



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2022 – 10:14 am BST

PDB ID : 7O2L
Title : Yeast 20S proteasome in complex with the covalently bound inhibitor b-lactone (2R,3S)-3-isopropyl-4-oxo-2-oxetane-carboxylate (IOC)
Authors : Shi, Y.M.; Hirschmann, M.; Shi, Y.N.; Shabbir, A.; Abebew, D.; Tobias, N.J.; Gruen, P.; Crames, J.J.; Poeschel, L.; Kuttelochner, W.; Richter, C.; Herrmann, J.; Mueller, R.; Thanwisai, A.; Pidot, S.J.; Stinear, T.P.; Groll, M.; Kim, Y.; Bode, H.
Deposited on : 2021-03-30
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

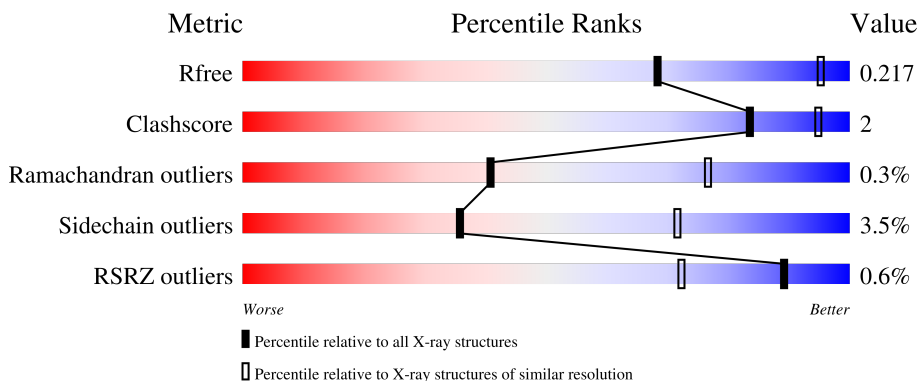
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	96%
1	O	250	96%
2	B	258	86% 8% 5%
2	P	258	87% 8% 5%
3	C	254	87% 6% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	2% 87% 6% • 6%
4	D	260	85% • • 10%
4	R	260	85% 5% 10%
5	E	234	91% 7% ••
5	S	234	2% 91% 7% •
6	F	288	78% 5% • 16%
6	T	288	78% 6% 16%
7	G	252	88% 7% •
7	U	252	88% 7% •
8	H	232	3% 84% 13% •
8	V	232	3% 86% 12% •
9	I	205	94% 5%
9	W	205	94% 5%
10	J	198	1% 91% 7% ••
10	X	198	1% 91% 7% ••
11	K	212	88% 11% •
11	Y	212	86% 13% •
12	L	222	90% 9% •
12	Z	222	90% 10%
13	M	246	86% 6% • 7%
13	a	246	90% • 7%
14	N	196	92% 8% •
14	b	196	98%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49492 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 HLJ1_G0039880.mRNA.1.CDS.1.

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

- Molecule 2 is a protein called BJ4_G0021480.mRNA.1.CDS.1.

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

- Molecule 3 is a protein called HLJ1_G0048980.mRNA.1.CDS.1.

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

- Molecule 4 is a protein called 20S proteasome.

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

- Molecule 5 is a protein called BJ4_G0043800.mRNA.1.CDS.1.

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 BJ4_G0020160.mRNA.1.CDS.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 endopeptidase complex.

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

- Molecule 9 is a protein called Proteasome endopeptidase complex.

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.

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

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 12 is a protein called Proteasome endopeptidase complex.

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	228	Total	C	N	O	S	0	0	0
			1786	1131	305	343	7			
13	a	228	Total	C	N	O	S	0	0	0
			1786	1131	305	343	7			

- Molecule 14 is a protein called Proteasome endopeptidase complex.

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

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

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

Continued on next page...

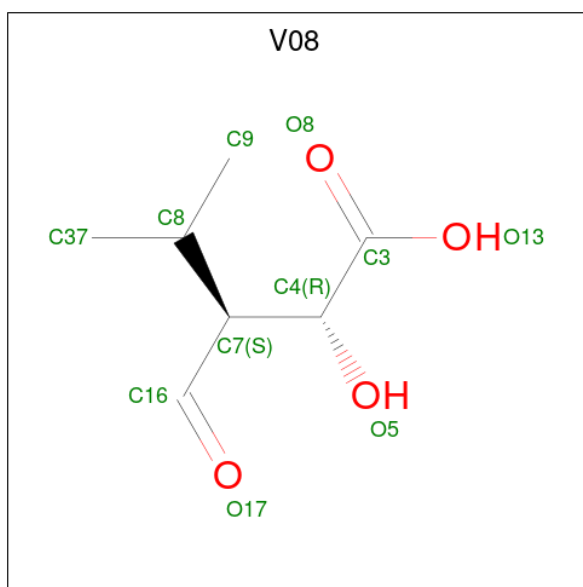
Continued from previous page...

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

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 17 is (2 {R},3 {S})-3-methanoyl-4-methyl-2-hydroxy-pentanoic acid (three-letter code: V08) (formula: C₇H₁₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	H	1	Total	C	O	0	0
			11	7	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	K	1	Total	C	O	0	0
			11	7	4		
17	N	1	Total	C	O	0	0
			11	7	4		
17	V	1	Total	C	O	0	0
			11	7	4		
17	Y	1	Total	C	O	0	0
			11	7	4		
17	b	1	Total	C	O	0	0
			11	7	4		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	4	Total	O	0	0
			4	4		
18	B	9	Total	O	0	0
			9	9		
18	C	5	Total	O	0	0
			5	5		
18	D	2	Total	O	0	0
			2	2		
18	E	3	Total	O	0	0
			3	3		
18	F	3	Total	O	0	0
			3	3		
18	G	4	Total	O	0	0
			4	4		
18	H	6	Total	O	0	0
			6	6		
18	I	3	Total	O	0	0
			3	3		
18	J	5	Total	O	0	0
			5	5		
18	K	8	Total	O	0	0
			8	8		
18	L	7	Total	O	0	0
			7	7		
18	M	10	Total	O	0	0
			10	10		
18	N	5	Total	O	0	0
			5	5		

Continued on next page...

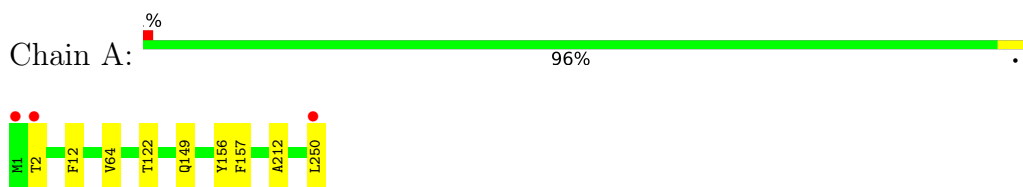
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	P	5	Total O 5 5	0	0
18	Q	1	Total O 1 1	0	0
18	R	1	Total O 1 1	0	0
18	S	2	Total O 2 2	0	0
18	T	5	Total O 5 5	0	0
18	U	3	Total O 3 3	0	0
18	V	2	Total O 2 2	0	0
18	W	1	Total O 1 1	0	0
18	X	5	Total O 5 5	0	0
18	Y	9	Total O 9 9	0	0
18	Z	4	Total O 4 4	0	0
18	a	8	Total O 8 8	0	0
18	b	6	Total O 6 6	0	0

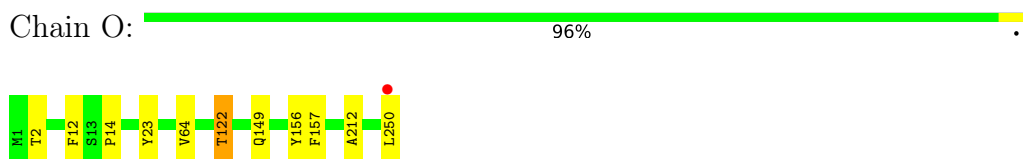
3 Residue-property plots [i](#)

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.

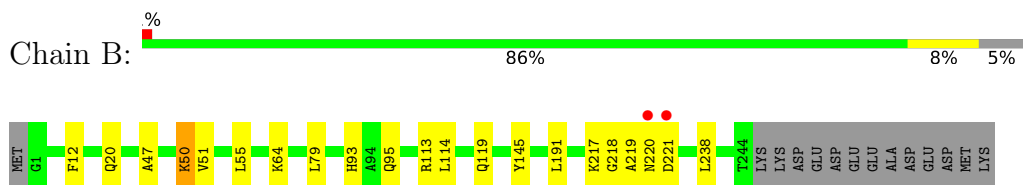
- Molecule 1: HLJ1_G0039880.mRNA.1.CDS.1



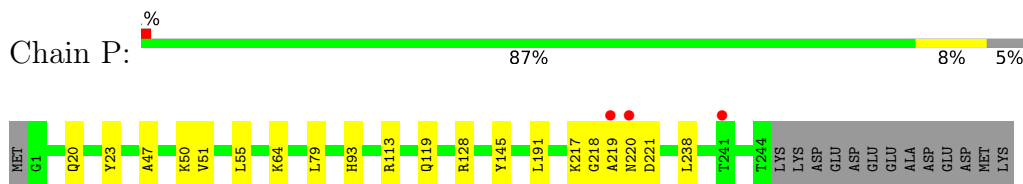
- Molecule 1: HLJ1_G0039880.mRNA.1.CDS.1



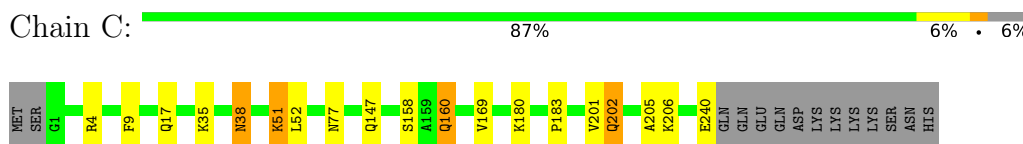
- Molecule 2: BJ4_G0021480.mRNA.1.CDS.1



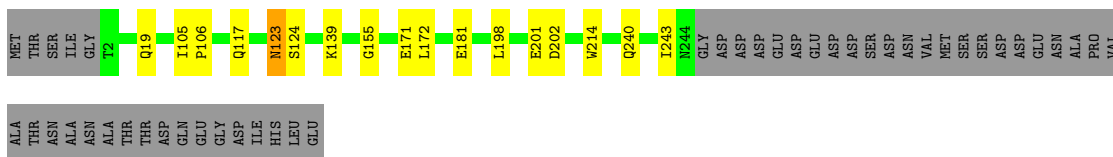
- Molecule 2: BJ4_G0021480.mRNA.1.CDS.1



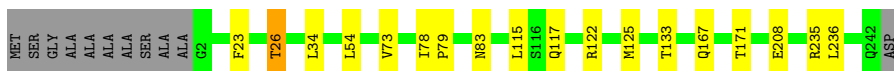
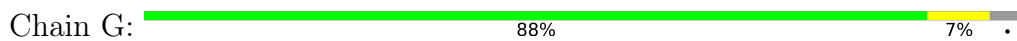
- Molecule 3: HLJ1_G0048980.mRNA.1.CDS.1



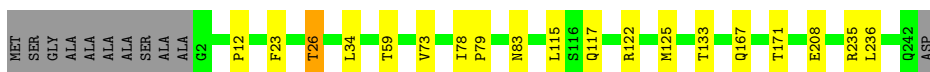
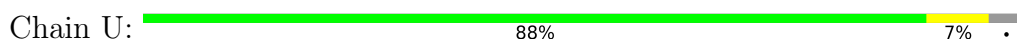
- Molecule 3: HLJ1_G0048980.mRNA.1.CDS.1



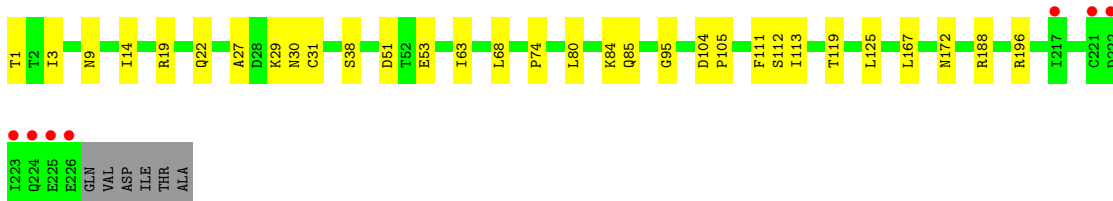
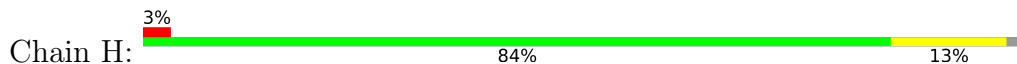
• Molecule 7: BJ4_G0020160.mRNA.1.CDS.1



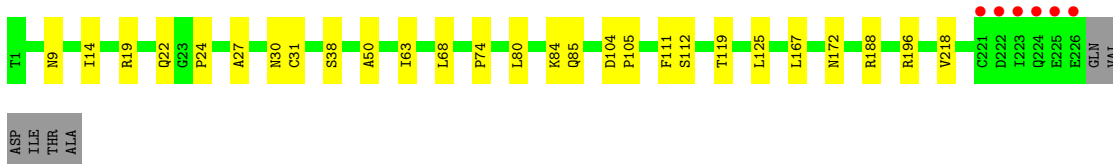
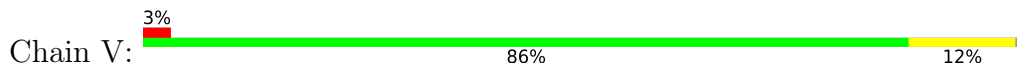
• Molecule 7: BJ4_G0020160.mRNA.1.CDS.1



• Molecule 8: Proteasome endopeptidase complex



• Molecule 8: Proteasome endopeptidase complex



• Molecule 9: Proteasome endopeptidase complex




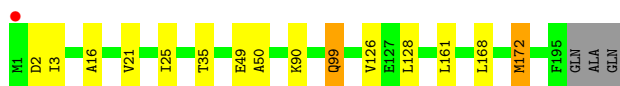
• Molecule 9: Proteasome endopeptidase complex

Chain W:  94% 5%




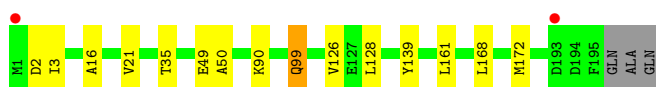
- Molecule 10: Proteasome subunit beta

Chain J:  91% 7% ..




- Molecule 10: Proteasome subunit beta

Chain X:  91% 7% ..




- Molecule 11: Proteasome subunit beta type-5

Chain K:  88% 11% .




- Molecule 11: Proteasome subunit beta type-5

Chain Y:  86% 13% .




- Molecule 12: Proteasome endopeptidase complex

Chain L:  90% 9% .




- Molecule 12: Proteasome endopeptidase complex

Chain Z:  90% 10%




- Molecule 13: Proteasome subunit beta type-7

Chain M:  86% 6% • 7%




- Molecule 13: Proteasome subunit beta type-7

Chain a:  90% • 7%



- Molecule 14: Proteasome endopeptidase complex

Chain N:  92% 8% •



- Molecule 14: Proteasome endopeptidase complex

Chain b:  98% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.12Å 301.50Å 144.25Å 90.00° 112.93° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 48.78 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-3.00) 96.4 (48.78-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.178 , 0.216 0.182 , 0.217	Depositor DCC
R_{free} test set	10185 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	76.5	Xtrriage
Anisotropy	0.867	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	49492	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: MG, V08, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	0/1952	0.70	0/2642
1	O	0.66	0/1952	0.70	0/2642
2	B	0.66	0/1934	0.72	0/2618
2	P	0.66	0/1934	0.72	0/2618
3	C	0.67	0/1910	0.72	0/2586
3	Q	0.67	0/1910	0.72	0/2586
4	D	0.67	0/1837	0.71	0/2475
4	R	0.67	0/1837	0.71	0/2475
5	E	0.67	0/1800	0.72	0/2433
5	S	0.67	0/1800	0.72	0/2433
6	F	0.66	0/1932	0.70	0/2609
6	T	0.66	0/1932	0.70	0/2609
7	G	0.65	0/1945	0.70	0/2634
7	U	0.65	0/1945	0.70	0/2634
8	H	0.66	0/1750	0.72	0/2373
8	V	0.66	0/1750	0.72	0/2373
9	I	0.66	0/1611	0.71	0/2174
9	W	0.66	0/1611	0.71	0/2174
10	J	0.65	0/1589	0.70	0/2142
10	X	0.65	0/1589	0.70	0/2142
11	K	0.66	0/1681	0.72	0/2274
11	Y	0.66	0/1681	0.72	0/2274
12	L	0.65	0/1795	0.71	0/2420
12	Z	0.65	0/1795	0.71	0/2420
13	M	0.66	0/1817	0.72	0/2465
13	a	0.66	0/1817	0.72	0/2465
14	N	0.66	0/1541	0.70	0/2087
14	b	0.66	0/1541	0.71	0/2087
All	All	0.66	0/50188	0.71	0/67864

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3	0
1	O	1915	0	1929	6	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	12	0
5	S	1773	0	1775	10	0
6	F	1892	0	1883	7	0
6	T	1892	0	1883	6	0
7	G	1907	0	1901	7	0
7	U	1907	0	1901	8	0
8	H	1719	0	1718	19	0
8	V	1719	0	1718	16	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	8	0
10	X	1561	0	1569	7	0
11	K	1644	0	1594	14	0
11	Y	1644	0	1594	17	0
12	L	1757	0	1711	17	0
12	Z	1757	0	1711	15	0
13	M	1786	0	1790	7	0
13	a	1786	0	1790	0	0
14	N	1512	0	1480	8	0
14	b	1512	0	1480	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	W	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	11	0	0	3	0
17	K	11	0	0	2	0
17	N	11	0	0	1	0
17	V	11	0	0	1	0
17	Y	11	0	0	2	0
17	b	11	0	0	0	0
18	A	4	0	0	0	0
18	B	9	0	0	1	0
18	C	5	0	0	0	0
18	D	2	0	0	0	0
18	E	3	0	0	0	0
18	F	3	0	0	0	0
18	G	4	0	0	0	0
18	H	6	0	0	0	0
18	I	3	0	0	0	0
18	J	5	0	0	0	0
18	K	8	0	0	0	0
18	L	7	0	0	0	0
18	M	10	0	0	1	0
18	N	5	0	0	0	0
18	P	5	0	0	1	0
18	Q	1	0	0	0	0
18	R	1	0	0	0	0
18	S	2	0	0	0	0
18	T	5	0	0	0	0
18	U	3	0	0	0	0
18	V	2	0	0	0	0
18	W	1	0	0	0	0
18	X	5	0	0	0	0
18	Y	9	0	0	0	0
18	Z	4	0	0	1	0
18	a	8	0	0	0	0
18	b	6	0	0	0	0
All	All	49492	0	49040	210	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 2.

The worst 5 of 210 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)
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.41	0.85
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.41	0.84
13:M:2:GLN:NE2	18:M:301:HOH:O	2.24	0.69
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.60	0.66
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.61	0.66

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%)	238 (96%)	9 (4%)	1 (0%)	34	72
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	72
2	B	242/258 (94%)	231 (96%)	7 (3%)	4 (2%)	9	39
2	P	242/258 (94%)	231 (96%)	7 (3%)	4 (2%)	9	39
3	C	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	12	45
3	Q	238/254 (94%)	229 (96%)	6 (2%)	3 (1%)	12	45
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	239/252 (95%)	233 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	U	239/252 (95%)	233 (98%)	6 (2%)	0	100	100
8	H	224/232 (97%)	222 (99%)	2 (1%)	0	100	100
8	V	224/232 (97%)	221 (99%)	3 (1%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	226/246 (92%)	218 (96%)	8 (4%)	0	100	100
13	a	226/246 (92%)	218 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6274/6614 (95%)	6094 (97%)	164 (3%)	16 (0%)	41	76

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	88
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	72
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	72
3	C	212/226 (94%)	202 (95%)	10 (5%)	26	63
3	Q	212/226 (94%)	202 (95%)	10 (5%)	26	63
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	64
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	64
5	E	190/193 (98%)	182 (96%)	8 (4%)	30	66
5	S	190/193 (98%)	182 (96%)	8 (4%)	30	66
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	60
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	60
7	G	206/210 (98%)	197 (96%)	9 (4%)	28	65
7	U	206/210 (98%)	197 (96%)	9 (4%)	28	65
8	H	185/190 (97%)	177 (96%)	8 (4%)	29	66
8	V	185/190 (97%)	179 (97%)	6 (3%)	39	74
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	85
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	85
10	J	173/175 (99%)	167 (96%)	6 (4%)	36	71
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	76
11	K	169/169 (100%)	160 (95%)	9 (5%)	22	58
11	Y	169/169 (100%)	160 (95%)	9 (5%)	22	58
12	L	185/185 (100%)	181 (98%)	4 (2%)	52	81
12	Z	185/185 (100%)	181 (98%)	4 (2%)	52	81
13	M	195/208 (94%)	189 (97%)	6 (3%)	40	75
13	a	195/208 (94%)	189 (97%)	6 (3%)	40	75
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	79
14	b	162/162 (100%)	159 (98%)	3 (2%)	57	84
All	All	5312/5540 (96%)	5124 (96%)	188 (4%)	36	71

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	240	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	26	THR
4	R	176	LEU
5	S	188	LEU
7	U	235	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
12	Z	3	ASN
12	Z	70	ASN
11	K	208	ASN
11	K	176	ASN
12	Z	158	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	V08	H	901	8	7,10,10	1.47	2 (28%)	8,13,13	1.41	2 (25%)
17	V08	K	901	11	7,10,10	1.40	1 (14%)	8,13,13	1.60	2 (25%)
17	V08	V	901	8	7,10,10	1.17	0	8,13,13	0.81	0
17	V08	Y	901	11	7,10,10	1.62	2 (28%)	8,13,13	1.99	3 (37%)
17	V08	b	901	14	7,10,10	1.34	1 (14%)	8,13,13	1.03	1 (12%)
17	V08	N	901	14	7,10,10	0.91	0	8,13,13	1.14	1 (12%)

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	V08	H	901	8	-	3/10/14/14	-
17	V08	K	901	11	-	4/10/14/14	-
17	V08	V	901	8	-	0/10/14/14	-
17	V08	Y	901	11	-	4/10/14/14	-
17	V08	b	901	14	-	1/10/14/14	-
17	V08	N	901	14	-	0/10/14/14	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	901	V08	C7-C8	-3.23	1.50	1.55
17	Y	901	V08	C7-C4	-3.02	1.51	1.54
17	H	901	V08	C7-C8	-3.02	1.50	1.55
17	Y	901	V08	C7-C8	-2.83	1.50	1.55
17	b	901	V08	C7-C16	2.57	1.54	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	901	V08	C3-C4-C7	-3.52	107.19	112.69
17	Y	901	V08	C9-C8-C7	-3.38	105.47	111.74
17	K	901	V08	C9-C8-C7	-2.97	106.23	111.74
17	H	901	V08	C37-C8-C7	-2.49	107.11	111.74
17	b	901	V08	O17-C16-C7	-2.34	119.30	125.23

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

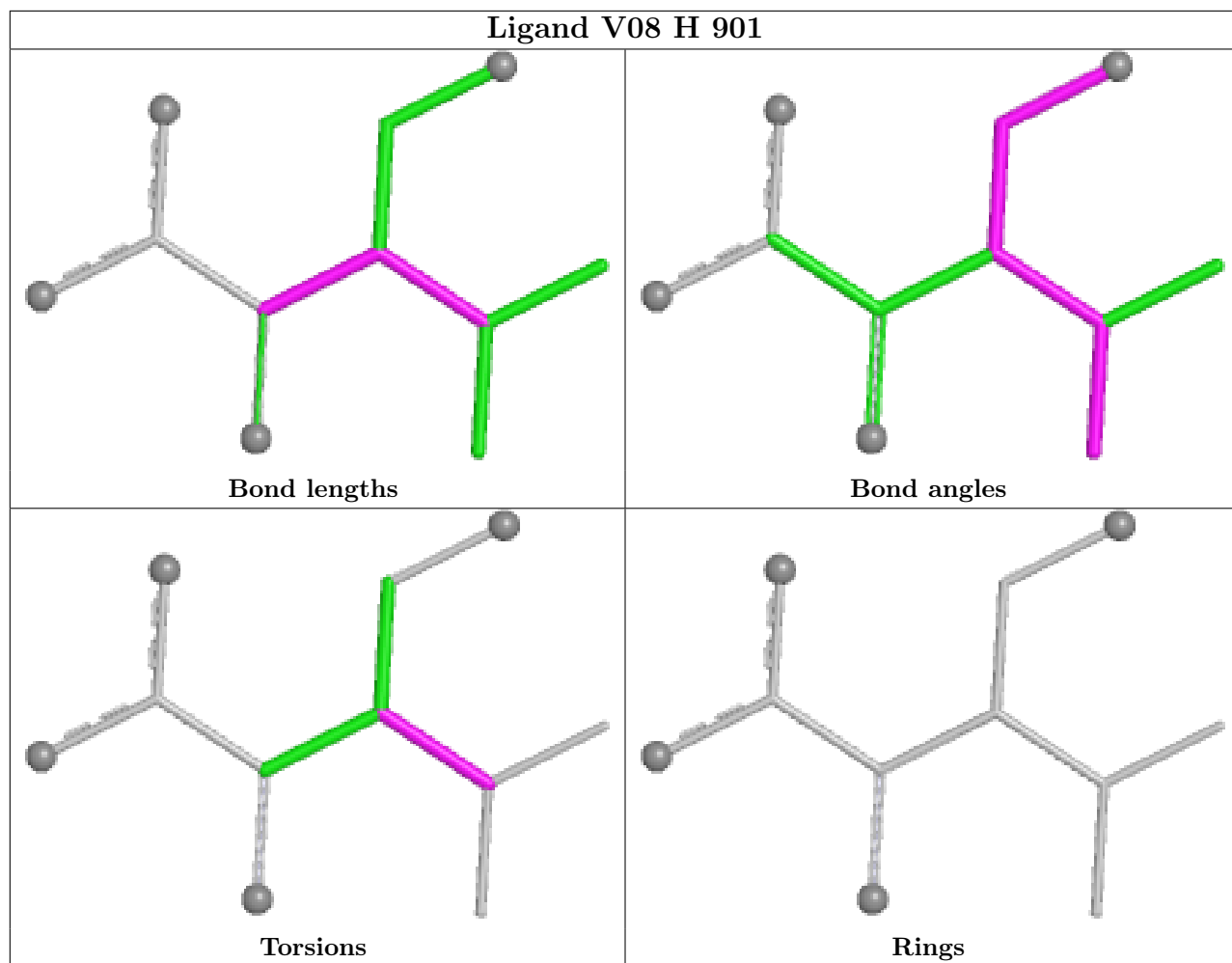
Mol	Chain	Res	Type	Atoms
17	H	901	V08	C16-C7-C8-C37
17	K	901	V08	C3-C4-C7-C8
17	K	901	V08	C3-C4-C7-C16
17	K	901	V08	O5-C4-C7-C8
17	K	901	V08	O5-C4-C7-C16

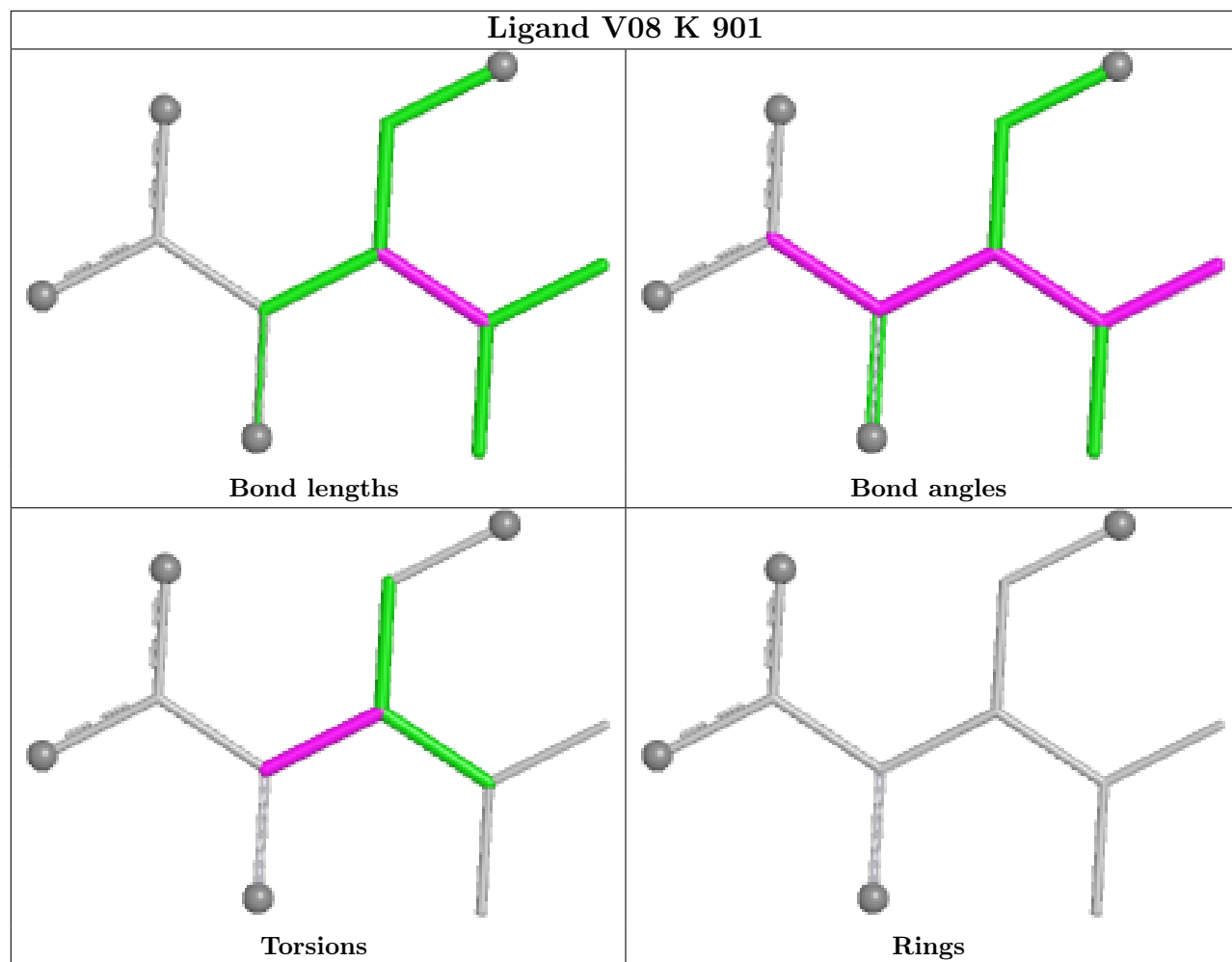
There are no ring outliers.

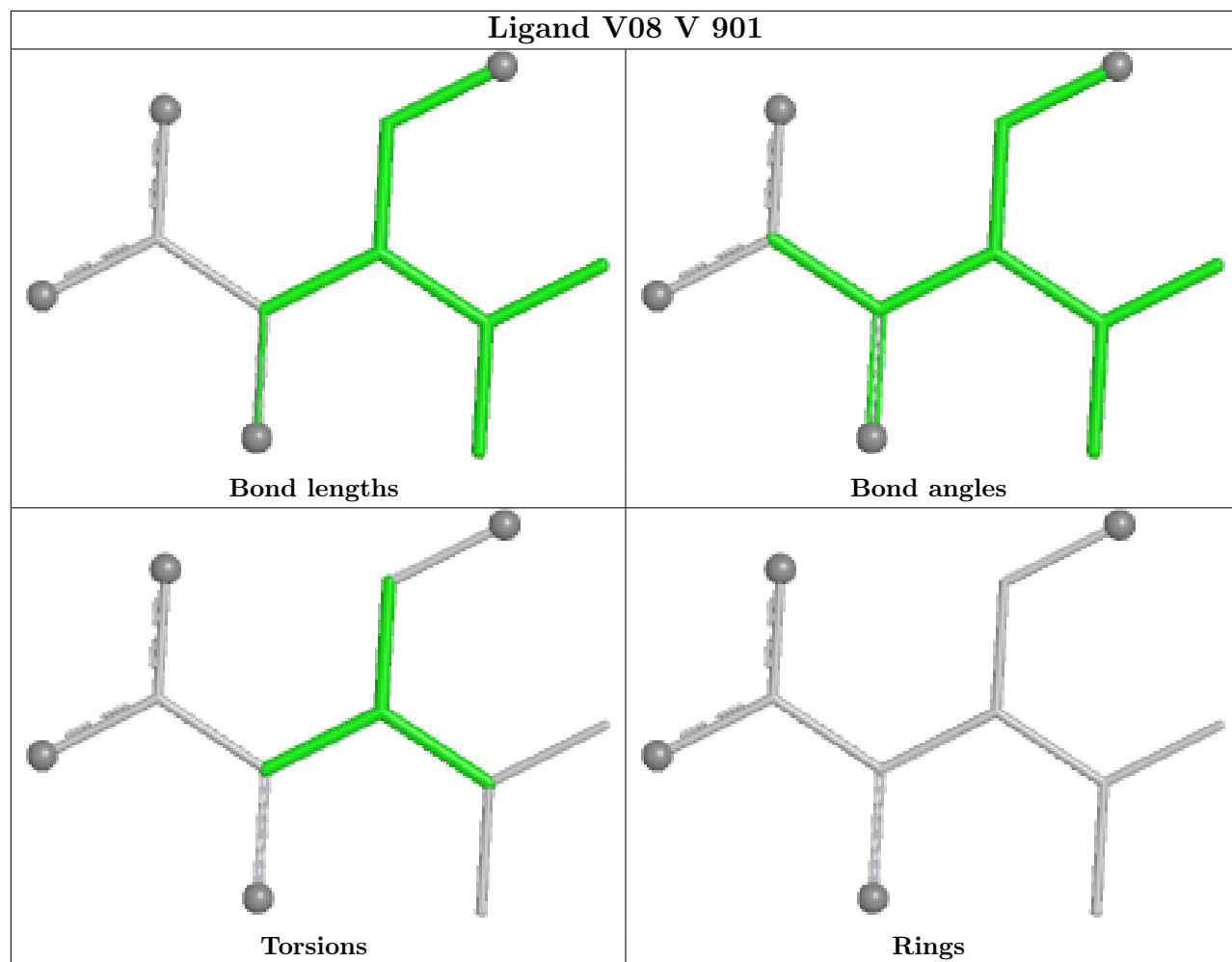
5 monomers are involved in 9 short contacts:

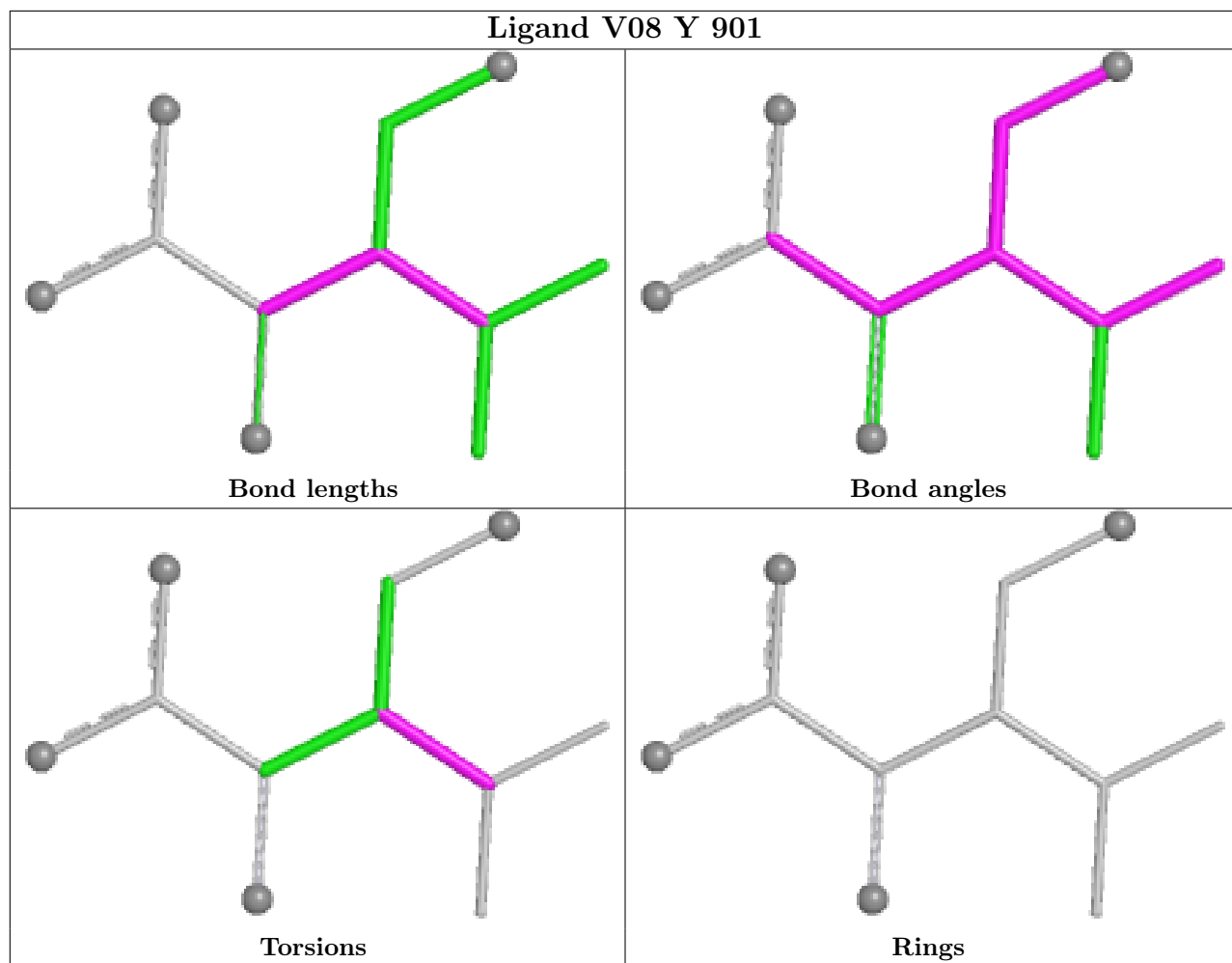
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	901	V08	3	0
17	K	901	V08	2	0
17	V	901	V08	1	0
17	Y	901	V08	2	0
17	N	901	V08	1	0

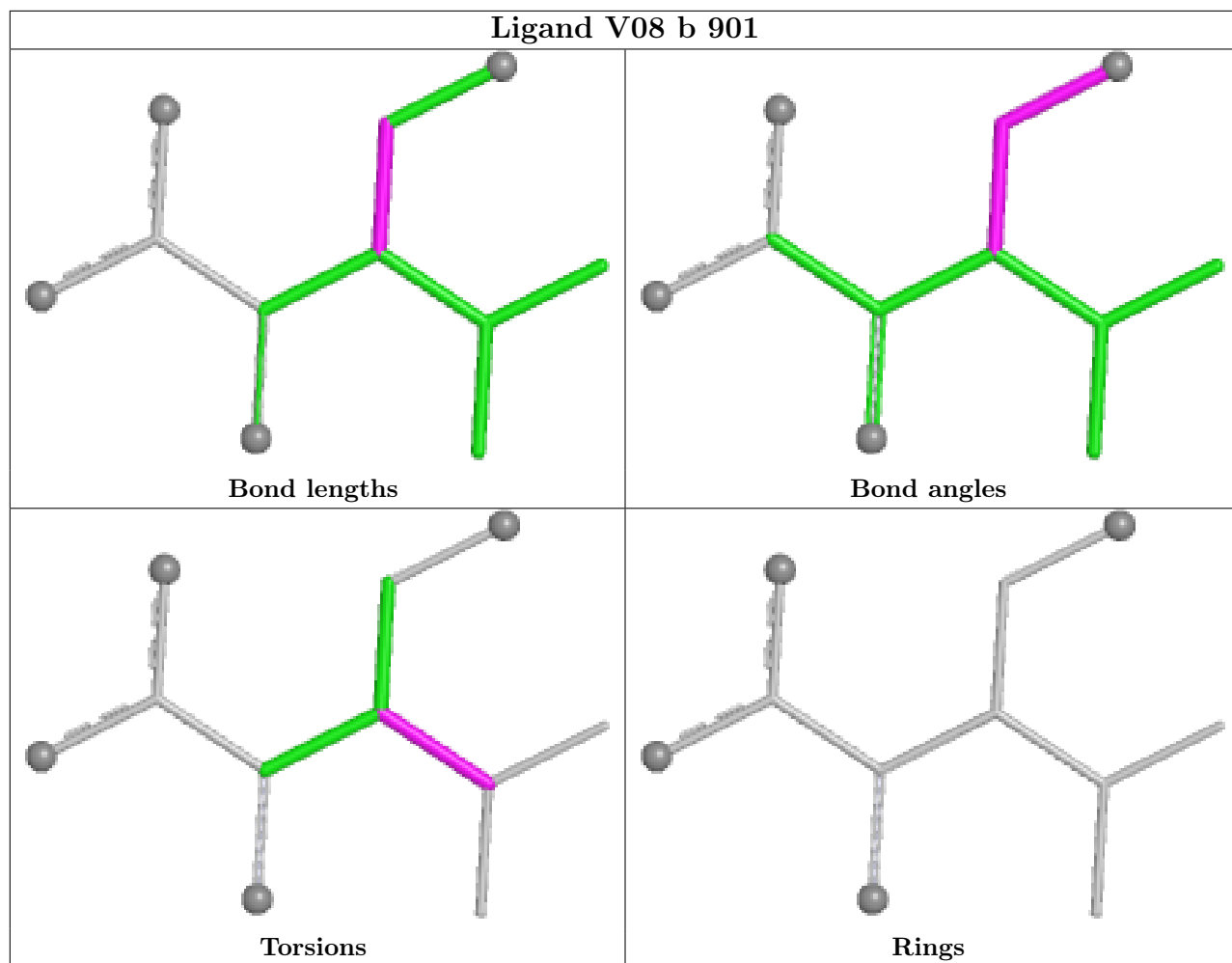
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

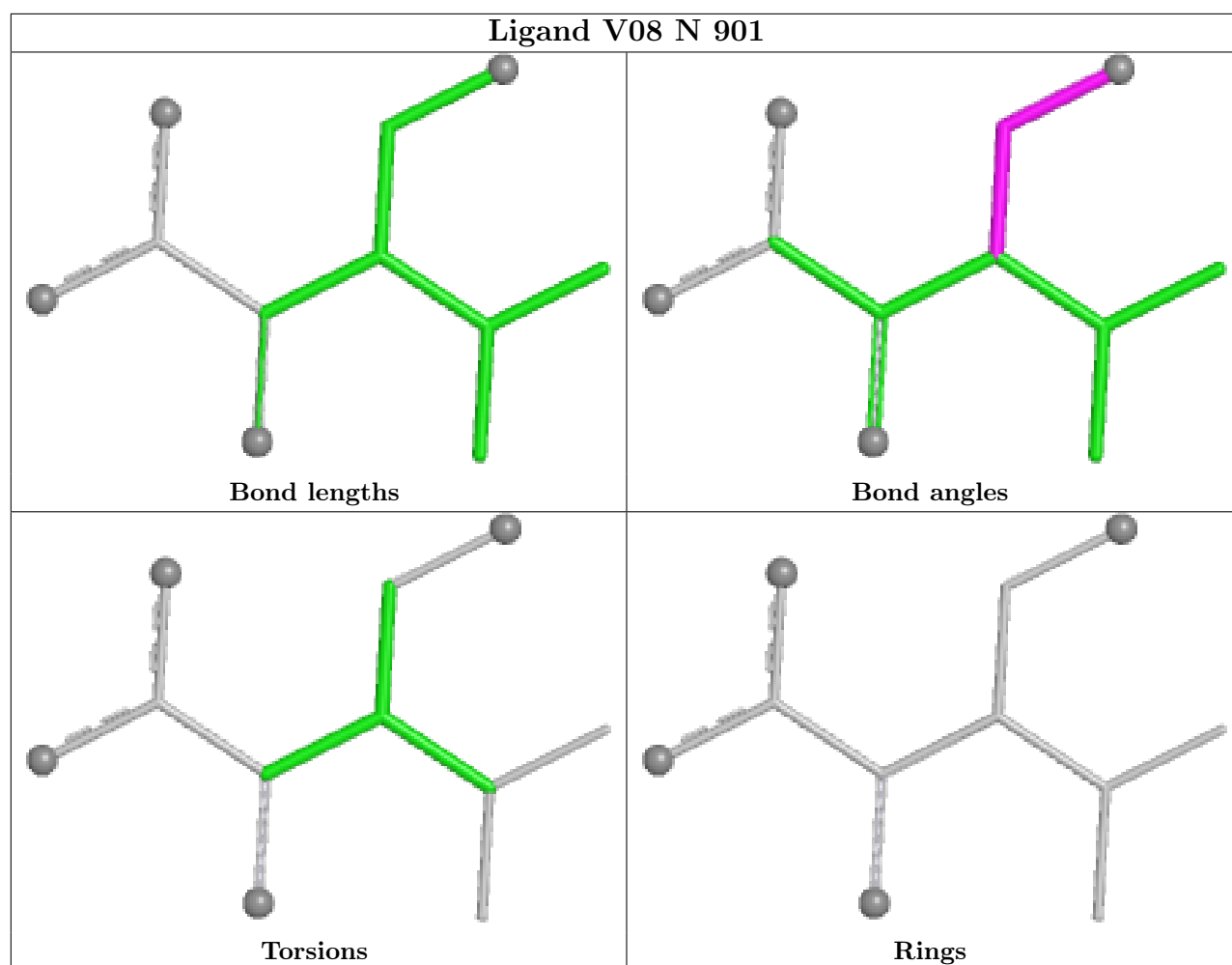












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.43	3 (1%) 79 54	72, 90, 121, 158	0
1	O	250/250 (100%)	-0.34	1 (0%) 92 79	74, 102, 134, 158	0
2	B	244/258 (94%)	-0.33	2 (0%) 86 65	74, 97, 151, 202	0
2	P	244/258 (94%)	-0.25	3 (1%) 79 54	80, 99, 155, 187	0
3	C	240/254 (94%)	-0.26	0 100 100	73, 100, 153, 163	0
3	Q	240/254 (94%)	-0.10	6 (2%) 57 29	84, 113, 172, 193	0
4	D	235/260 (90%)	-0.46	0 100 100	76, 100, 126, 147	0
4	R	235/260 (90%)	-0.32	0 100 100	82, 108, 140, 153	0
5	E	231/234 (98%)	-0.32	1 (0%) 92 79	76, 103, 134, 150	0
5	S	231/234 (98%)	-0.18	5 (2%) 62 33	84, 109, 144, 158	0
6	F	243/288 (84%)	-0.40	0 100 100	71, 94, 132, 155	0
6	T	243/288 (84%)	-0.32	0 100 100	75, 103, 144, 161	0
7	G	241/252 (95%)	-0.45	0 100 100	70, 88, 121, 150	0
7	U	241/252 (95%)	-0.41	0 100 100	76, 95, 125, 161	0
8	H	226/232 (97%)	-0.25	7 (3%) 49 21	68, 87, 119, 200	0
8	V	226/232 (97%)	-0.35	6 (2%) 54 26	73, 91, 119, 207	0
9	I	204/205 (99%)	-0.47	0 100 100	69, 86, 109, 128	0
9	W	204/205 (99%)	-0.38	0 100 100	73, 87, 115, 135	0
10	J	195/198 (98%)	-0.48	1 (0%) 91 75	69, 88, 111, 140	0
10	X	195/198 (98%)	-0.51	2 (1%) 82 59	76, 92, 112, 156	0
11	K	212/212 (100%)	-0.45	0 100 100	69, 87, 110, 122	0
11	Y	212/212 (100%)	-0.53	0 100 100	74, 90, 110, 123	0
12	L	222/222 (100%)	-0.38	1 (0%) 91 75	68, 88, 119, 143	0
12	Z	222/222 (100%)	-0.37	0 100 100	72, 92, 120, 147	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	228/246 (92%)	-0.44	1 (0%) 92 79	68, 86, 116, 133	0
13	a	228/246 (92%)	-0.45	1 (0%) 92 79	69, 87, 119, 138	0
14	N	196/196 (100%)	-0.51	0 100 100	70, 82, 111, 133	0
14	b	196/196 (100%)	-0.46	0 100 100	70, 83, 112, 137	0
All	All	6334/6614 (95%)	-0.37	40 (0%) 89 72	68, 94, 136, 207	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	222	ASP	8.1
8	H	223	ILE	6.7
8	V	222	ASP	6.2
8	H	225	GLU	6.1
8	H	224	GLN	5.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

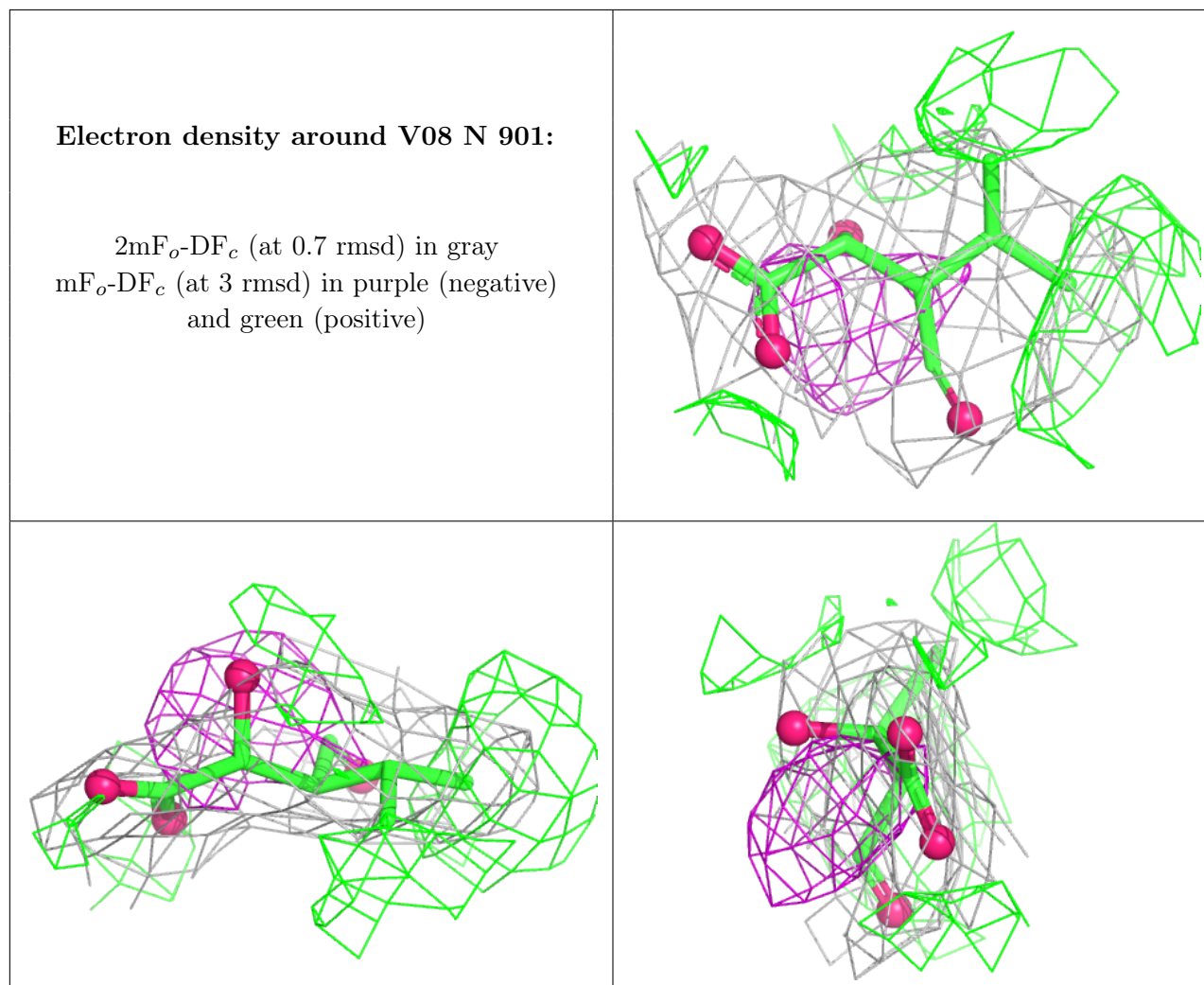
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	V08	N	901	11/11	0.76	0.33	107,112,119,119	0
17	V08	H	901	11/11	0.80	0.32	109,116,132,135	0
17	V08	V	901	11/11	0.85	0.27	100,112,121,125	0
17	V08	b	901	11/11	0.87	0.24	97,106,121,129	0
17	V08	Y	901	11/11	0.92	0.17	92,97,104,109	0
15	MG	G	301	1/1	0.93	0.18	86,86,86,86	0
17	V08	K	901	11/11	0.93	0.18	88,94,107,115	0

Continued on next page...

Continued from previous page...

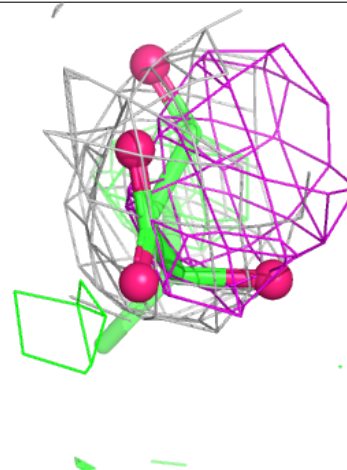
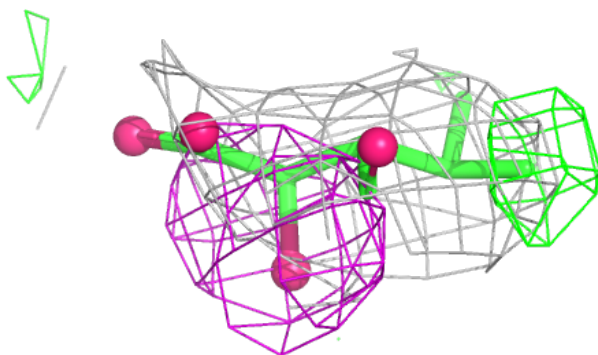
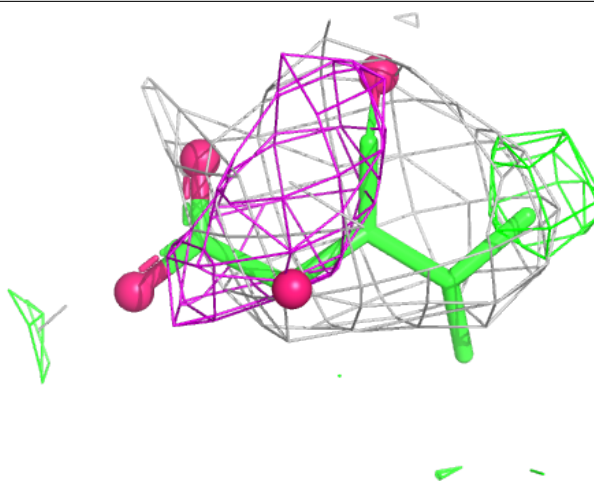
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	CL	G	302	1/1	0.94	0.11	72,72,72,72	0
16	CL	U	301	1/1	0.94	0.10	85,85,85,85	0
15	MG	N	902	1/1	0.95	0.19	66,66,66,66	0
15	MG	Z	301	1/1	0.96	0.08	96,96,96,96	0
15	MG	V	902	1/1	0.96	0.17	100,100,100,100	0
15	MG	Y	902	1/1	0.96	0.21	103,103,103,103	0
15	MG	I	301	1/1	0.97	0.44	98,98,98,98	0
15	MG	W	301	1/1	0.98	0.47	90,90,90,90	0
15	MG	K	902	1/1	0.99	0.16	85,85,85,85	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.



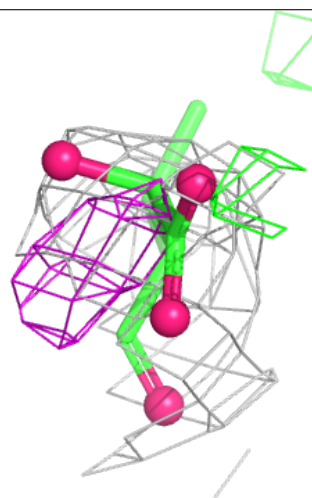
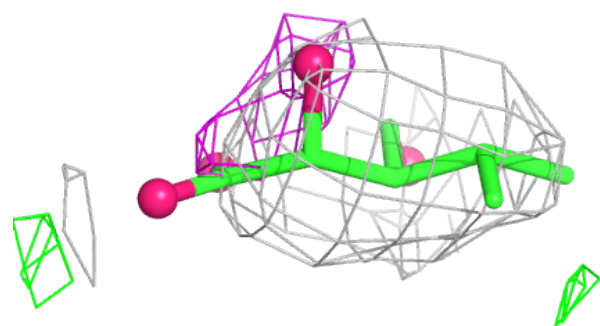
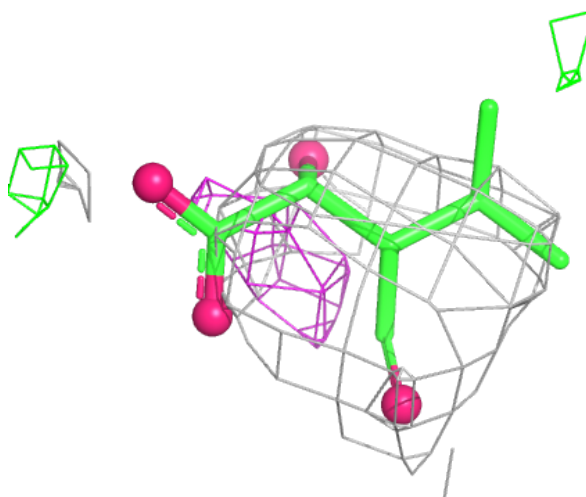
Electron density around V08 H 901:

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



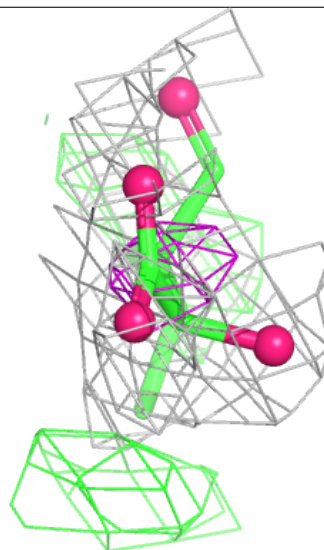
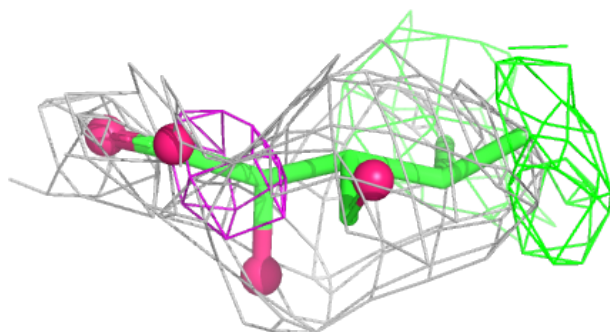
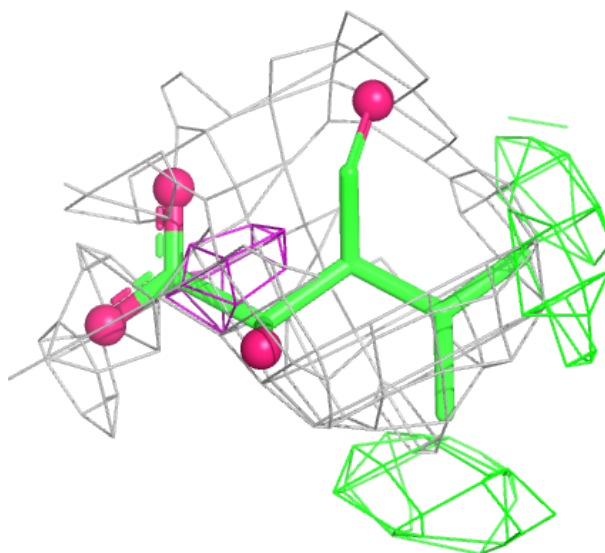
Electron density around V08 V 901:

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



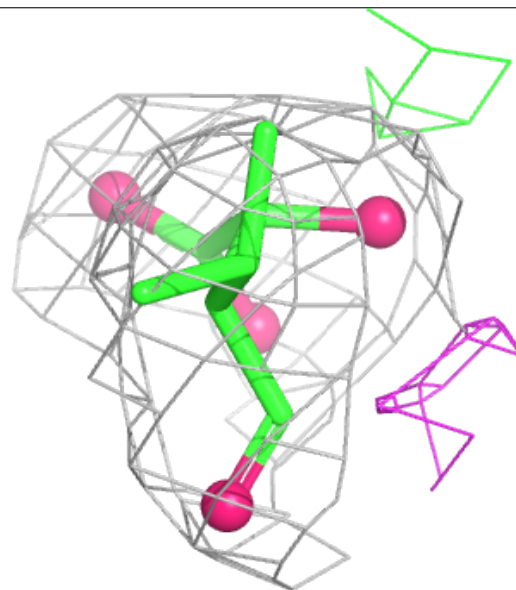
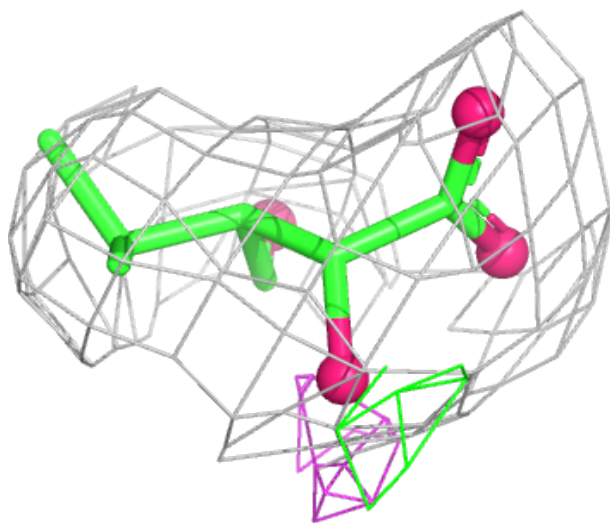
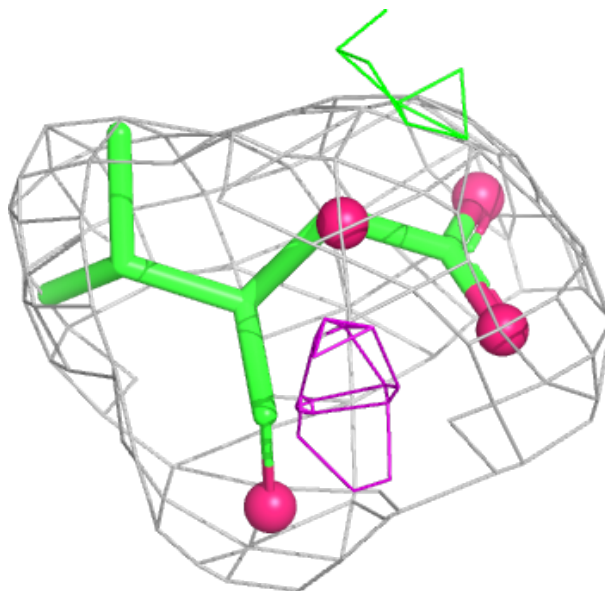
Electron density around V08 b 901:

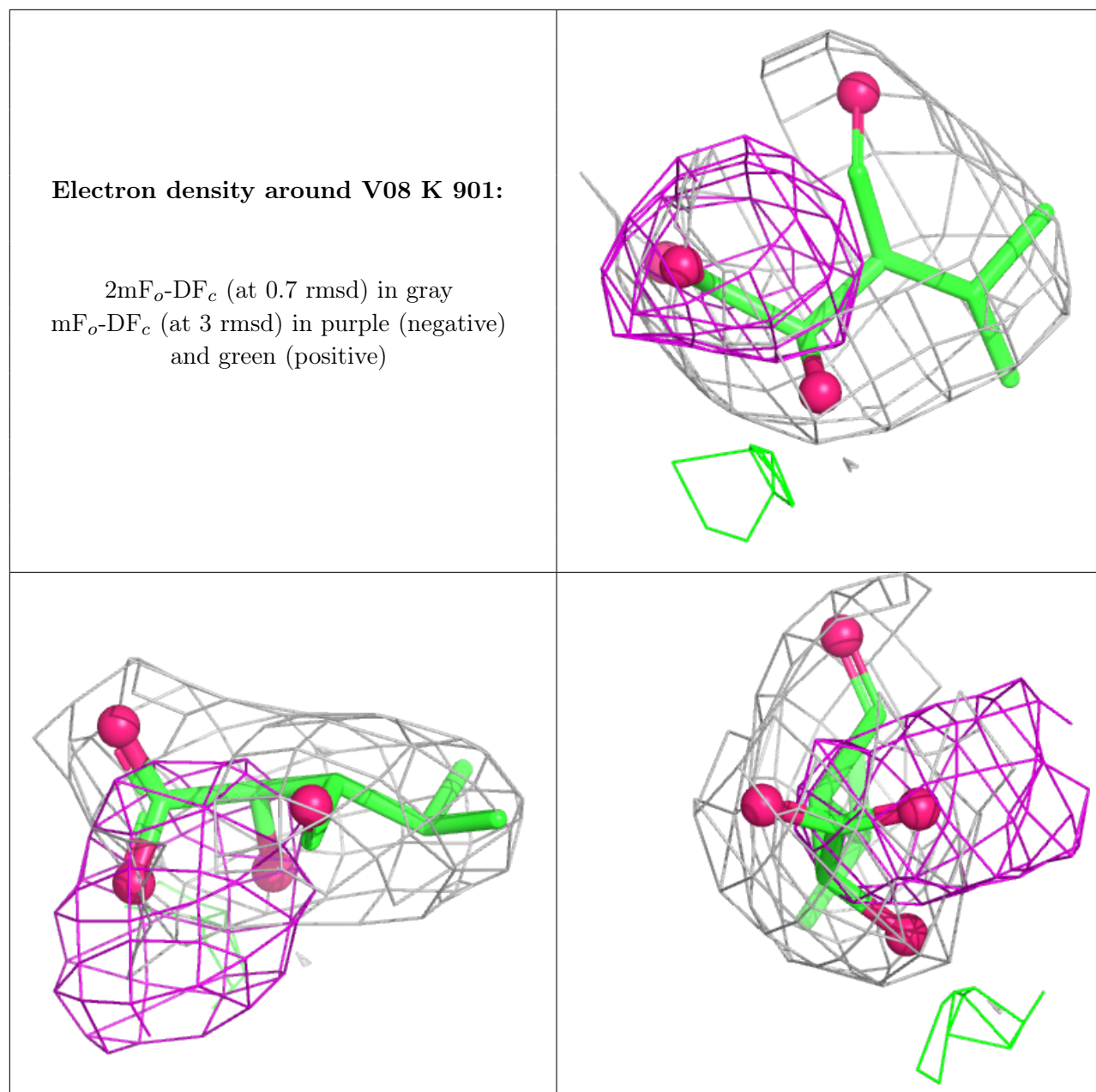
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around V08 Y 901:

$2mF_o-DF_c$ (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.