT | PHE | N3 | T9 | L25 | K29 | L55 | L71 | A77
P78 | L87 | A107 | T119 | T174
L175 | F178 | L188 | T219 | I233 |
|-----|-----|----|----|-----|-----|-----|-----|------------|-----|------|------|--------------|------|------|------|------|

- | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|
| ALA | ASN | ALA | THR | THR | ASP | GLN | GLU | GLY | ASP | ILE | HIS | LEU | GLU | MET | THR | SER | ILE | GLY | T2 | D14 | R68 | S94 | F95 | K96 | N123 | L172 | E181 | E187 | I195 | M203 | K206 | C215 | M221 | N244 | GLY | ASP | ASP | GLU | ASP | GLU | ASP | ASP | ASP | ASN | VAL | MET | SER | SER | ASP | GLU | ASN | ALA | PRO | VAL | ALA | THR | ASN |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|

- 

Chain T:  80% 16%



- Molecule 7: Proteasome subunit alpha type-1

Chain G:  89% 6%



- Molecule 7: Proteasome subunit alpha type-1

Chain U:  90% 6%



- Molecule 8: Proteasome subunit beta type-2

Chain H:  91%

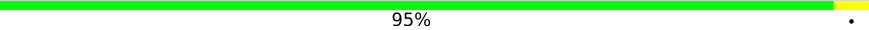


- Molecule 8: Proteasome subunit beta type-2

Chain V:  91%

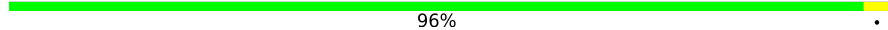


- Molecule 9: Proteasome subunit beta type-3

Chain I:  95%

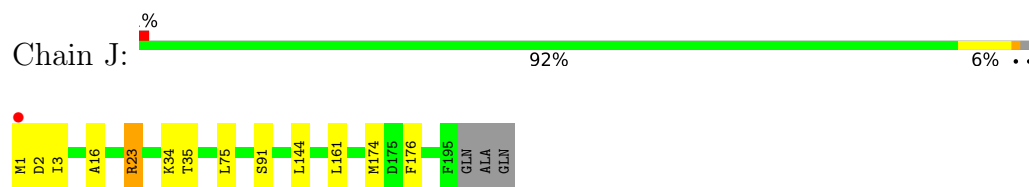


- Molecule 9: Proteasome subunit beta type-3

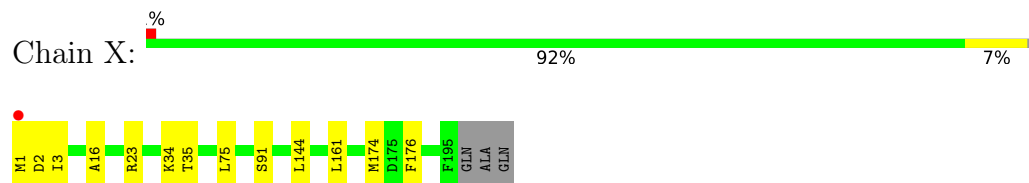
Chain W:  96%



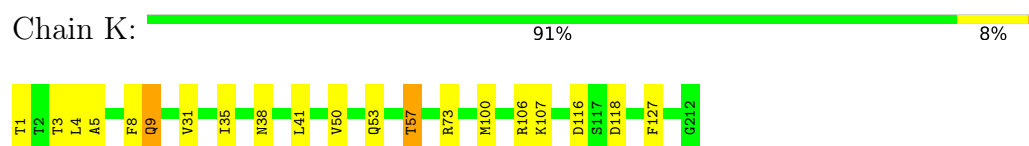
- Molecule 10: Proteasome subunit beta type-4



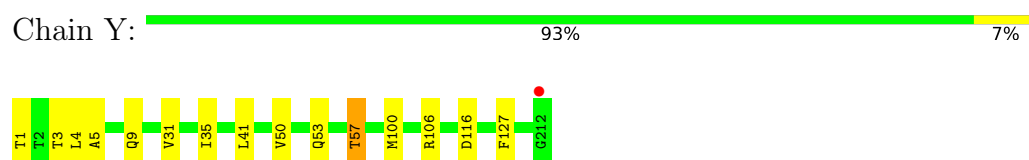
- Molecule 10: Proteasome subunit beta type-4



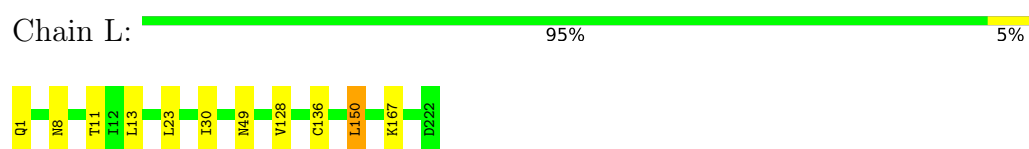
- Molecule 11: Proteasome subunit beta type-5



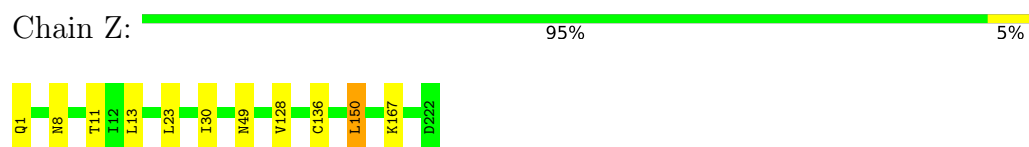
- Molecule 11: Proteasome subunit beta type-5



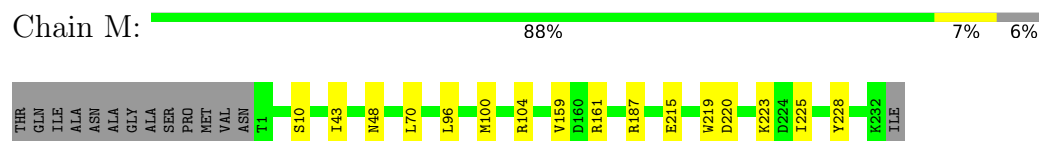
- Molecule 12: Proteasome subunit beta type-6



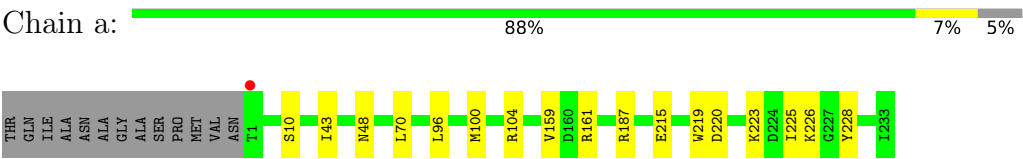
- Molecule 12: Proteasome subunit beta type-6



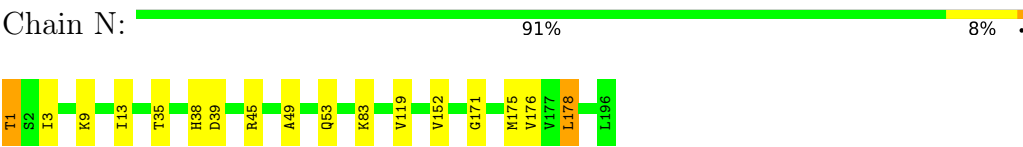
- Molecule 13: Proteasome subunit beta type-7



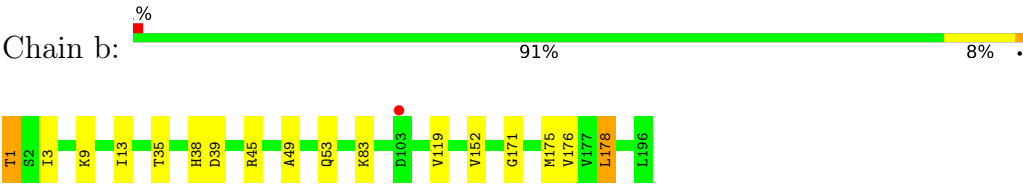
• Molecule 13: Proteasome subunit beta type-7



• 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	135.79Å 300.31Å 146.09Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (15.00-2.80) 96.8 (15.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.213 0.181 , 0.214	Depositor DCC
R_{free} test set	12769 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.8	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	0.96	EDS
Total number of atoms	49808	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MG, MES, 04C

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	0.70	0/2642
1	O	0.41	0/1952	0.70	0/2642
2	B	0.41	0/1934	0.69	0/2618
2	P	0.40	0/1934	0.69	0/2618
3	C	0.40	0/1910	0.71	1/2586 (0.0%)
3	Q	0.40	0/1910	0.72	1/2586 (0.0%)
4	D	0.39	0/1837	0.67	0/2475
4	R	0.39	0/1837	0.66	0/2475
5	E	0.40	0/1800	0.67	0/2433
5	S	0.40	0/1800	0.67	0/2433
6	F	0.40	0/1932	0.71	0/2609
6	T	0.40	0/1932	0.71	0/2609
7	G	0.39	0/1945	0.70	0/2634
7	U	0.40	0/1945	0.70	0/2634
8	H	0.38	0/1715	0.67	0/2326
8	V	0.38	0/1715	0.67	0/2326
9	I	0.38	0/1611	0.69	0/2174
9	W	0.38	0/1611	0.68	0/2174
10	J	0.41	0/1589	0.68	0/2142
10	X	0.41	0/1589	0.67	0/2142
11	K	0.37	0/1683	0.67	0/2277
11	Y	0.36	0/1683	0.67	0/2277
12	L	0.38	0/1795	0.65	0/2420
12	Z	0.38	0/1795	0.65	0/2420
13	M	0.40	0/1846	0.68	0/2503
13	a	0.40	0/1855	0.68	0/2514
14	N	0.37	0/1541	0.69	1/2087 (0.0%)
14	b	0.37	0/1541	0.70	1/2087 (0.0%)
All	All	0.39	0/50189	0.69	4/67863 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	201	VAL	N-CA-C	5.39	115.53	110.30
3	C	201	VAL	N-CA-C	5.36	115.50	110.30
14	N	1	THR	N-CA-C	5.16	125.45	111.00
14	b	1	THR	N-CA-C	5.15	125.41	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	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	2	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	4	0
8	H	1684	0	1685	4	0
8	V	1684	0	1685	4	0
9	I	1581	0	1574	4	0
9	W	1581	0	1574	3	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	5	0
11	K	1646	0	1596	11	0
11	Y	1646	0	1596	7	0
12	L	1757	0	1711	5	0
12	Z	1757	0	1711	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1815	0	1821	6	0
13	a	1824	0	1832	6	0
14	N	1512	0	1478	10	0
14	b	1512	0	1478	10	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	42	0	42	1	0
17	K	42	0	42	0	0
17	N	42	0	42	4	0
17	V	42	0	42	0	0
17	Y	42	0	42	0	0
17	b	42	0	42	4	0
18	K	12	0	13	0	0
18	Y	12	0	13	0	0
19	A	6	0	0	0	0
19	B	8	0	0	0	0
19	C	10	0	0	0	0
19	D	3	0	0	0	0
19	E	3	0	0	0	0
19	F	8	0	0	0	0
19	G	10	0	0	0	0
19	H	10	0	0	0	0
19	I	6	0	0	0	0
19	J	10	0	0	0	0
19	K	9	0	0	1	0
19	L	11	0	0	0	0
19	M	9	0	0	0	0
19	N	6	0	0	0	0
19	O	3	0	0	0	0
19	P	8	0	0	0	0
19	Q	6	0	0	0	0
19	R	5	0	0	0	0
19	S	6	0	0	0	0
19	T	9	0	0	0	0
19	U	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	V	10	0	0	0	0
19	W	5	0	0	0	0
19	X	12	0	0	0	0
19	Y	14	0	0	0	0
19	Z	16	0	0	0	0
19	a	11	0	0	0	0
19	b	8	0	0	0	0
All	All	49808	0	49325	123	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.

The worst 5 of 123 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:100:MET:HE3	11:Y:127:PHE:HB2	1.70	0.72
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.71	0.71
17:N:201:04C:O21	17:N:201:04C:O13	2.07	0.70
11:Y:53:GLN:O	11:Y:57:THR:OG1	2.13	0.66
11:K:53:GLN:O	11:K:57:THR:OG1	2.16	0.62

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	9 (4%)	0	100	100
1	O	248/250 (99%)	239 (96%)	9 (4%)	0	100	100
2	B	242/258 (94%)	232 (96%)	8 (3%)	2 (1%)	16	44
2	P	242/258 (94%)	231 (96%)	9 (4%)	2 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	238/254 (94%)	229 (96%)	7 (3%)	2 (1%)	16	44
3	Q	238/254 (94%)	229 (96%)	7 (3%)	2 (1%)	16	44
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%)	220 (96%)	9 (4%)	0	100	100
5	S	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	234 (97%)	7 (3%)	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	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	55
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	55
11	K	210/212 (99%)	206 (98%)	3 (1%)	1 (0%)	24	55
11	Y	210/212 (99%)	206 (98%)	3 (1%)	1 (0%)	24	55
12	L	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
12	Z	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
13	M	230/246 (94%)	223 (97%)	7 (3%)	0	100	100
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	b	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6275/6614 (95%)	6091 (97%)	172 (3%)	12 (0%)	43	72

5 of 12 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
3	C	239	GLN

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%)	204 (98%)	5 (2%)	43	77
1	O	209/209 (100%)	204 (98%)	5 (2%)	43	77
2	B	203/216 (94%)	196 (97%)	7 (3%)	32	68
2	P	203/216 (94%)	195 (96%)	8 (4%)	28	64
3	C	212/226 (94%)	203 (96%)	9 (4%)	26	61
3	Q	212/226 (94%)	203 (96%)	9 (4%)	26	61
4	D	194/215 (90%)	180 (93%)	14 (7%)	13	39
4	R	194/215 (90%)	180 (93%)	14 (7%)	13	39
5	E	190/193 (98%)	183 (96%)	7 (4%)	30	65
5	S	190/193 (98%)	183 (96%)	7 (4%)	30	65
6	F	201/239 (84%)	189 (94%)	12 (6%)	17	47
6	T	201/239 (84%)	189 (94%)	12 (6%)	17	47
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	59
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	59
8	H	181/190 (95%)	176 (97%)	5 (3%)	38	73
8	V	181/190 (95%)	176 (97%)	5 (3%)	38	73
9	I	172/173 (99%)	168 (98%)	4 (2%)	44	78
9	W	172/173 (99%)	168 (98%)	4 (2%)	44	78
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	73
10	X	173/175 (99%)	169 (98%)	4 (2%)	44	78
11	K	170/170 (100%)	164 (96%)	6 (4%)	32	67
11	Y	170/170 (100%)	164 (96%)	6 (4%)	32	67
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	70
12	Z	185/185 (100%)	179 (97%)	6 (3%)	34	70
13	M	198/208 (95%)	189 (96%)	9 (4%)	24	58
13	a	199/208 (96%)	189 (95%)	10 (5%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	158 (98%)	4 (2%)	42	76
14	b	162/162 (100%)	158 (98%)	4 (2%)	42	76
All	All	5313/5542 (96%)	5108 (96%)	205 (4%)	28	64

5 of 205 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	4	ARG
5	S	188	LEU
13	a	225	ILE
3	Q	160	GLN
4	R	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
10	X	55	GLN
10	X	147	HIS
13	a	48	ASN
9	I	88	GLN
9	I	63	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 17 ligands modelled in this entry, 9 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
18	MES	K	303	-	12,12,12	2.33	1 (8%)	15,16,16	1.17	2 (13%)
17	04C	K	301	11	44,44,44	1.36	3 (6%)	54,58,58	1.28	8 (14%)
17	04C	Y	301	11	44,44,44	1.38	3 (6%)	54,58,58	1.28	8 (14%)
17	04C	H	301	8	44,44,44	1.23	3 (6%)	54,58,58	1.12	7 (12%)
17	04C	V	301	8	44,44,44	1.20	3 (6%)	54,58,58	1.11	6 (11%)
17	04C	b	201	14	44,44,44	1.59	4 (9%)	54,58,58	1.34	9 (16%)
17	04C	N	201	14	44,44,44	1.62	4 (9%)	54,58,58	1.33	9 (16%)
18	MES	Y	303	-	12,12,12	2.27	1 (8%)	15,16,16	1.14	2 (13%)

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
18	MES	K	303	-	-	0/6/14/14	0/1/1/1
17	04C	K	301	11	-	9/44/52/52	0/3/3/3
17	04C	Y	301	11	-	9/44/52/52	0/3/3/3
17	04C	H	301	8	-	15/44/52/52	0/3/3/3
17	04C	V	301	8	-	14/44/52/52	0/3/3/3
17	04C	b	201	14	-	16/44/52/52	0/3/3/3
17	04C	N	201	14	-	16/44/52/52	0/3/3/3
18	MES	Y	303	-	-	0/6/14/14	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	303	MES	C8-S	-7.79	1.66	1.77
18	Y	303	MES	C8-S	-7.56	1.67	1.77
17	N	201	04C	C10-C9	7.20	1.65	1.53
17	b	201	04C	C10-C9	7.07	1.65	1.53
17	Y	301	04C	C10-C9	5.71	1.63	1.53

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	201	04C	C11-C10-C12	-4.18	104.44	109.76
17	b	201	04C	C11-C10-C12	-4.08	104.56	109.76
17	Y	301	04C	O13-C12-C10	-3.34	104.66	111.51
17	K	301	04C	O13-C12-C10	-3.25	104.83	111.51
17	b	201	04C	C29-C30-N31	-3.20	105.98	113.41

There are no chirality outliers.

5 of 79 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	K	301	04C	C11-C10-C9-C8
17	K	301	04C	C12-C10-C9-C8
17	N	201	04C	C11-C10-C9-C8

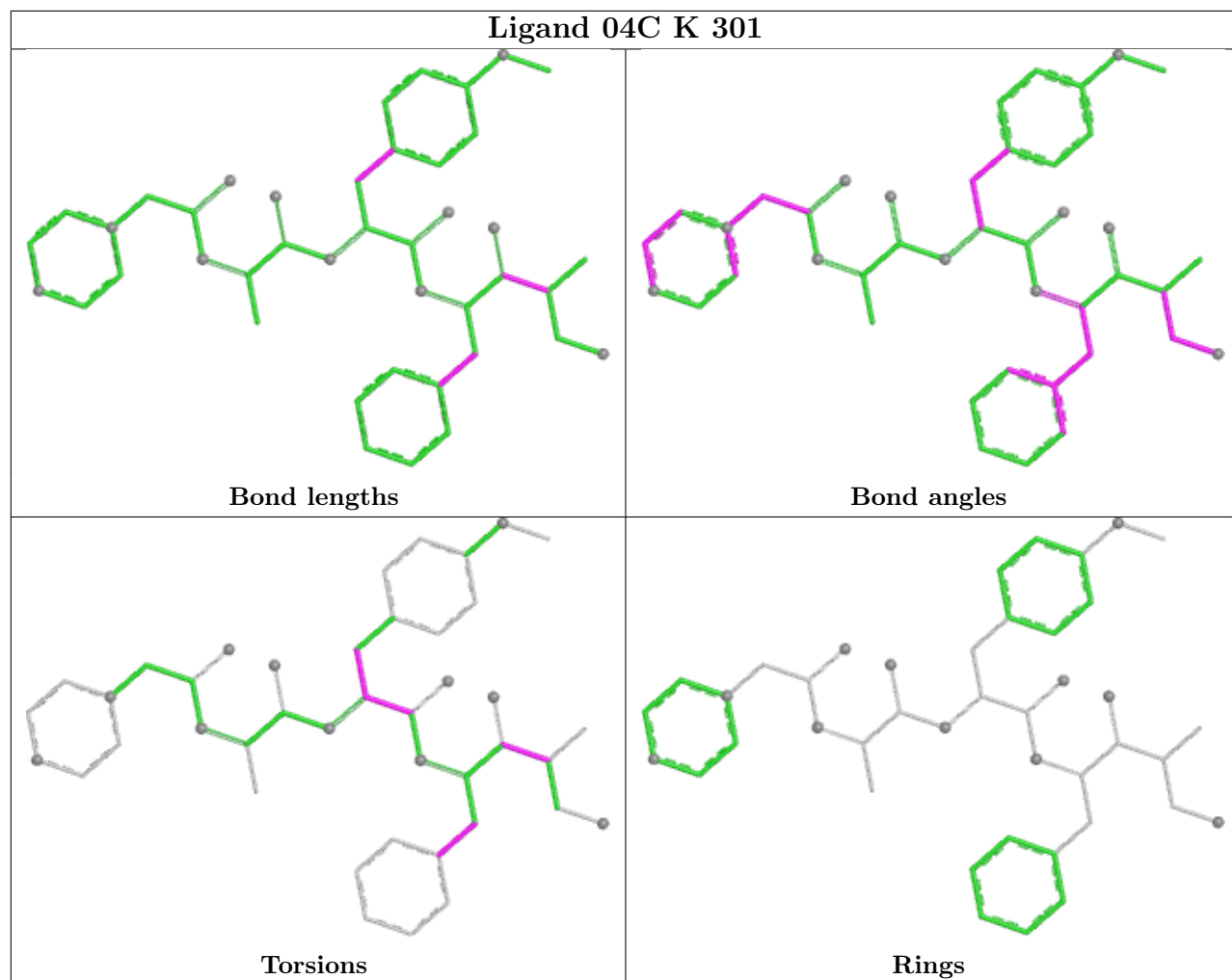
There are no ring outliers.

3 monomers are involved in 9 short contacts:

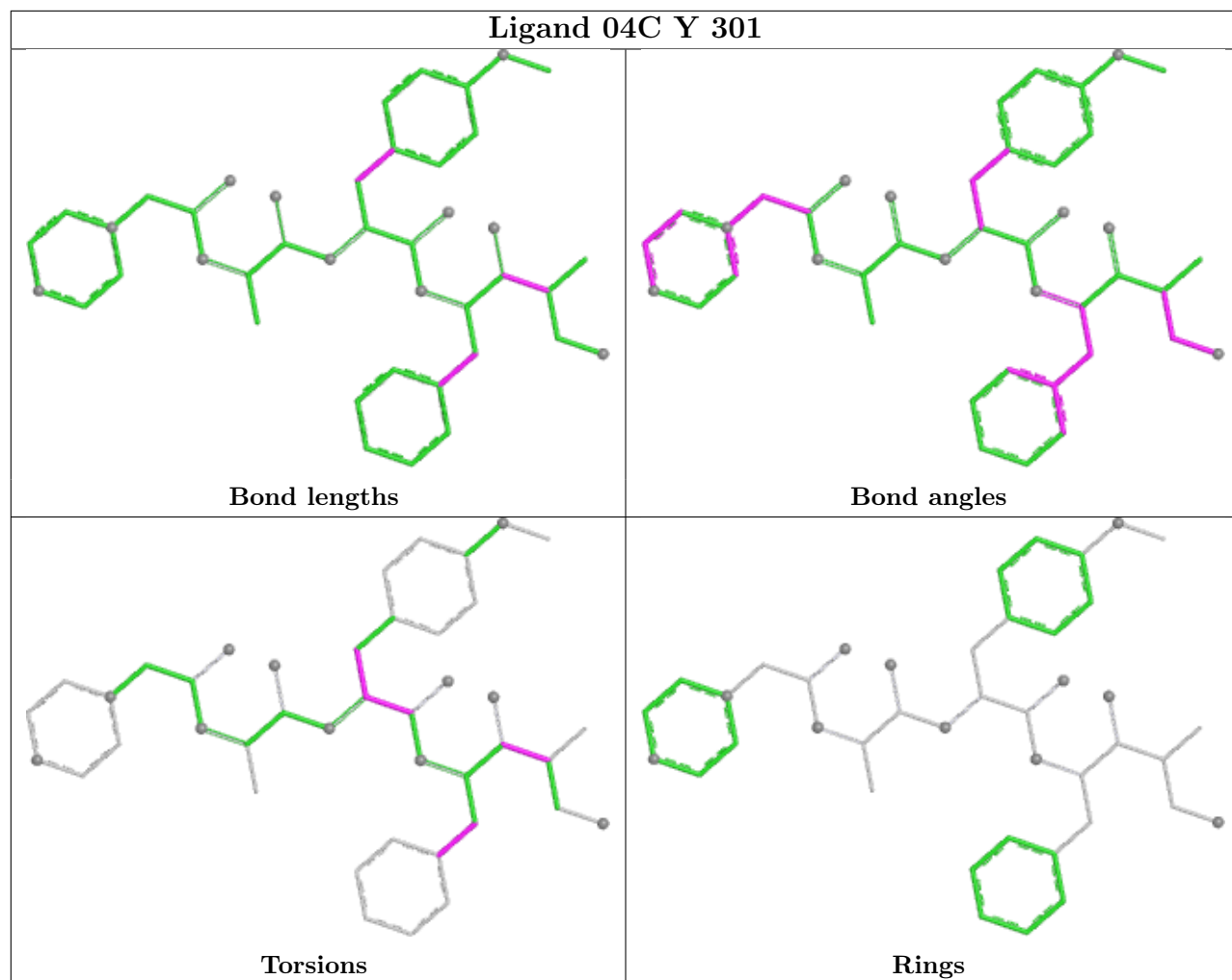
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	04C	1	0
17	b	201	04C	4	0
17	N	201	04C	4	0

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.

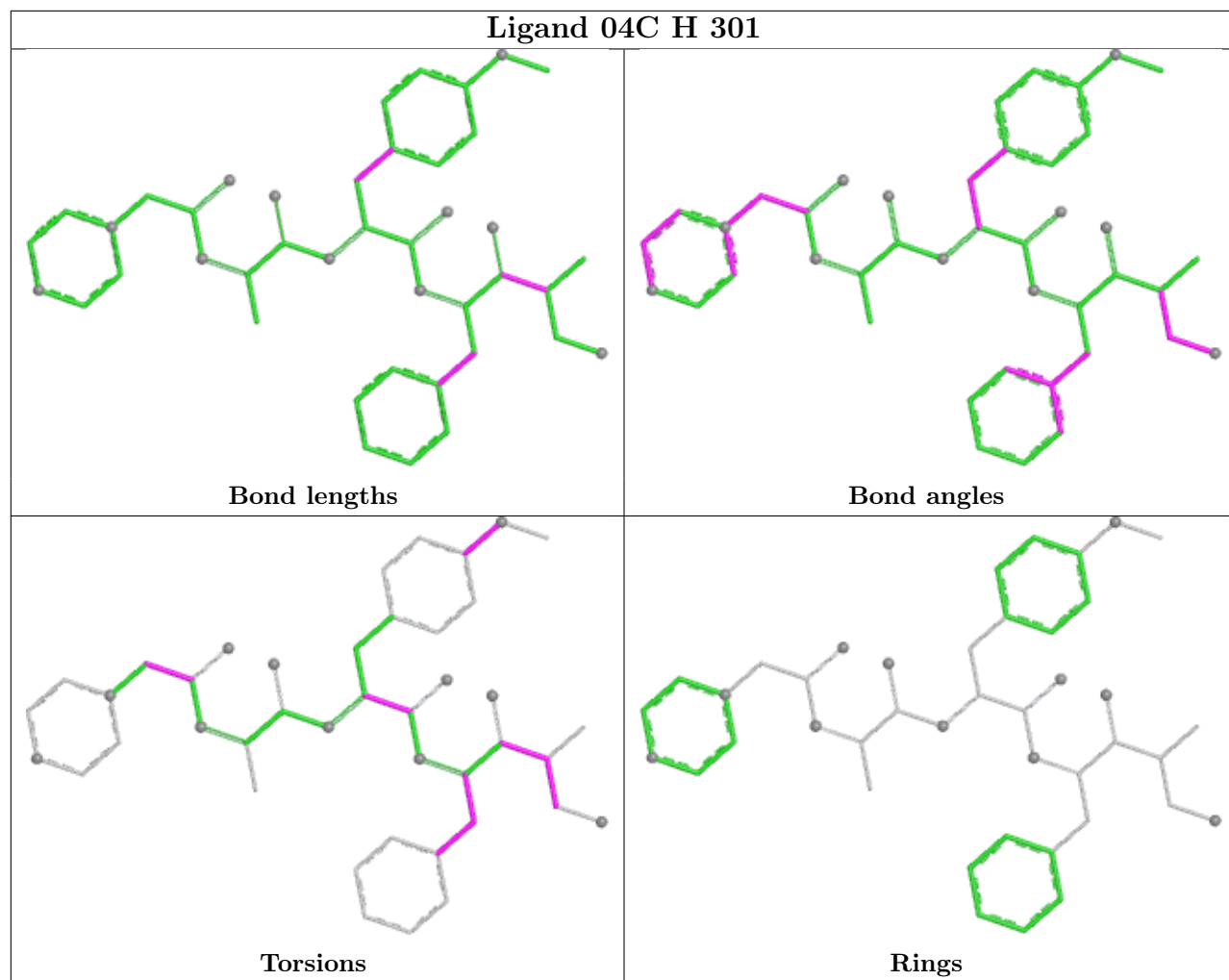
Ligand 04C K 301



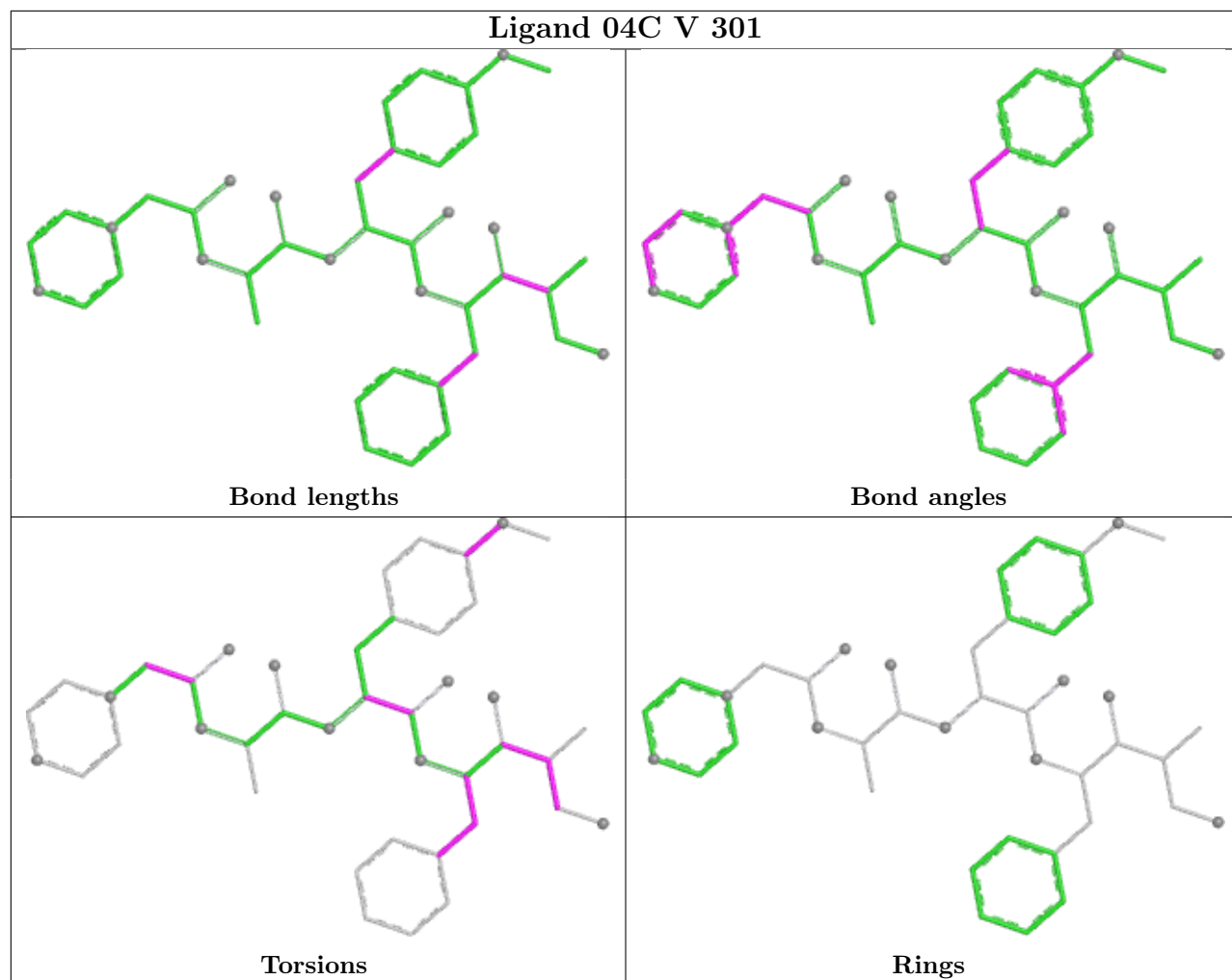
Ligand 04C Y 301

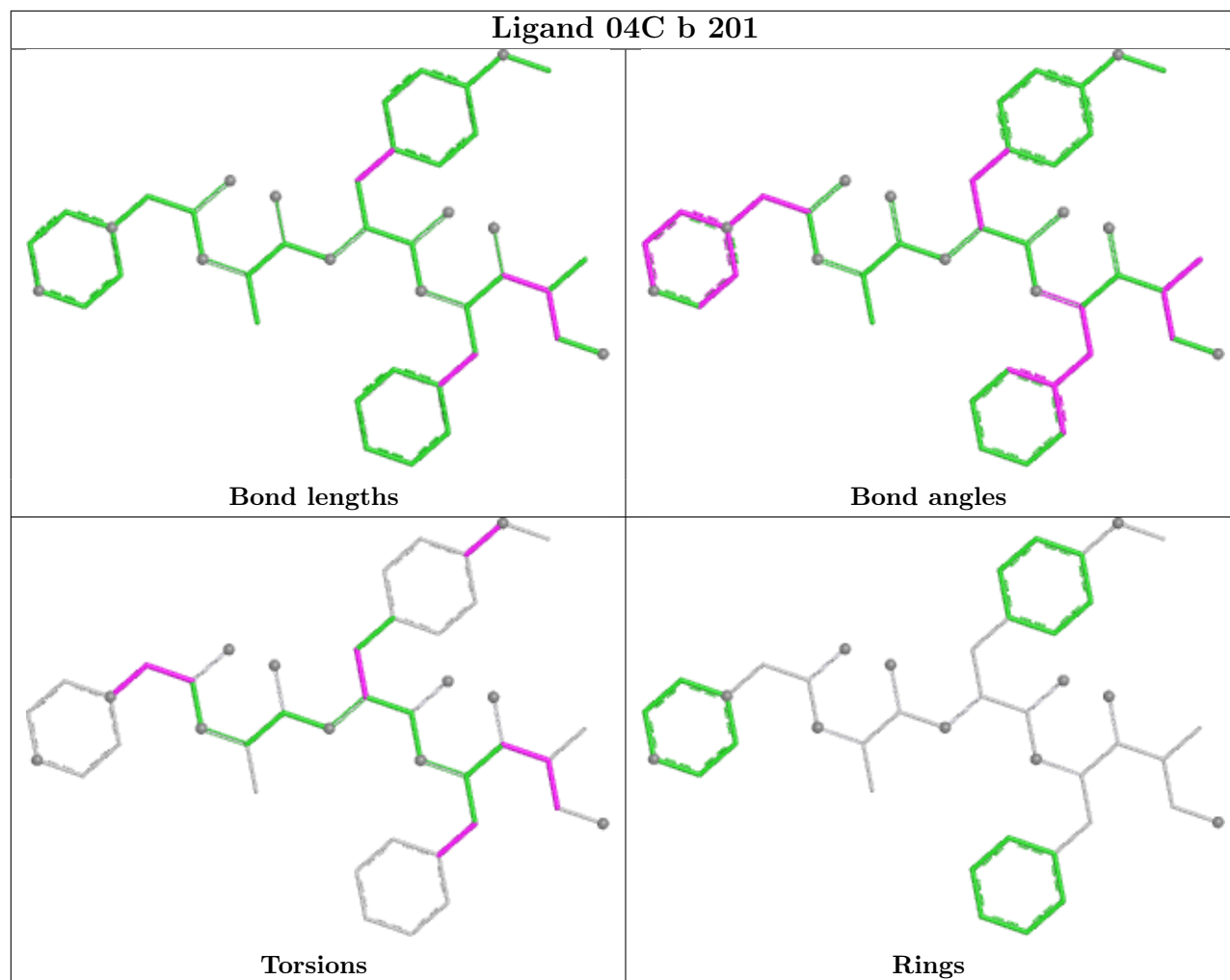


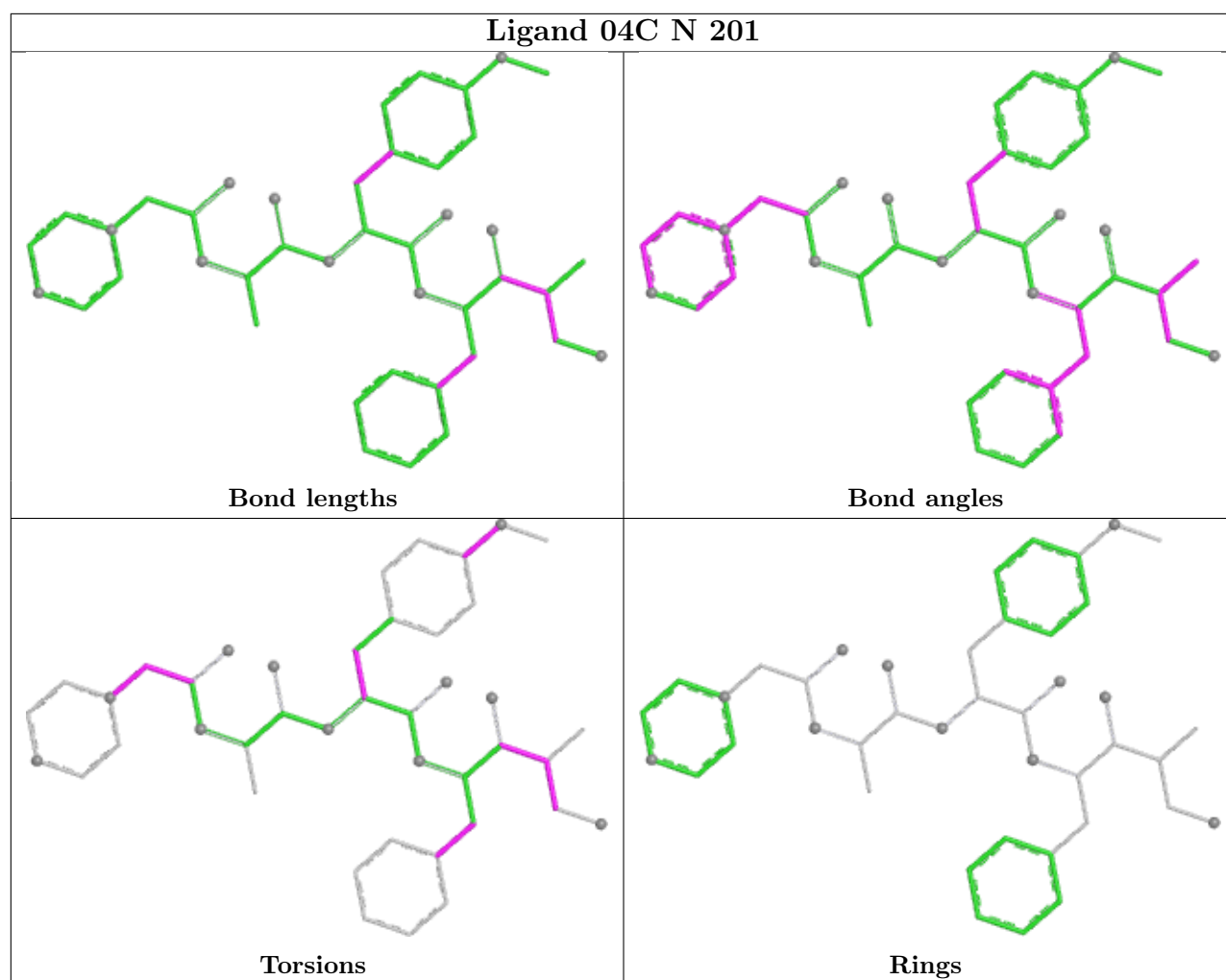
Ligand 04C H 301



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%)	-0.61	1 (0%) 88 84	44, 61, 96, 137	0
1	O	250/250 (100%)	-0.55	2 (0%) 82 75	45, 66, 109, 144	0
2	B	244/258 (94%)	-0.47	3 (1%) 76 68	44, 66, 113, 176	0
2	P	244/258 (94%)	-0.43	1 (0%) 88 84	45, 67, 114, 173	0
3	C	240/254 (94%)	-0.40	1 (0%) 88 84	45, 71, 128, 160	0
3	Q	240/254 (94%)	-0.27	1 (0%) 88 84	47, 78, 153, 178	0
4	D	235/260 (90%)	-0.48	1 (0%) 88 84	50, 71, 104, 143	0
4	R	235/260 (90%)	-0.42	1 (0%) 88 84	52, 73, 106, 149	0
5	E	231/234 (98%)	-0.46	0 100 100	52, 78, 110, 149	0
5	S	231/234 (98%)	-0.40	0 100 100	49, 76, 112, 143	0
6	F	243/288 (84%)	-0.52	0 100 100	48, 70, 110, 147	0
6	T	243/288 (84%)	-0.45	0 100 100	43, 70, 116, 141	0
7	G	241/252 (95%)	-0.55	0 100 100	42, 64, 99, 137	0
7	U	241/252 (95%)	-0.57	0 100 100	42, 61, 95, 119	0
8	H	222/232 (95%)	-0.60	0 100 100	45, 61, 85, 121	0
8	V	222/232 (95%)	-0.61	0 100 100	45, 63, 87, 125	0
9	I	204/205 (99%)	-0.72	0 100 100	37, 57, 90, 115	0
9	W	204/205 (99%)	-0.68	0 100 100	41, 59, 91, 115	0
10	J	195/198 (98%)	-0.72	1 (0%) 87 82	39, 56, 83, 128	0
10	X	195/198 (98%)	-0.68	1 (0%) 87 82	42, 58, 86, 144	0
11	K	212/212 (100%)	-0.71	0 100 100	43, 58, 84, 115	0
11	Y	212/212 (100%)	-0.69	1 (0%) 87 82	42, 58, 80, 110	0
12	L	222/222 (100%)	-0.69	0 100 100	46, 63, 86, 105	0
12	Z	222/222 (100%)	-0.68	0 100 100	40, 60, 85, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	232/246 (94%)	-0.61	0 100 100	43, 61, 88, 112	0
13	a	233/246 (94%)	-0.58	1 (0%) 88 84	41, 59, 88, 127	0
14	N	196/196 (100%)	-0.70	0 100 100	41, 58, 86, 109	0
14	b	196/196 (100%)	-0.68	1 (0%) 87 82	42, 57, 88, 114	0
All	All	6335/6614 (95%)	-0.56	16 (0%) 90 86	37, 64, 106, 178	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.7
10	X	1	MET	4.3
3	Q	50	LEU	3.6
2	P	219	ALA	3.6
1	O	1	MET	3.5

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
17	04C	N	201	42/42	0.72	0.17	75,89,117,122	0
17	04C	b	201	42/42	0.83	0.16	65,95,123,126	0
17	04C	V	301	42/42	0.85	0.14	80,88,118,122	0
17	04C	H	301	42/42	0.86	0.14	73,89,121,124	0
17	04C	Y	301	42/42	0.95	0.08	39,51,74,76	0
15	MG	V	302	1/1	0.95	0.09	81,81,81,81	0
17	04C	K	301	42/42	0.96	0.07	38,48,80,84	0

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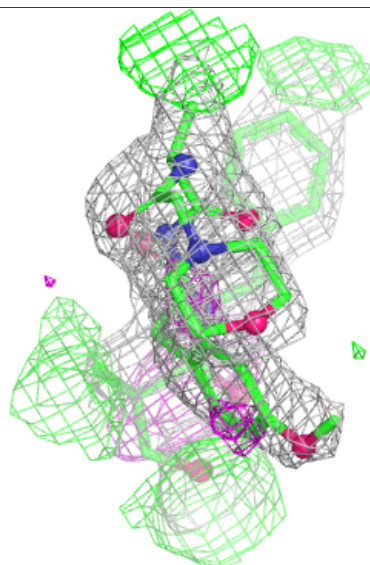
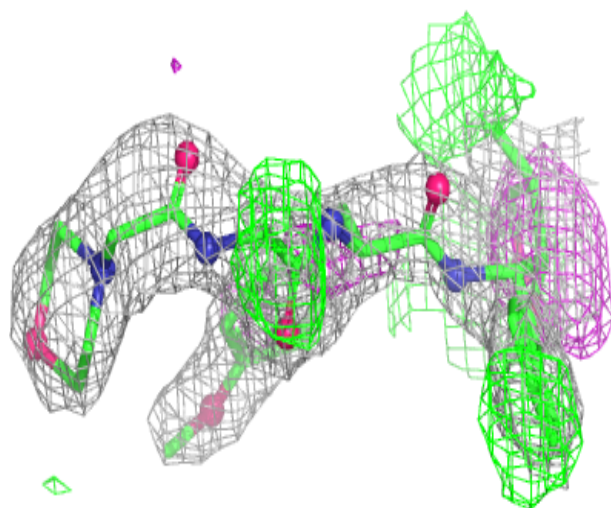
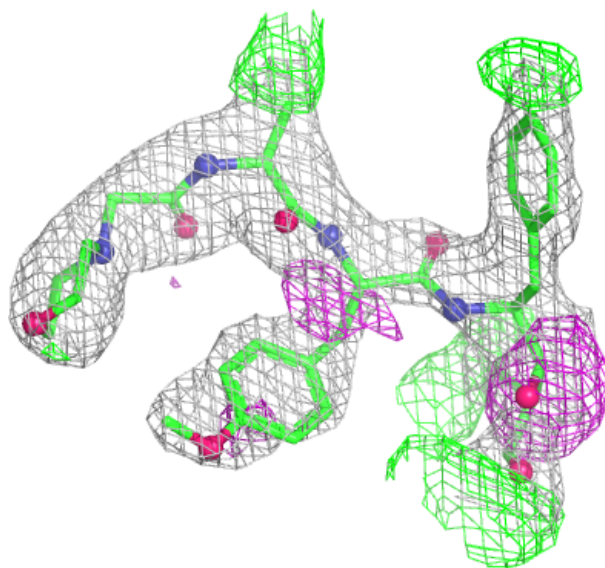
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	MES	K	303	12/12	0.96	0.10	58,64,65,68	0
15	MG	I	301	1/1	0.98	0.07	60,60,60,60	0
15	MG	Z	301	1/1	0.98	0.04	70,70,70,70	0
15	MG	N	202	1/1	0.98	0.04	56,56,56,56	0
18	MES	Y	303	12/12	0.98	0.07	49,60,62,65	0
16	CL	G	302	1/1	0.99	0.07	50,50,50,50	0
16	CL	U	301	1/1	0.99	0.09	49,49,49,49	0
15	MG	K	302	1/1	0.99	0.07	63,63,63,63	0
15	MG	Y	302	1/1	0.99	0.08	39,39,39,39	0
15	MG	G	301	1/1	0.99	0.04	55,55,55,55	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.

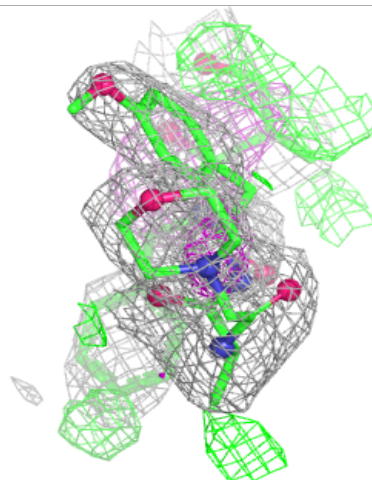
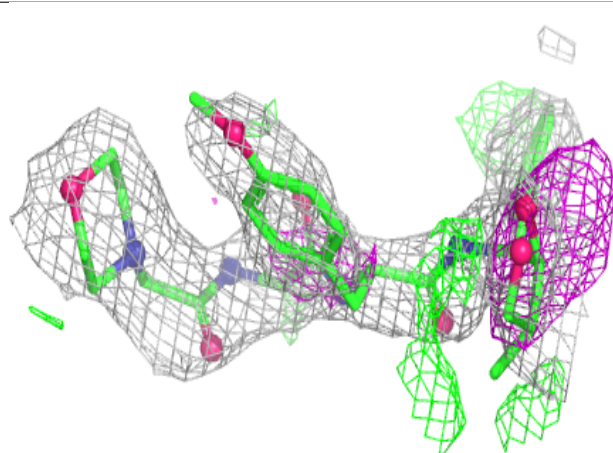
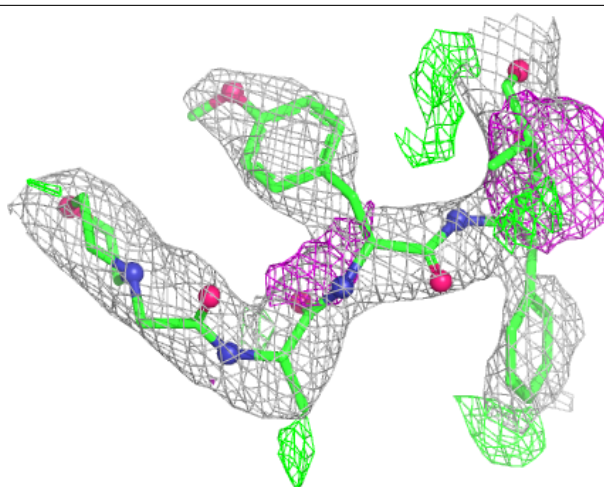
Electron density around 04C N 201:

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



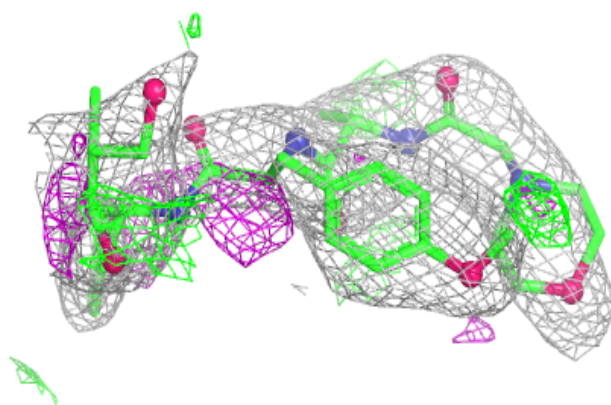
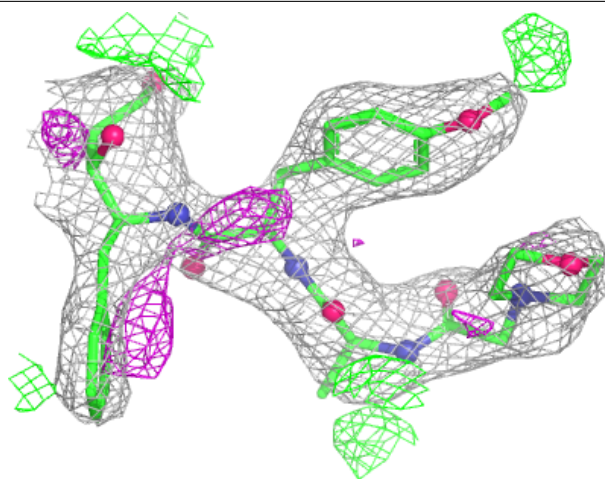
Electron density around 04C b 201:

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



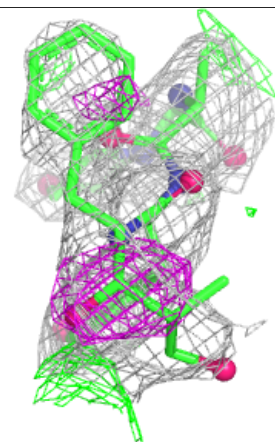
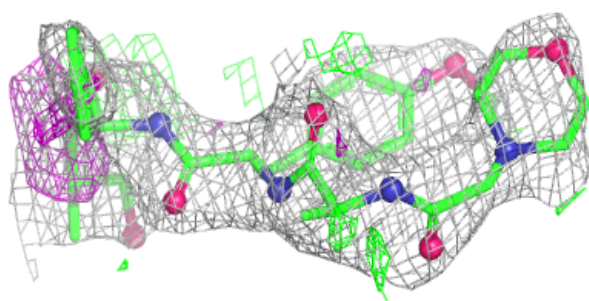
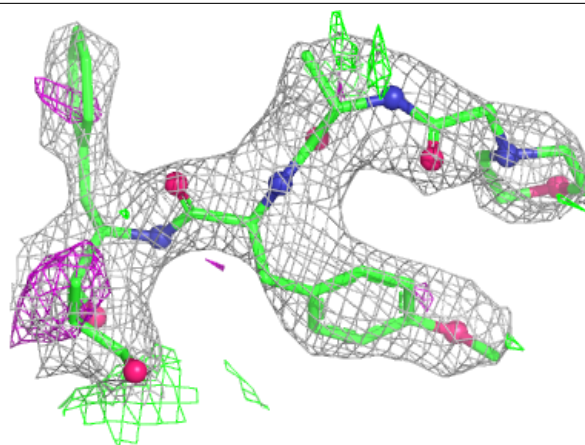
Electron density around 04C V 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

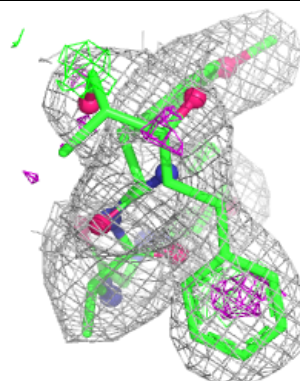
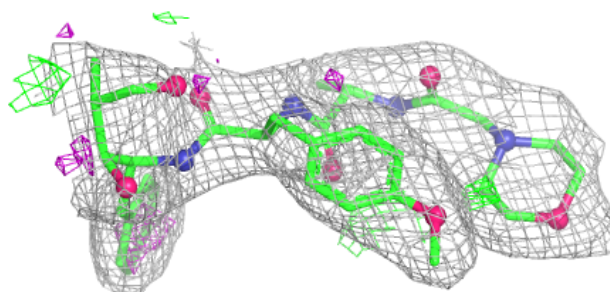
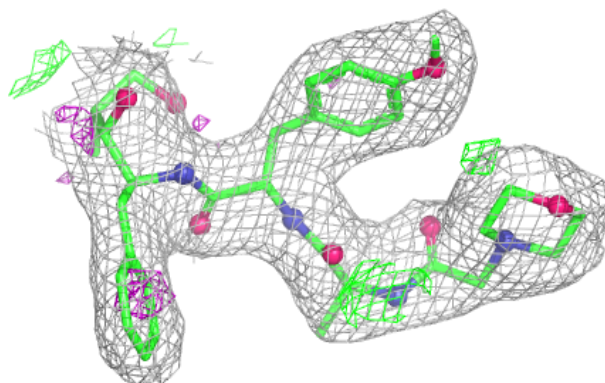


Electron density around 04C H 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

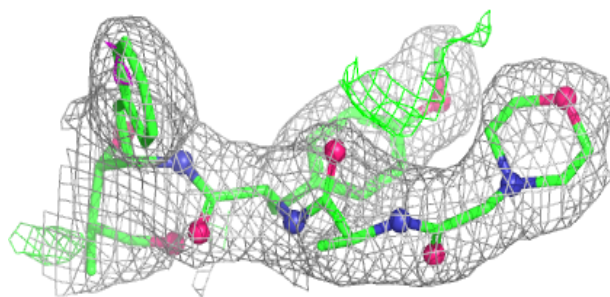
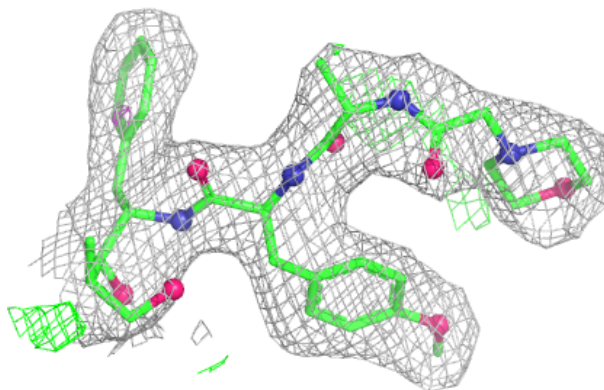
**Electron density around 04C Y 301:**

$2mF_o-DF_c$ (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.